Program & Abstracts

51st Vietnam Conference on Theoretical Physics

Galina Hotel
31 Hung Vuong,
Nha Trang, Vietnam

3-6 August, 2026

Contents

Welcome Message

It is a great pleasure to welcome you to the 51st Vietnam Conference on Theoretical Physics (VCTP-51).

VCTP-51 is organized by the Institute of Physics, Vietnam Academy of Science and Technology (IOP-VAST), with the support of the Vietnam Theoretical Physics Society (VTPS). It is sponsored by the International Centre of Physics (ICP) at the Institute of Physics, VAST in Hanoi, Vietnam, and the Asia Pacific Center for Theoretical Physics (APCTP) in Pohang, Korea.

VCTP, formerly known as the National Conference on Theoretical Physics (NCTP), has been an annual event of the VTPS since 1976. VCTP aims to be an international conference for physicists in Vietnam, the region, and worldwide. Our mission is to foster scientific exchange and to promote high-quality research and education in Vietnam and Southeast Asia.

This year, the conference brings together nearly 179 participants. The program features 13 invited talks, 48 oral presentations, and 96 poster contributions.

We hope you enjoy the scientific atmosphere at this conference.

The Organizing Committee

Committees

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- Institute of Physics, Vietnam Academy of Science and Technology (IOP-VAST)

Organizing Committee

- Tran Minh Tien (Institute of Physics, VAST), Chair
- Trinh Xuan Hoang (Institute of Physics, VAST)
- Do Thi Huong (Institute of Physics, VAST)
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Sponsors

- International Centre of Physics (ICP), Institute of Physics, Vietnam Academy of Science and Technology
- Asia Pacific Center for Theoretical Physics (APCTP)

General Information

Conference venue

The VCTP-51 conference takes place in:

Galina Hotel
31 Hung Vuong street,
Nha Trang City, Khanh Hoa, Vietnam

Instructions for participation

- Participation takes place at the conference site.
- Oral presenters present their talks as in a normal conference.
- Poster presenters present the posters as in a normal conference.

Instructions for speakers

The duration of a regular invited talk is 40 minutes. This includes 35 minutes for the presentation itself and 5 minutes for Q&A. The duration of a regular presentation is 20 minutes. This includes 18 minutes for presentation itself and 2 minutes for Q&A. We would appreciate it if all presenters can adhere strictly to these time limits.

Instructions for posters

Poster should be prepared as one page of size A0 (841 mm x 1189 mm) in portrait (vertical) mode. The presenting author of the poster should be present during the poster session. A PDF file of the poster of size less than 5 MB must be uploaded to the conference website before the conference dates. Please follow the instructions on the conference website on how to present your poster online.

Meeting rooms

Please follow the direction in the lobby to go to the conference rooms.

Conference Date	Room Type	Notes
03 August	Function Room 3 + 4	Oral Session 1, 2, 3
04 August	Function Room 3	Session 4A, 5A, 6A, 7A
	Function Room 6	Session 4B, 5B, 6B, 7B
06 August	Function Room 3	Session 8A, 9A, 10A, 11A
	Function Room 6	Session 8B, 9B, 10B, 11B

Lunches

Lunches will be provided for conference participants at **the Galina Hotel**, on the **2nd Floor**. Lunch coupons are included in your name badge holder. A limited number of additional lunch coupons may be purchased for accompanying family members at the registration desk.

Gala dinner

All offline participants are invited to the Gala dinner:

Date: **Wednesday, 5 August 2026.**
Time: **19:00.**
Place: **Function Room 3, 2nd Floor, Galina Hotel**.

For your family members to attend the Gala Dinner, please buy tickets from the conference secretary on 3 August.

VTPS Meeting

A regular meeting of the Vietnamese Theoretical Physics Society (VTPS) will be held on the first day of the conference.

Date: **Monday, 3 August 2026**.
Time: **17:00 - 18:00.**
Place: **Function Room 3, 2nd Floor, Galina Hotel.**

VTPS Young Research Award

At the opening session of the conference will be an announcement and the delivery of the 2026 VTPS Young Research Award.

Program timetable

Time	Monday, 3 August Function 3+4, 2nd floor	Tuesday, 4 August		Wednesday, 5 August	Thursday, 6 August	
		Session A-Function 3, 2nd floor	Session B-Function 6, 2nd floor		Session A-Function 3, 2nd floor	Session B-Function 6, 2nd floor
08:30 – 09:30	Opening (8:50) VTPS Young Researcher Award Tran Dinh Cuong (I.1) *(Chair: Tran Minh Tien)*	Anton Baushev (O.8) F. Karan (O.9) Ngo P. D. Loc (O.10) *(Chair: Do Quoc Tuan)*	Le X. T. Tai (O.11) T. K. T. Nguyen (O.12) V. P. Villegas (O.13) *(Chair: Bach H. Giang)*		Dao Nhut Anh (O.30) V. A. Filippov (O.31) Tran Vu Dong (O.32) *(Chair: Nguyen Le Anh)*	Hieu T. T. Nguyen (O.33) Khoa D. D. Le (O.34) Nguyen D. T. Duy (O.35) *(Chair: Bui Dinh Hoi)*
09:30 – 10:30	Photo Session Coffee break	Poster Session 1 + Coffee break **(Function 4+5, 2nd floor)** *(Chair:Trinh Xuan Hoang)*			Poster Session 2 + Coffee break **(Function 4+5, 2nd floor)** *(Chair: Nguyen Hong Quang)*	
10:30 – 12:10	D. I. Kazakov (I.2) Hoang Ngoc Long (O.1) Tran Van Que (O.2) Do Quoc Tuan (O.3) *(Chair: Phung Van Dong)*	M. M. Muhlleitner (I.5) Senaha Eibun (O.14) Tran Van Ngoc (O.15) Vu Hoa Binh (O.16) *(Chair: Do Thị Huong)*	Y. Morikawa (I.6) Do Minh Hoat (O.17) Nguyen T. Kien (O.18) *(Chair: Nguyen N. Linh)*		A. Gusev (I.9) Nguyen Q. Hung (O.36) Tran Chien Thang (O.37) *(Chair: Nguyen Ngoc Anh)*	Yang Zhesen (I.10) Nguyen Hai Son (I.11) *(Chair: T. K. T. Nguyen)*
12:10 – 14:00	Lunch (2nd floor)	Lunch (2nd floor)		Excursion	Lunch (2nd floor)	
14:00 – 15:40	Mei-Yin Chou (I.3) N. Linh Nguyen (O.4) To Quy Dong (O.5) Nguyen D. Khanh (O.6) *(Chair: Tran Nguyen Lan)*	Nguyen Le Anh (O.19) Saxena Gaurav (O.20) Moiseev Nikita (O.21) Le Tan Phuc (O.22) *(Chair: Nguyen Q. Hung)*	Jiangping Hu (I.7) Hoa Nghiem (O.23) Hirobumi Mineo (O.24) Thanh Tran (O.25) *(Chair:Tran Minh Tien)*		Tran Nguyen Lan (I.12) Dung-Van Lu (O.38) Luong Le Hai (O.39) Thanh D. T. Nguyen (O.40) *(Chair: Nguyen Van Duy)*	L. Siurakshina (I.13) G. Kalagov (O.41) Tran Ky Vi (O.42) *(Chair: Phan T. Long)*
15:40 – 16:00	Coffee break	Coffee break			Coffee break	
16:00 – 17:00	V. Yushankhai (I.4) Hoang-Trong D. D. (O.7) *(Chair: Do Ngoc Son)*	Nguyen Thi Phuong (O.26) Le Van Cuong (O.27) Nguyen T. N. Nga (O.28) *(Chair: Pham T. T. Nhung)*	Hidetomo Usui (I.8) Hung The Dang (O.29) *(Chair: Nguyen Q. Bau)*		Lott Tell Peter (O.43) Afzal Adeela (O.44) Pham T. T. Nhung (O.45) (*Chair: Cao Hoang Nam)*	Dang Phuc Dam (O.46) Le N. B. Thu (O.47) Nguyen Minh Phi (O.48) *(Chair: Nguyen N. Hieu)*
	VTPS Meeting **(17:00)** Function 3, 2nd floor			Gala dinner **(19:00)** Function 3, 2nd floor		

Conference Program

Monday, 3 August 2026

Opening Session
Chair: Tran Minh Tien

08:30 - 09:00	Registration
09:00 - 09:10	Opening
09:10 - 09:20	Announcement of VTPS Young Researcher Award
09:20 - 10:00	I.1 – Invited Simple theory for the molecular dynamics of superionic crystals under extreme conditions **Tran Dinh Cuong** (Phenikaa Institute for Advanced Study)
10:00 - 10:10	Photo Session
10:00 - 10:30	Coffee break

Oral Session 1: *Particle, Nuclear and Astrophysics*
Chair: Phung Van Dong

10:30 - 11:10	I.2 – Invited New solutions for RG equations in QCD **Kazakov Dmitry** (Bogoliubov Laboratory of Theoretical Physics, JINR)
11:10 - 11:30	O.1 – Oral Probing axion in the DFSZ model **Hoang Ngoc Long** (Van Lang University)
11:30 - 11:50	O.2 – Oral Freeze-in production of non-Abelian millicharged vector dark matter **Tran Van Que** (NCTS, National Taiwan University and Phenikaa University)
11:50 - 12:10	O.3 – Oral Which phase of universe is favored by fourth-order gravity models? **Do Quoc Tuan** (Phenikaa University)
12:10 - 14:00	Lunch

Oral Session 2: *Condensed Matter Physics*
Chair: Trần Nguyen Lan

14:00 - 14:40 I.3 – Invited
First-principles electronic structure calculations: past, present and future
Mei-Yin Chou (Institute of Atomic and Molecular Sciences, Academia Sinica, Taipei, Taiwan)

14:40 - 15:00 O.4 – Oral
Ab initio Simulation for Electronic Transport in Charged Defect Materials
Nguyen Ngoc Linh (Faculty of Materials Science and Engineering, Phenikaa University)

15:00 - 15:20 O.5 – Oral
Helium transport in silicon channels: a coupled study using DFT, molecular dynamics, machine learning and Monte Carlo simulations
To Quy Dong (Université Gustave Eiffel)

15:20 - 15:40 O.6 – Oral
High-performance sensor design based on co-doped 2D materials using first-principles and machine learning approaches
Nguyen Duy Khanh (Van Lang University)

15:40 - 16:00 Coffee break

Oral Session 3: *Condensed Matter Physics*
Chair: Do Ngoc Son

16:00 - 16:40 I.4 – Invited
DNA molecule as an effective quantum wire for the long-distance transfer of a charged carrier
Yushankhai Victor (Bogoliubov Laboratory of Theoretical Physics, JINR)

16:40 - 17:00 O.7 – Oral
Construction of a machine-learned soft-Coulomb potential along the HCN–HNC isomerization pathway
Hoang-Trong D. Duong (Van Lang University)

17:00 - 18:00 VTPS meeting

Tuesday, 4 August 2026

Oral Session 4A: *Particle, Nuclear and Astrophysics*
Chair: Do Quoc Tuan

08:30 - 08:50 O.8 – Oral
How empty are the voids in the large-scale structure of the Universe?
Anton Baushev (BLTP)

08:50 - 09:10 O.9 – Oral

Gravitational wave observables and soft factors from Wilson lines

Fernandes Karan (National Taiwan Normal University, Taiwan)

09:10 - 09:30 O.10 – Oral

Pathways for primordial black holes to resolve the dark matter problem

Ngo Loc (National Taiwan University)

Oral Session 4B: *Condensed Matter Physics*
Chair: Bach H. Giang

08:30 - 08:50 O.11 – Oral

Nonlinear Transport in a one-dimensional superconducting wire within the time-dependent Ginzburg–Landau framework

Lê xuân Thế Tài (Van Lang University)

08:50 - 09:10 O.12 – Oral

Effects of weak electron-electron interactions on transport in a two-site charge Kondo circuit

Nguyen Thi Kim Thanh (Institute of Physics, VAST)

09:10 - 09:30 O.13 – Oral

Noise and memory profiles of spin-chain multichannel Kondo model with image impurity boundaries

Villegas Paat Vladimir (Mapúa University)

Poster Session 1
Chair: Trinh Xuan Hoang

09:30 - 10:30 P.1 – Poster

Bayesian Parameter Estimation and Uncertainty Quantification in Radiative Charmonium Transitions

Nguyen Nguyen Dang Khoa (Ho Chi Minh City University of Technology and Engineering)

09:30 - 10:30 P.2 – Poster

Effects of temperature and SiO_2 content on the structure of lithium silicate glasses: A Molecular dynamics simulation study

Pham Thi Lien (Faculty of Applied Sciences, University of Economics – Technology for Industries (UNETI), Hanoi, Vietnam)

09:30 - 10:30 P.3 – Poster

Fourier transformation for non-parametric CPT testing with neutrino oscillation data

Lê Cẩm Vi (IFIRSE, ICISE)

09:30 - 10:30 P.4 – Poster

Resolving Singularities in Sign-Changeable Interacting Dark Energy via Observational Constraints from Type Ia Supernovae

Dang Minh Nhut (Dalat University)

09:30 - 10:30 P.5 – Poster

First-principles elucidation of hydrogen insertion in Sr3Co3O8 in Grenier Phase

Pham Ngoc Thanh (An Giang University)

09:30 - 10:30 P.6 – Poster

Thermodynamic properties and melting temperature of FCC Cu–Ni alloys under high pressure

Nguyen Thi Hong (Hong Duc university)

09:30 - 10:30 P.7 – Poster

A Density Functional Theory Investigation into the Application Potential of an MBene Material Ti2B2 as an Anode Material for Sodium-Ion Batteries

Phạm Tuấn Kiệt (Institute of Physics)

09:30 - 10:30 P.8 – Poster

Dual-site methylammonium-zinc co-doping enhances phase stability and tunable optoelectronic properties in α-CsPbI3 perovskites: a first-principles study

Nguyen Chi Ben (Can Tho University)

09:30 - 10:30 P.9 – Poster

Reservoir-controlled topological triplet excitonic condensations

Do Thi Hong Hai (Hanoi University of Mining and Geology)

09:30 - 10:30 P.10 – Poster

Investigating the role of protein folding in G6PD deficiency

Trinh Xuan Hoang (Institute of Physics, VAST)

09:30 - 10:30 P.11 – Poster

Theoretical predictions for triple Z boson production at the LHC

LE Duc Ninh (Phenikaa University)

09:30 - 10:30 P.12 – Poster

Metric Variation of the Energy-Momentum Tensor of a Perfect Fluid and Its Applications to Cosmology and Neutron Stars

Pham Van Ky (Institute of physics, Vietnam academy of science and technology (VAST))

09:30 - 10:30 P.13 – Poster

Spectral signatures of the BCS–BEC crossover in mass-imbalanced Semimetal / Semiconductor Microcavities

Nguyen Thi Hau (HaNoi University of mining and geology)

09:30 - 10:30 P.14 – Poster

Computational Design and Emergent Physical Characteristics of Novel 2D Janus Materials

Nguyen Ngoc Hieu (Duy Tan University)

09:30 - 10:30 P.15 – Poster

Enhancement of two-mode sum squeezing and quantum entanglement through

two-photon addition and two-photon subtraction in Pair coherent states

Ho Sy Chuong (Dong Nai University)

09:30 - 10:30 P.16 – Poster

Material-Dependent Hot-Electron Energy Dissipation in GaAs-, GaSb-, and InAs-Based Asymmetric Gaussian Quantum Wells: Implications for Infrared and Terahertz Optoelectronics

Pham Tuan Vinh (Dong Thap University)

09:30 - 10:30 P.17 – Poster

Non-Gaussianity and nonclassicality of generalized superpositions of displaced Fock states

Nguyen Thi Thu Thuy (Dong Nai University; University of Education, Hue University.)

09:30 - 10:30 P.18 – Poster

Exploring Single-Molecule Magnets by Methods of Computational Quantum Chemistry

Syrakshin Anton (Institute of Mathematical Problems of Biology)

09:30 - 10:30 P.19 – Poster

Estimating the magnitude of coherent ring current In π-conjugated aromatic molecules

Ho Quang Huy (Faculty of Engineering Technology & Interdisciplinary Research Transfer and Innovation Center, University of Phan Thiet, Lam Dong, Vietnam)

09:30 - 10:30 P.20 – Poster

In silico disease outbreak dynamics using stochastically-resetting 2D Ising and Blume-Capel models

Lamento-Villegas Barbarona Em-Em (University of the Philippines Manila)

09:30 - 10:30 P.21 – Poster

Investigating physical properties of nano tungsten trioxide under the adsorption of liver cancer-related gases using density functional theory

Phan Thi Hong Hoa (Ho Chi Minh City University of Technology)

09:30 - 10:30 P.22 – Poster

Synergistic multi-doping effect on thermal-electrical properties of $Ce_{0.8-x}(La_{1/3}Sm_{1/3}Gd_{1/3})_{0.2}M_xO_{2-y}$ (M = Ca, Sr) electrolytes for intermediate temperature solid oxide fuel cells

Le Thu Lam (Tay Bac University)

09:30 - 10:30 P.23 – Poster

Unveiling Vacancy-Induced Magnetism in TiO2 via Electronic Structure Calculations

Nguyen Duc Phong (University of Science, VNU)

09:30 - 10:30 P.24 – Poster

Optimization of Light Collection in a Miniature Water Cherenkov Detector

Using Geant4 Simulations

Nguyen Hoang (IFIRSE, ICISE Centre)

09:30 - 10:30 P.25 – Poster

A computational framework for solving the few-body schrodinger equation with quantum interactions

Phan Quang Sơn (Department of Theoretical Physics, Faculty of Physics and Engineering Physics, University of Science, VNU-HCM)

09:30 - 10:30 P.26 – Poster

Microscopic description of Quarkyonic matter in neutron stars using the miscroscopic interaction

Ngo Hai Tan (Phenikaa University)

09:30 - 10:30 P.27 – Poster

Detecting Volatile Organic Compounds in Exhaled Breath: A Theoretical Perspective

Do Ngoc Son (Ho Chi Minh City University of Technology, VNU-HCM)

09:30 - 10:30 P.28 – Poster

Defect and dopant engineering in silicene/MoS2 van der Waals heterostructures for next-generation gas sensing

Duong Trong Nhan (Van Lang University)

09:30 - 10:30 P.29 – Poster

A DFT study of acetone adsorption on the zinc oxide nanosheets

Nguyen Vu Dang Khoa (Vietnam National University Ho Chi Minh City, Ho Chi Minh City University of Technology)

09:30 - 10:30 P.30 – Poster

Enhancement of stability and electronic properties of ultra-high nickel cathodes by aluminium and boron codoping studied by combined density functional theory and neural network models.

Duy Vo Anh Nguyen (FPT High School Can Tho, FPT University)

09:30 - 10:30 P.31 – Poster

Formic Acid Decomposition on Pd–Au Catalysts for Green Hydrogen Production

Huỳnh Thị Lan Trinh (Quy Nhơn University)

09:30 - 10:30 P.32 – Poster

Magnetic and transport properties of bilayer honeycomb lattice: Magnetization processes, magneto-caloric effect, and tunneling magneto-conductivity in CrI_2 thin films

Bach Huong Giang (VNU University of Science)

09:30 - 10:30 P.33 – Poster

Understanding the ferromagnetism in two-dimensional Hubbard model with application to twisted bilayer structures

Nguyen Hoang Duy (Phenikaa University)

09:30 - 10:30 P.34 – Poster

Study of non-Fermi liquid behavior in the low-energy flat bands of twisted transition metal dichalcogenides

Nguyen Trong Son (Phenikaa University)

09:30 - 10:30 P.35 – Poster

Chiral Redistribution of Quantum Entanglement: Spectral Mechanisms and Delayed Correlation Transfer in a Rhombic Spin Network

Tran Cong Phong (Ton Duc Thang University)

09:30 - 10:30 P.36 – Poster

De Sitter vacuum on nucleated D-branes with stringy corrections

Cao Hoang Nam (Duy Tan University)

09:30 - 10:30 P.37 – Poster

Excited Exciton States and Hydrogenic Convergence in Anisotropic Two-Dimensional Materials

Le Hoang Viet (Ho Chi Minh City University of Education)

09:30 - 10:30 P.38 – Poster

Transition metal dichalcogenides heterostructures for lung cancer diagnosis via alveolar gas analysis

Ong Kim Le (Institute of Fundamental and Applied Sciences, Duy Tan University)

09:30 - 10:30 P.39 – Poster

Electronic and thermoelectric properties of WSe_2 under the adsorption of VOCs: First-principles study

Nguyễn Lưu Thanh Ngân (Ho Chi Minh City University of Technology - nltngan.sdh242@hcmut.edu.vn)

09:30 - 10:30 P.40 – Poster

Investigating the binding of agonists to the stability of μ-opioid receptor

Lai T. T. Hien (VNU University of Science, Vietnam National University)

09:30 - 10:30 P.41 – Poster

Twin hypercharge

Phung Van Dong (Phenikaa University)

09:30 - 10:30 P.42 – Poster

Tuning Noncollinear RKKY Interactions in Altermagnets via Adiabatic Electron–Phonon Coupling

Bui D. Hoi (Hue University of Education)

09:30 - 10:30 P.43 – Poster

First-Principles Study of the Electronic and Optical Properties of Oxygen Vacancy Defects in Bismuth Vanadate

Nguyen Le Bao Tran (Phenikaa University)

09:30 - 10:30 P.44 – Poster

The influence of confined phonon and electromagnetic wave on the Hall effect in asymmetric infinite semi-parabolic Quantum Wells

Nguyen Dinh Nam (Department of Theoretical Physics, Faculty of Physics, VNU University of Science, Vietnam National University, Hanoi, Vietnam)

09:30 - 10:30 P.45 – Poster

Structure-informed α–nucleus optical potentials: from repulsive-core effects in α decay to deformed nonlocal (α, n) reactions

Nguyen Nhu Le (Faculty of Physics, University of Education, Hue University)

09:30 - 10:30 P.46 – Poster

Study of diffusion in sodium silicate glasses by molecular dynamics simulation

Nguyen Thi Thao (Faculty of Physics, Hanoi National University of Education)

09:30 - 10:30 P.47 – Poster

Frontal-Parietal Disruption in AD and FTD: A Multidimensional EEG Assessment via Symbolic Transfer Entropy

Le Duy Manh (Viện Công Nghệ Tiên Tiến, ĐH Tôn Đức Thắng)

10:00 - 10:30 Coffee break

Oral Session 5A: *Particle, nuclear, and astrophysics*
Chair: Do Thi Huong

10:30 - 11:10 I.5 – Invited

The cosmic origin of matter: Higgs physics, gravitational waves and collider probes of baryogenesis

Milada M. Muhlleitner (Karlsruhe Institute of Technology)

11:10 - 11:30 O.14 – Oral

Sphalerons in the general two-Higgs-doublet model

Senaha Eibun (Van Lang University)

11:30 - 11:50 O.15 – Oral

Testing Maximal Leggett–Garg inequality violation with two-detector accelerator-based neutrino experiments

Tran Van Ngoc (IFIRSE, ICISE)

11:50 - 12:10 O.16 – Oral

Physical state of axion in DFSZ model

Vũ Hoà Bình (Institute of Physics, VAST)

Oral Session 5B: *Condensed Matter Physics*
Chair: Nguyen Ngọc Linh

10:30 - 11:10 I.6 – Invited

Multi-scale simulations of chemical reactions at surfaces and interfaces

Morikawa Yoshitada (The University of Osaka)

11:10 - 11:30 O.17 – Oral

Exploring SnSe2 monolayer as a promising 2D material for the removal of heavy metals in wastewater

Hoat Do Minh (Duy Tan University)

11:30 - 11:50 O.18 – Oral

Quantum confinement effects on thermoelectric transport in nonuniform ultrathin films

Nguyễn Trung Kiên (Nano and Energy Center, VNU University of Science)

12:10 - 14:00 Lunch

Oral Session 6A: *Particle, nuclear, and astrophysics*
Chair: Nguyễn Quang Hung

14:00 - 14:20 O.19 – Oral

Toward a unified microscopic description of astrophysical capture reactions

Nguyen Le Anh (Ho Chi Minh City University of Education)

14:20 - 14:40 O.20 – Oral

Nuclear shape coexistence and its impact on decay properties across the nuclear chart

Saxena Gaurav (Dept. of Physics, Govt. Women Engg. College, Ajmer, Rajasthan, India)

14:40 - 15:00 O.21 – Oral

Empirical systematics for spontaneous fission and alpha-decay half-lives of heavy and superheavy nuclei

Moiseev Nikita (Bogoliubov Laboratory of Theoretical Physics, Joint Institute for Nuclear Research)

15:00 - 15:20 O.22 – Oral

Low-energy enhancement in the gamma-ray strength function

Le Tan Phuc (Institute of Fundamental and Applied Sciences, Duy Tan University)

Oral Session 6B: *Condensed Matter Physics*
Chair: Tran Minh Tien

14:00 - 14:40 I.7 – Invited

Loop current states in correlated electron systems

Jiangping Hu (Institute of Physics, Chinese Academy of Sciences)

14:40 - 15:00 O.23 – Oral

Efficient two-time lesser Green's function calculation via non-uniform pole expansions

Nghiem Hoa (Phenikaa University)

15:00- 15:20 O.24 – Oral

Unidirectional π-electron rotations for the helical-photo-dressed states in aromatic ring molecules

Mineo Hirobumi (Van Lang University)

15:20 - 15:40 O.25 – Oral
Compact indicator set of intrinsic molecular asymmetry in high-order harmonic generation from polar molecules
Tran Thanh (Ho Chi Minh City University of Education)

15:40 - 16:00 Coffee break

Oral Session 7A: *Particle, nuclear, and astrophysics*
Chair: Pham Thi Tuyet Nhung

16:00- 16:20 O.26 – Oral
A multiwavelength ALMA view of gas and dust in binary protoplanetary system AS 205: evidence of dust asymmetric distribution
Nguyen Thi Phuong (Vietnam National Space Center)

16:00 - 16:25 O.27 – Oral
First predictions for triply polarized WWW cross sections production at the LHC at LO
Le Van Cuong (Phenikaa Institute for Advanced Study)

16:50 - 17:15 O.28 – Oral
Quasi-Dirac fermion: A source of neutrino mass and dark matter
Nguyễn Thị Nguyệt Nga (Hung Vương university)

Oral Session 7B: *Condensed Matter Physics*
Chair: Nguyen Quang Bau

16:00 - 16:40 I.8 – Invited
First-principles study of thermoelectric materials design: high-entropy and goniopolar systems
Usui Hidetomo (The University of Electro-Communications)

16:40 - 17:00 O.29 – Oral
Role of van Hove singularity in moiré structures of twisted bilayer transition metal dichalcogenides
Dang The Hung (Phenikaa University)

Wednesday, 5 August 2026

08:00 - 16:00 Excursion

19:00 - 21:00 Gala dinner

Thursday, 6 August 2026

Oral Session 8A: *Particle, nuclear, and astrophysics*
Chair: Nguyen Le Anh

08:30 - 08:50 O.30 – Oral

From the First Radiative Capture Reactions to the Primordial Deuterium Abundance

Dao Nhut Anh (Ho Chi Minh City University of Education)

08:50 - 09:10 O.31 – Oral

General approach to the effective potentials in curved spacetime

Filippov Aleksandrovich Vladislav (Joint Institute for Nuclear Research)

09:10 - 09:30 O.32 – Oral

Proton-neutron pairing correlations in hot nuclei

Tran Vu Dong (Bogoliubov Laboratory of Theoretical Physics, JINR)

Oral Session 8B: *Molecular physics, quantum optics and quantum information*
Chair: Bui Dinh Hoi

08:30 - 08:50 O.33 – Oral

Approximate solution of the Schrodinger equation with the Mie potential

Nguyen-Truong T. Hieu (Van Lang University)

08:50 - 09:10 O.34 – Oral

Anisotropic Exciton in Monolayer Black Phosphorus with Exact Center-of-Mass Separation

Le Do Dang Le (HCMUE)

09:10 - 09:30 O.35 – Oral

Controlling high-order harmonic peak shifts in two-color laser fields

Nguyễn Đinh Thanh Duy (Ho Chi Minh city University of Education)

Poster Session 2
Chair: Nguyen Hong Quang

09:30 - 10:30 P.48 – Poster

Investigating the Structure of Two-Dimensional Penta-Silicene via Machine Learning and Classical MD

Nguyen Thanh Tien (College of Natural Sciences, Can Tho University)

09:30 - 10:30 P.49 – Poster

Significant variations of resonance energy transfer at magic angles

Nguyen Dung Chinh (posts and telecommunications institute of technology)

09:30 - 10:30 P.50 – Poster

Double exchange altermagnetism in the Lieb lattice

Nguyen Thi Hai Yen (Institute of Physics)

09:30 - 10:30 P.51 – Poster

Machine-Learning Molecular Dynamics Study of Wear Processes at Diamond – Iron Interfaces

Nguyen Trinh Bao Anh (The University of Osaka)

09:30 - 10:30 P.52 – Poster

Photon blockade in a system of two micro-cavities with nonlinear coupling kicked by periodic laser pulses

Le Duc Vinh (Atomic Molecular and Optical Physics Research Group, Institute for Advanced Study in Technology, Ton Duc Thang University, Ho Chi Minh City, Vietnam)

09:30 - 10:30 P.53 – Poster

Controlled Remote Implementation of Operators via Non-Maximal Hyperentanglement

Cao Thi Bich (Institute of Physics)

09:30 - 10:30 P.54 – Poster

Tunable Magneto-Optical Anisotropy in Nodal-Line Semimetals

Huynh V. Phuc (Dong Thap University)

09:30 - 10:30 P.55 – Poster

Microscopic signatures of quadrupole and hexadecapole softness in even-even nuclei

Hoang Thai An (Department of Physics, Ho Chi Minh City University of Education)

09:30 - 10:30 P.56 – Poster

Collective excitations in double-bilayer graphene: Spin polarization effects

Đỗng Thị Kim Phượng (Can Tho University; An Giang University - VNUHCM)

09:30 - 10:30 P.57 – Poster

Two-dimensional graphene: Peltier coefficient with electron - optical phonon scattering under the influence of intense electromagnetic wave

Nguyen Thu Huong (Air Defence-Air Force Academy)

09:30 - 10:30 P.58 – Poster

Two-dimensional graphene: Magneto - optical phonon resonance in hall coefficient under terahertz radiation

Nguyen Quang Son (Air Defence-Air Force Academy)

09:30 - 10:30 P.59 – Poster

Observation of the magnetic dipole scissors resonance in 182Ta(n,2γ) experiment

Nguyen Ngoc Anh (Phenikaa University)

09:30 - 10:30 P.60 – Poster

Spin–Valley Hall Transport in Jacutingaite under Finite Temperature Conditions

Muoi Do (Department of Physics, Pham Van Dong University)

09:30 - 10:30 P.61 – Poster

Thermodynamics of higher-dimensional Black Holes in dRGT Massive Gravity with Power Yang-Mills source

Phùng Huy Hiệu (Phenikaa Institute for Advanced Study)

09:30 - 10:30 P.62 – Poster

Synthesis and structural stability investigation of Fe_3GeTe_2 van-der-Waals ferromagnet

Phan T. Long (VNU University of Engineering and Technology)

09:30 - 10:30 P.63 – Poster

A Capillary Bundle Model for Relative Permeability in Unsaturated Porous Media

Nguyen Van Nghia (Thuyloi University)

09:30 - 10:30 P.64 – Poster

Simulation of the Talbot Effect in Nonlinear Binary Waveguide Arrays

Tran Cong Minh (Van Lang University)

09:30 - 10:30 P.65 – Poster

Two-component dark matter in an extended inert doublet model

N.T.Duy (Institute of Physics, VAST)

09:30 - 10:30 P.66 – Poster

Interaction-Induced Noise Enhancement in a Single-Channel Charge Kondo Circuit

Nguyen Hong Quang (Institute of Physics, VAST)

09:30 - 10:30 P.67 – Poster

Systematic Evaluation of ^{187}W Statistical Properties via Experimental Two-Step γ-Cascade Intensities

Phan Bao Quoc Hieu (Dalat Nuclear Research Institute)

09:30 - 10:30 P.68 – Poster

Emergence of altermagnetism on the Lieb lattice with depleted local correlations

Tran Minh Tien (Institute of Physics, Vietnam Academy of Science and Technology)

09:30 - 10:30 P.69 – Poster

Entanglement and quantum teleportation with the generalized superposition of two-mode coherent states SU(1, 1)

Truong Minh Duc (University of Education, Hue University)

09:30 - 10:30 P.70 – Poster

DFT-Calibrated Machine-Learning Screening of Off-Stoichiometric Na_xSbS_4 Solid Electrolytes

Tran Van Thien (Can Tho University)

09:30 - 10:30 P.71 – Poster

Energy-Based Downfolding with One-Body MP2 for Molecular and Periodic Systems

Vũ Công Ngọc Thái (Phenikaa university)

09:30 - 10:30 P.72 – Poster

Microscopic alpha-nucleus potentials constrained by the Bohr-Sommerfeld quantization condition for alpha decay

Nguyen Gia Huy (Ho Chi Minh City University of Education)

09:30 - 10:30 P.73 – Poster

Enhanced Magneto-Optical and Transport Properties of InSb-, InAs-, and GaSb-Based Asymmetric Gaussian Quantum Wells under Confined Optical Phonons: Material-Dependent Behavior and Prospects for Infrared Photodetectors and Terahertz Optoelectronic Devices

Nguyen Dinh Hien (Ton Duc Thang University)

09:30 - 10:30 P.74 – Poster

Influence of laser wavelength on the cross-shaped structure in the nonsequential double ionization of noble gas atom

Chau Bao Khoa (Ho Chi Minh City Univeristy of Education)

09:30 - 10:30 P.75 – Poster

Structural and thermal stability of pentagonal PtN_2/PdN_2 heterostructures: Insights from machine learning interatomic potentials trained on first-principles data

Mai Ngoc Qui (College of Natural Sciences - Can Tho University; Vinh Long University of Technology Education)

09:30 - 10:30 P.76 – Poster

A New Set of Combining Rules for the Mie (λ, 6) Potential for Predicting Thermophysical Properties of Fluid Mixtures

Nguyen Van Phuoc (Trường ĐH Tôn Đức Thắng)

09:30 - 10:30 P.77 – Poster

Structures and Dynamics of α-Synuclein in Different States: A Molecular Dynamics Study

Tran Thi Minh Thu (University of Science, VNU - HCM)

09:30 - 10:30 P.78 – Poster

A Hierarchical Binding Mechanism Governs the SARS-CoV-2 N Protein-G3BP1 Interaction: A Computational Insight

Nguyễn Hoàng Linh (Duy Tan University)

09:30 - 10:30 P.79 – Poster

Temperature-dependent EXAFS parameters of wurtzite CdSe derived from a classical correlated Einstein model

Tong Sy Tien (University of Fire Prevention & Fighting)

09:30 - 10:30 P.80 – Poster

Gravitational waves from CP domain wall collapse and electron EDM in a complex singlet model with dimension-five Yukawa interactions

PHAM THE HIEU (National Tsing Hua University, Taiwan)

09:30 - 10:30 P.81 – Poster

A new effecient scan tool of the NMSSM parameter space: NMSSMScanner
Dao Thi Nhung (Phenikaa Unversity)

09:30 - 10:30 P.82 – Poster
One-loop gauge boson contributions to decays $h \to e_a e_b$ in the general gauge R_ξ
Trịnh Thị Hồng (Đại học An Giang, VNU-HCM)

09:30 - 10:30 P.83 – Poster
Power-law Bianchi type I inflation with multiple vector fields
Nguyen Hoang Duy (Phenikaa Institute for Advanced Study)

09:30 - 10:30 P.84 – Poster
Topological edge states in one-dimensional off-diagonal mosaic lattices
Nguyen Ba Phi (Mientrung University of Civil Engineering)

09:30 - 10:30 P.85 – Poster
LFV decays in a 3-3-1 model with singlet leptoquark
Nguyen Hua Thanh Nha (Van Lang University)

09:30 - 10:30 P.86 – Poster
Design of polaron confinement by Ta doping in rutile TiO_2 for colossal permittivity
Dinh Ngoc Dung (The University of Osaka)

09:30 - 10:30 P.87 – Poster
The structural stability of monomeric Glucose-6-phosphate dehydrogenase and its relationship to G6PD deficiency
Nguyen Thi Thuy Nhung (Center for Computational Physics, Institute of Physics, VAST)

09:30 - 10:30 P.88 – Poster
Tracking the HCN isomerization process by HHG spectra simulations
Hai Thi Huynh (Department of Engineering Physics)

09:30 - 10:30 P.89 – Poster
Doubly holography for understanding the dynamics of entanglement entropy
Tran Ngoc Hung (Phenikaa University)

09:30 - 10:30 P.90 – Poster
Floquet band engineering in graphene from perturbative to extreme driving: a multi-photon driven-Dirac observability map
Nguyen Duc Long (Simulation in Materials Science Research Group, Science and Technology Advanced Institute, Van Lang University, Ho Chi Minh City, Vietnam)

09:30 - 10:30 P.91 – Poster
Magnetocaloric effect in the skyrmion material Cu_2OSeO_3
Hoang Nam Nhat (Faculty of Physics Engineering and Nanotechnology)

09:30 - 10:30 P.92 – Poster
Machine-Learning Hamiltonian Approach to Electronic Structures and Moiré Physics in Twisted Transition Metal Dichalcogenides
Nguyễn Thị Phương Thảo (Dept. of Theoretical Nanotechnology, SANKEN, The University of Osaka)

09:30 - 10:30 P.93 – Poster
Optoelectronic properties of WSe 2 monolayer with local deformation
Nguyen Hoang Hieu (Can Tho University)

09:30 - 10:30 P.94 – Poster
Investigation of phase transitions in hot $^{166-170}$Er nuclei
Le Thi Quynh Huong (University of Khanh Hoa)

09:30 - 10:30 P.95 – Poster
Two-Mode Photon-Added Displaced Fock States: Non-Gaussianity and Nonclassical Properties
Lê Phước Định (University of Education, Hue University)

09:30 - 10:30 P.96 – Poster
Electron dynamics in nonsequential triple ionization of neon atoms: laser-wavelength dependence
Pham Nguyen Thanh Vinh (Ho Chi Minh City University of Education)

10:00 - 10:30 Coffee break

Oral Session 9A: *Particle, nuclear, and astrophysics*
Chair: Nguyen Ngoc Anh

10:30 - 11:10 I.9 – Invited
Finite element method for collective nuclear models
Gusev Alexander (Meshcheryakov Laboratory of Information Technologies Joint Institute for Nuclear Research)

11:10 - 11:30 O.36 – Oral
Classification of phase transitions in hot nuclei
Nguyen Quang Hung (Institute of Fundamental and Applied Sciences, Duy Tan University)

11:45 - 12:10 O.37 – Oral
Electromagnetic transitions of mesons in Covariant Confined Quark Model
Tran Chien-Thang (Ho Chi Minh City University of Technology and Engineering)

Oral Session 9B: *Condensed Matter Physics*
Chair: Nguyen Thi Kim Thanh

10:30 - 11:10 I.10 – Invited
Generalized non-Hermitian physics
Yang Zhesen (APCTP)

11:10 - 11:50 I.11 – Invited
Non-Hermitian topological singularities in photonic crystal slabs
Nguyen Hai Son (CNRS-International-NTU-Thales Research Alliance (CINTRA), IRL 3288, Singapore)

12:10 - 14:00 Lunch

Oral Session 10A: *Molecular physics, quantum optics and quantum information*
Chair: Nguyen Van Duy

14:00 - 14:40 I.12 – Invited
Development of quantum computing algorithms for quantum molecular simulations
Tran Nguyen Lan (University of Science, VNUHCM)

14:40 - 15:00 O.38 – Oral
Variational quantum simulation of the Bose-Hubbard model
Dụng-Văn Lữ (The University of Danang - University of Science and Education)

15:00 - 15:20 O.39 – Oral
Magnetically compressed hydrogen atom in spherical coordinates
Luong Le Hai (Ho Chi Minh city University of Education)

15:20 - 15:40 O.40 – Oral
Teraherzt-induced frequency shift of high - harmonic generation in transition metal dichalcogenide monolayers
Nguyen Dang Trong Thanh (Ho Chi Minh University of Education)

Oral Session 10B: *Condensed matter physics*
Chair: Trinh Xuan Hoang

14:00 - 14:40 I.13 – Invited
Cluster quantum-chemical approach to studying electronic and magnetic properties of complex transition metal xxides
Siurakshina Liudmila (Meshcheryakov Laboratory of Information Technologies, Joint Institute for Nuclear Research)

14:40 - 15:00 O.41 – Oral
Renormalization group study of the Aharony fixed point in dipolar magnets.
Kalagov Georgii (Joint Institute for Nuclear Research)

15:00 - 15:20 O.42 – Oral
Ginzburg–Landau dynamics in dissipative nonlinear systems: superconductors, PT-symmetric photonics, and interfacial Bose–Einstein condensates
Tran Ky Vi (School of Materials Science and Engineering (SMSE), Hanoi University of Science and Technology (HUST); Van Lang University)

15:30 - 16:00 Coffee break

Oral Session 11A: *Particle, nuclear, and astrophysics*
Chair: Cao Hoang Nam

16:00 - 16:20 O.43 – Oral
Gravitational-waves from oscillons in a generalized exponential plateau potential
Lott Tell Peter (Phenikaa Institute for Advanced Study)

16:20 - 16:40 O.44 – Oral
Topological defects and gravitational waves
Afzal Adeela (BLTP, JINR)

16:40 - 17:00 O.45 – Oral
Relating stellar and light curve parameters along the asymptotic giant branch
Pham Thi Tuyet Nhung (Vietnam National Space Center (VNSC/VAST))

Oral Session 11B: *Condensed Matter Physics*
Chair: Nguyen Ngoc Hieu

16:00 - 16:20 O.46 – Oral
Efficient tuning essential properties of semiconducting silicon carbide nanoribbons through rich p-type fluorination effects
Dang Phuc Dam (College of natural sciences, Can Tho University)

16:20 - 16:40 O.47 – Oral
DFT study of volatile organic compound adsorption on metal oxide thin films
Le Nguyen Bao Thu (Ho Chi Minh City University of Technology)

16:40 - 17:00 O.48 – Oral
Pressure-dependent structural and mechanical properties of Kaolin group minerals: a first-principles and molecular simulation study
Nguyen Minh Phi (Institute of Fundamental and Applied Sciences - Duy Tan University)

17:00 - 17:15 Closing

Conference Abstracts

I.1 – Invited, VCTP-51

Simple theory for the molecular dynamics of superionic crystals under extreme conditions

Tran Dinh Cuong

Phenikaa Institute for Advanced Study, Phenikaa University

Recently, the physics community has seen a surge of interest in superionic crystals. Possessing liquid-like mobile atoms in the solid state, these materials have opened up exciting prospects in planetary science, battery technology, and nuclear engineering. However, since superionic crystals primarily exist under extreme conditions, determining their physical properties remains a huge challenge for both theorists and experimentalists. To escape this predicament, we develop a simple theory based on strong similarities between superionic solids and supercooled liquids. The elastically collective nonlinear Langevin equation is leveraged to construct the dynamic free-energy profile. The impacts of local interaction, cooperative excitation, chemical composition, isobaric heating, and isothermal squeezing on activated hopping processes are fully evaluated. Our microscopic theory can quantitatively explain how superionic crystals relax, diffuse, and deform at various pressures and temperatures. Its predictive power and computational efficiency are validated in the cases of iron (the most abundant metal in planetary cores), uranium oxide (the predominant fuel in nuclear reactors), and mixed oxide fuel (the leading candidate for plutonium disposition). These interesting results would foster more research projects on superionic crystals to actualize their enormous potential. Keywords: superionic crystals, supercooled liquids, the elastically collective nonlinear Langevin equation.

Presenter: Tran Dinh Cuong

I.2 – Invited, VCTP-51

New solutions for RG equations in QCD

Dmitry Kazakov

Bogoliubov Laboratory of Theoretical Physics, JINR, Dubna, Russia

We construct simple analytical solutions of RG equations for the running coupling and for the Green functions in QCD in the asymptotic regime. These solutions have explicit form and subsequently sum up the leading, subleading, etc. logarithms in all orders of PT. They easily reproduce the inverselogarithm expansion and allow for further summation and improvement of the asymptotic behaviour.

Presenter: Kazakov Dmitry

I.3 – Invited, VCTP-51

First-principles electronic structure calculations: past, present and future

Mei-Yin Chou

Institute of Atomic and Molecular Sciences, Academia Sinica, Taipei, Taiwan 106319

Over the past several decades, first-principles electronic structure calculations have evolved from an original theoretical endeavor into an indispensable tool across physics, chemistry, materials science, and engineering. Starting from the foundational quantum-mechanical description of interacting electrons, efficient methodologies have been developed based on density functional theory and many other extensions, which have enabled quantitative predictions of structural, electronic, magnetic, optical, and dynamical properties for systems of increasing complexity. Today, electronic structure methods play a central role in many important fields, including the discovery and design of materials, the understanding of chemical processes, the interpretation of experimental observations, etc. In this talk, I will introduce the historical development of first-principles approaches, highlighting key conceptual advances that transformed electronic structure calculations into a predictive tool. I will then discuss the current state of the field, including challenges associated with the growing demand for accuracy and scalability, the treatment of excited states, and the integration of machine learning interatomic potentials. The continuing interplay between fundamental theory, algorithmic innovation, and computational power suggests that first-principles electronic structure calculations will remain at the forefront of efforts to understand and engineer matter at the atomic scale.

Presenter: Mei-Yin Chou

I.4 – Invited, VCTP-51

DNA molecule as an effective quantum wire for the long-distance transfer of a charged carrier

Victor Yushankhai

Bogoliubov Laboratory of Theoretical Physics, JINR, Dubna, Russia

Soon after the discovery of the double helical structure of DNA by J. Watson and F. Crick in 1953, a theoretical prediction was made about the conductive properties of the DNA molecule [1]. This was confirmed by a group led by J. Barton [2], who observed rapid charge transfer between a donor and an acceptor intercalated into the DNA molecule, and later by experimental studies by B. Giese and his colleagues [3] of the propagation of a photoinduced charge carrier over long distances in artificially created DNA oligonucleotide chains. Some key features of the charge transfer behavior observed in [3] can be described within the framework of a relatively simple one-dimensional quantum-statistical model [4], an extended version of which was also chosen in our study [5]. The DNA containing an extra charged carrier is considered as an open quantum system weakly coupled to its environment. The single-particle density operator $\rho(t)$ for the charged carrier obeys the Lindblad master equation with two different dissipative processes involved, including (i) a capture of the carrier by the environment and (ii) a decoherence of its quantum-wave motion due to the influence of stochastic environmental fields. To describe the time evolution of charged carrier wavefunction, numerical solutions of the Lindblad equation for the density operator $\rho(t)$ are found using the Lindblad MPO Solver program [6]. The results are interpreted in terms of two modes of charged carrier motion: the tunneling for a short-length DNA fragment and the ballistic propagation for the long-length fragment, in accordance with the experimentally observed crossover behavior. The obtained results can be conceptually inter-

preted from different perspectives. The first concept suggests viewing DNA as a one-dimensional quantum wire enabling to efficiently transfer a fermionic charge carrier between its two ends. A prototypical effect known as environment-assisted quantum transport has been shown to remarkably enhance the efficiency of charge transfer over long distances. The second concept, derived from quantum information processing and quantum communication theory, is to consider DNA as a quantum wire that serves to efficiently transmit localized quantum states over long distances. We consider in detail how a specially designed spin-1/2 chain model simulates such a transport process.

References:

[1] Eley D.D., Spivey D.I. Trans. Faraday Soc. 1962. V. 58. P. 411–415.

[2] Hall D.B., Holmlin R.E., Barton J.K. Nature. 1996. V. 382. P. 731–735.

[3] Giese B., Amaudrut J., Köhler A.K., Spormann M., Wessely S. Nature. 2001.V. 412. P.318–320.

[4] Skourtis S., Nitzan A. J. of Chem. Phys. 2003. V. 119. P. 6271–6276.

[5] Syurakshin A.V., Lakhno V.D., Yushankhai V.Yu. Mathematical Biology and Bioinformatics. 2024. Vol. 19. P. 212–231.

[6] Landa H., Misguich G. SciPost Phys. Core. 2023. V. 6. P. 037

Presenter: Yushankhai Victor

I.5 – Invited, VCTP-51

The cosmic origin of matter: Higgs physics, gravitational waves and collider probes of baryogenesis

Milada M. Muhlleitner

Karlsruhe Institute of Technology, Germany

One of the major open questions in the Standard Model (SM) is the origin of the observed matter–antimatter asymmetry of the Universe. A dynamical mechanism capable of generating the baryon asymmetry is electroweak baryogenesis. Although the SM qualitatively satisfies the necessary Sakharov conditions, its phenomenological predictions are not compatible with the observed baryon asymmetry. In this talk, I will explore possible vacuum phase histories of the early Universe, the resulting generation of gravitational waves, and the prospects for explaining the observed baryon asymmetry within various extensions of the Higgs sector beyond the SM. I will discuss the connections to current and future collider experiments as well as upcoming gravitational wave observatories, highlighting the prospects for experimentally testing these theoretical scenarios.

Presenter: Milada M. Muhlleitner

I.6 – Invited, VCTP-51

Multi-scale simulations of chemical reactions at surfaces and interfaces

*H. H. Halim, M.R. Al Fauzan, T.N. Pham, J.I.G. Enriquez and Y. Morikawa**

The University of Osaka

Chemical reactions at solid surfaces are important in wide range of fields, including heterogeneous catalysis, electrochemistry, semiconductor processes, adhesion, and so on. Understanding these elementary reaction processes at the atomic level is crucial for elucidating the factors governing surface reactivity for designing materials and reaction processes with more desirable

properties. Surface science research has actively explored the adsorption and reaction processes of atoms and molecules on well-defined surfaces at the atomic level, with the goal of elucidating the elementary processes of surface reactions. However, even for the same metal surfaces, the reactivity can differ significantly between a catalyst under realistic conditions and a clean solid surface under ultrahigh vacuum, a problem known as the "pressure gap" and/or "materials gap". The structure and chemical state of the interface during reactions constantly change dynamically due to the influence of finite temperature and ambient gases, making direct observation of these changes crucial. In this presentation, we will review our recent research works with multi-scale simulations of surface reaction processes, including strong metal-support interactions in heterogeneous catalysis[1], the graphitization of diamond surfaces[2], CO-induced cluster formation on Cu surfaces[3, 4] and NO reduction reactions by CO on Cu surfaces[5].

References:

[1] T. N. Pham, B. A. Choi Tan, Y. Hamamoto, K. Inagaki, I. Hamada, and Y. Morikawa, ACS Catal. 14, 1443-1458 (2024).

[2] J. I. G. Enriquez, H. H. Halim, T. Yamasaki, M. Michiuchi, K. Inagaki, M. Geshi, I. Hamada, Y. Morikawa, Carbon, 226, 119223 (2024).

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[5] M. R. Al Fauzan, T. N. Pham, H. H. Halim, and Y. Morikawa, ACS Catal., in press, DOI: 10.1021/acscatal.5c09328

Presenter: Morikawa Yoshitada

I.7 – Invited, VCTP-51

Loop current states in correlated electron systems

Jiangping Hu

Institute of Physics, Chinese Academy of Sciences, Beijing, China

In this talk, I will discuss new progress in understanding electronic loop current states in correlated electron systems. A brief review of this type of states will be given for cuprates and Kagome lattice superconductors. We will develop correlated electron models where the loop current states are ground states and discuss the physics behind it.

Presenter: Jiangping Hu

I.8 – Invited, VCTP-51

First-principles study of thermoelectric materials design: high-entropy and goniopolar systems

Hidetomo Usui

Department of Engineering Science, The University of Electro-Communications, Chofu, Tokyo 182-8585, Japan

Thermoelectric materials design requires an understanding of the relationship between crystal structure, electronic structure, and transport properties. In this study, we present first-principles evaluations of thermoelectric materials based on two different design concepts: high-entropy al-

loying and goniopolarity. High-entropy alloying is based on chemical disorder in multicomponent systems, whereas goniopolarity is characterized by crystallographic-direction-dependent carrier polarity for anisotropic thermoelectric responses.

High-entropy alloying has been shown to reduce lattice thermal conductivity and enhance thermoelectric performance in PbSe-based chalcogenides [1], while other high-entropy chalcogenides exhibit only moderate performance despite their ultra-low lattice thermal conductivity [2]. Motivated by these studies, we investigate PbSe-based high-entropy thermoelectric materials using the KKR-CPA method to clarify how elemental substitution affects the electronic states and thermoelectric properties.

For the goniopolar case, we focus on layered Zintl-phase Mg_3Sb_2 and Mg_3Bi_2, which exhibit axis-dependent conduction polarity [3]. First-principles calculations show that this behavior originates from band anisotropy near the Fermi level: electron bands mainly contribute to in-plane conduction, while hole bands dominate cross-plane conduction. This direction-dependent carrier polarity provides a possible route to transverse thermoelectric conversion.

By comparing these two cases, we discuss how elemental substitution and band anisotropy affect thermoelectric transport properties. Our results provide insight into thermoelectric materials design based on electronic-structure control.

References:

[1] B. Jiang et al., Science 371, 830 (2021).

[2] A. Yamashita et al., Materials Research Letters 9, 366 (2021).

[3] Y. Goto et al., Chemistry of Materials 36, 2018 (2024).

Presenter: Usui Hidetomo

I.9 – Invited, VCTP-51

Finite element method for collective nuclear models

Oleg O. Kovalev (1, 2), Alexander A. Gusev (1, 2, 3), Luong Le Hai (4), Ochbadrakh Chuluunbaatar (1, 2, 5), Evgenii V. Mardyban (1, 2, 6) and Sergue I. Vinitsky (1, 2, 7)

(1) Joint Institute for Nuclear Research, Dubna, Russian Federation

(2) Dubna State University, Dubna, Russian Federation

(3) School of Applied Sciences, Mongolian University of Science and Technology, Ulaanbaatar, Mongolia

(4) Ho Chi Minh city University of Education, Ho Chi Minh City, Viet Nam

(5) Institute of Mathematics and Digital Technology, Mongolian Academy of Sciences, Ulaanbaatar, Mongolia

(6) Korkyt Ata Kyzylorda University, Kyzylorda, Kazakhstan

(7) RUDN University, Moscow, Russian Federation

Finite element method schemes for solving elliptic boundary value problems with mixed partial derivatives describing collective nuclear models are presented. The coefficients of the elliptic equation and the potential energy surface are calculated in tabular form from the relativistic mean-field model. The finite element method scheme is implemented using Hermite interpolation polynomials with given multiplicity of nodes, which preserve the smooth of the desired solution at the finite element boundaries, unlike traditional schemes with Lagrange interpolation polynomials. To save the computer memory, especially in dimensions 4 and higher, we solve the

problem in a restricted domain where the solution is localized, for example in classically allowed region and exclude local basis functions with large total multiplicity of the derivatives. The effectiveness of the schemes is demonstrated by calculating the reference degenerate spectrum of the Moshinsky atomic model and the rotational-vibrational spectra and electric quadrupole transitions for the isotopes 154Gd and 238U, with single-well and double-well potential energy surfaces.

Presenter: Gusev Alexander

I.10 – Invited, VCTP-51

Generalized non-Hermitian physics

Zhesen Yang

APCTP

Over the last decade, non-Hermitian physics has experienced explosive growth. Nevertheless, for quantum systems, non-Hermitian physics is generally treated as a phenomenological theory. In this presentation, I will explain how we construct a microscopic basis for non-Hermitian physics and show how to go beyond the non-Hermitian approximation.

Presenter: Yang Zhesen

I.11 – Invited, VCTP-51

Non-Hermitian topological singularities in photonic crystal slabs

Nguyen Hai Son (1,2)

(1) CNRS-International-NTU-Thales Research Alliance (CINTRA), IRL 3288, Singapore 637553

(2) Ecole Centrale de Lyon, INSA Lyon, Université Claude Bernard Lyon 1, CPE Lyon, CNRS, Institut des Nanotechnologies de Lyon, UMR5270, Ecully 69130, France

Topological photonics has recently emerged as a powerful paradigm for controlling light, and when combined with non-Hermitian physics, it opens new routes to engineer radiative coupling, modal degeneracies, and light–matter interactions. In this talk, I will present how leaky eigenmodes in photonic crystal slabs can be rigorously described by a non-Hermitian Hamiltonian that treats guided-mode coupling and radiation losses on equal footing [1]. This framework enables accurate prediction of complex photonic band structures and unveils a rich variety of topological singularities: bound states in the continuum (BICs) associated with polarization singularities in the radiation topology, and exceptional points (EPs) arising from the coalescence of eigenmodes in both frequency and field profile. I will illustrate these concepts through recent experimental realizations, including non-Hermitian band inversion and the proper definition of topological charge for radiation topology[2], the unconventional enhancement of spontaneous emission at exceptional points occurring at the band-inversion transition[3], and the hybridization of topological interfaces formed by inverted band structures[4]. If time allows, I will also discuss optical trapping[5] and lasing action at on-demanded BICs[6,7] enabled by engineered radiation patterns. These results highlight the interplay between topology, non-Hermiticity, and light–matter interaction, and point toward novel photonic devices with unprecedented control over emission and scattering.

References:

[1] "Generalized Guided Mode Expansion for Non-Hermitian Resonances in Photonic Crystal Slabs", Nanophotonics 14, 17, 5229-5250 (2025)

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Presenter: Nguyen Hai Son

I.12 – Invited, VCTP-51

Development of quantum computing algorithms for quantum molecular simulations

Tran Nguyen Lan

Unversity of Science, VNUHCM

Quantum computing holds transformative promise for molecular simulations, yet practical deployment on near-term devices remains challenging. In this talk, I will survey the current landscape of quantum algorithms for molecular simulation focusing on Variational Quantum Eigensolver (VQE) and Sample-Based Quantum Diagonalization (SQD). I will then present our recent developments in quantum simulation algorithms. First, we tackle the gradient stagnation in ADAPT-VQE through an operator elimination strategy that reduces circuit depth and iteration count while preserving accuracy. Second, we augment ADAPT-VQE with one-body downfolding (OBDF) to capture out-of-active-space dynamical correlations via an effective Hamiltonian, recovering electron correlation missed by standard active-space approaches. Third, we introduce OBDF-SQD, which seamlessly integrates OBDF into SQD to achieve superior accuracy over conventional active-space SQD, with no additional circuit overhead. Overall, our results demonstrate that adaptive ansatz construction and effective Hamiltonian techniques offer practical, high-impact pathways toward accurate and efficient near-term quantum molecular simulations.

Presenter: Tran Nguyen Lan

I.13 – Invited, VCTP-51

Cluster quantum-chemical approach to studying electronic and magnetic properties of complex transition metal oxides

Liudmila Siurakshina

Meshcheryakov Laboratory of Information Technologies, JINR, Dubna, Russia

Synthesis of new functional materials based on transition metal (TM) oxides poses new challenges in the theoretical description of their electronic and magnetic properties, taking into account the effects of strong electron correlations. At the core of this challenge is the formulation and numerical justification of multiorbital Hubbard models, as well as their low-energy limit in the form of effective spin Hamiltonians. The models are aimed at the quantitative description of complex oxides of TM elements placed in three consecutive rows of the periodic table and

showing the increasing spin-orbit coupling within the unfilled nd-electron shells, n = 3, 4, 5. To address this problem, we proposed and developed an ab initio quantum-chemical method for calculating the local electronic structure (N-electron wave functions and their energies) of small crystalline fragments (clusters) of complex oxides of all three families of TMs. To account for the effects of strong electron correlations, the multielectron states of the cluster obtained at the first stage in the Hartree-Fock (HF) approximation are further refined and expanded at the stage of post-HF calculations of increasing complexity. The final numerical results determine the quantitative estimates for a set of interaction constants of the above-mentioned Hubbard and spin models. Applications of ab initio cluster calculations are given for the quantitative description of (i) the spectra of local multiplet states of electrons in a crystal field measured in copper and vanadium oxides by RIXS spectroscopy, (ii) the phenomenon of thermally induced spin transitions in cobalt oxides and (iii) superexchange interactions of pseudospins (Kramers doublet states) in iridium oxides with strong spin-orbit interactions [1-3].

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Presenter: Siurakshina Liudmila

O.1 – Oral, VCTP-51

Probing axion in the DFSZ model

Hoang Ngoc Long and Nguyen Hua Thanh Nha

Science and Technology Advanced Institute, Van Lang University, Ho Chi Minh City, Vietnam

We show that within new right-handed neutrinos N_R, the Peccei - Quinn (PQ) transformation in the DFSZ (Dine-Fischler-Srednicki-Zhitnitsky) depends only on PQ charge of scalar singlet ϕ, it depends on just PQ charge of the scalar singlet PQ_ϕ but not in the latter and sine/cosine of $\arctan(v_u/v_d)$. The model consists of four new scalars: charged $H^\pm$, CP-odd A and CP-even with masses at the EW scale (few hundreds GeVs) and a super heavy inflaton Φ. The invariance of the model under the PQ transformation leads to the form of axion state, in which VEVs lie in the nominators. The scalar fields have been presented in a form of unitary matrices in which there is no mixing among axion and Goldstone boson G_Z. As a result, there are two kinds of couplings between axion and fermions, namely Yukawa-like interactions and anomaly ones associated with derivative of the axion. The branching decay of Higgs boson into an axion pair is derived.

Presenter: Hoang Ngoc Long

O.2 – Oral, VCTP-51

Freeze-in production of non-abelian millicharged vector dark matter

Van Que Tran (1) and Tzu-Chiang Yuan (2)

(1) National Center for Theoretical Sciences, National Taiwan University, Taiwan and Phenikaa Institute for Advanced Study, Phenikaa University, Vietnam

(2) Institute of Physics, Academia Sinica, Taiwan

We present the first predictive realization of vector freeze-in dark matter from a hidden non-Abelian gauge sector, spontaneously broken to a residual $U(1)$ with a massless dark photon mediator. A massive dark vector particle-antiparticle pair acquires small millicharges via a dimension-five kinetic mixing operator that induces a dimension-four mixing term with effective coefficient ϵ, and interacts through the hidden gauge coupling g_D, linking it weakly to the Standard Model. Solving the relic abundance with a two-temperature Boltzmann evolution including plasmon decays, we find a wide region of parameter space that reproduces the observed density while satisfying astrophysical and cosmological bounds. This minimal framework links non-Abelian vector dynamics, long-range dark forces, and dark matter, and can be testable with upcoming sub-GeV dark matter direct-detection experiments.

Presenter: Tran Van Que

O.3 – Oral, VCTP-51

Which phase of universe is favored by fourth-order gravity models?

Tuan Q. Do

Phenikaa Institute for Advanced Study, Phenikaa University

In this talk, I will present recent results on investigating the stability of de Sitter solution in four novel higher-order gravity models, namely the Einstein-Grisaru-Zanon gravity, Starobinsky-Grisaru-Zanon gravity, generalized Einsteinian cubic gravity, and Starobinsky-generalized Einsteinian cubic gravity. These investigations are an important criterion to determine which phase of universe would be compatible with these fourth-order gravity models. Furthermore, we are able, thanks to the obtained results, to identify potential extensions of the well-known Starobinsky inflationary model that may resolve its tension with the latest Atacama Cosmology Telescope data.

Presenter: Do Quoc Tuan

O.4 – Oral, VCTP-51

Ab initio simulation for electronic transport in charged defect materials

Ngoc Linh Nguyen

MSE, Phenikaa University

Predictive simulations of charge transport from first principles are crucial for the rational design of semiconductor devices. Although electron–phonon interactions can now be routinely described using density functional theory (DFT) combined with scattering-based transport theories, a comparable treatment of carrier scattering by defects, particularly charged defects, remains elusive. The challenge arises from the coexistence of short-range defect perturbations and long-range screened Coulomb interactions, which have thus far been treated predominantly using simplified models. Here, we introduce a fully ab initio framework that combines a finite-field approach

within many-body perturbation theory [1] with DFT to accurately determine the screening response associated with charged defects. The resulting electron–defect scattering rates are incorporated into the Boltzmann transport equation to predict carrier mobilities without empirical parameters. Applying this approach to vacancy defects in monolayer MoS2, we quantify the role of charged defects in limiting charge transport. Our method establishes a general route for ab initio simulations of defect-limited transport in low-dimensional materials and substantially extends the applicability of first-principles transport theory to complex materials relevant to electronic, energy, and quantum technologies.

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Presenter: Nguyen Ngoc Linh

O.5 – Oral, VCTP-51

Helium transport in silicon channels: a coupled study using DFT, molecular dynamics, machine learning and Monte Carlo simulations

Quy-Dong To , Céline Léonard and Christian Soize

Laboratoire MSME, Université Gustave Eiffel, France

Helium and silicon are two important materials in nanotechnology. Semiconductors are primarily made of silicon, and helium is known for its excellent cooling capacity. Modeling and characterizing He–Si interactions at the atomic scale are crucial for understanding helium transport in silicon micro- and nanochannels. It is well known that fluid flows in extremely confined channels are complex and strongly influenced by adsorption/desorption processes and surface diffusion mechanisms at the boundary walls. In this work, density functional theory (DFT) calculations are performed for a system composed of a helium atom and a silicon cluster, from which the interatomic pair potential for this material system is derived. Next, molecular dynamics (MD) simulations of helium atoms impacting a silicon substrate at different temperatures are carried out. Based on the resulting collision data—including velocity, residence time, and surface displacement—a surrogate stochastic wall model is constructed using probabilistic Machine Learning (ML) approaches [1]. Since the data are generated under equilibrium conditions, special attention is paid to preserving the equilibrium distribution of classical particle velocities and ensuring compliance with the principle of time reversibility [2]. The stochastic model is then used in Monte Carlo (MC) simulations of Knudsen diffusion for gas particles traveling between two parallel walls. It is also employed to determine interfacial coefficients, such as velocity slip and temperature jump coefficients, for fluid flows in the continuum regime based on the Navier–Stokes–Fourier equations [3].

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Presenter: To Quy Dong

O.6 – Oral, VCTP-51

High-performance sensor design based on co-doped 2D materials using first-principles and machine learning approaches

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Air pollution caused by toxic gases has become a significant global issue through human transportation and industrial activities. Moreover, the potential risks of leakage and diffusion of CO, CO2 and NH3 in case of accidents are extremely important. Thereby, the development of gas sensor flatform with high sensitivity, selectivity and other essential characteristics have been and are being vigorously promoted. In this work, first-principles calculations with effective machine learning approach were conducted to explore the adsorption of CO, CO2, and NH3 molecules on B–O and B–N co-doped MoS2 monolayer surfaces at atomic scale. The B–O and B–N co-doping creates active sites, improves the adsorption capacity and interaction with gas molecules of the MoS2 monolayer, thereby improving its gas selectivity. The co-doping reveals good selectivity toward CO and outstanding selectivity toward NH3, however, manifesting limited response to CO2. Most prominently, NH3 exhibits outstanding electronic sensitivity, gas selectivity, and recovery behavior on the B–O and B–N co-doped MoS2 monolayer surfaces. The electronic sensitivity of NH3 increases by approximately 400% for B–O–MoS2 and 900% for B–N–MoS2 compared with the non-adsorbed state, while the work function change reaches –1.347 eV and –1.269 eV, respectively. Furthermore, the recovery time for NH3 decreases monotonically with increasing temperature and converges to about 31 s (B–O–MoS2) and 25 s (B–N–MoS2). These results indicate that hetero-co-doping with B–N/B–O significantly enhances the electronic properties and key sensing metrics of the MoS2 monolayer toward CO and NH3 molecules; importantly, showing strong potential for practical gas-sensing applications under high-temperature operating conditions in the case of NH3 adsorption.

Presenter: Nguyen Duy Khanh

O.7 – Oral, VCTP-51

Construction of a machine-learned soft-coulomb potential along the hcn – hnc isomerization pathway

Duong D. Hoang-Trong (1,2), Minh-Nhut Tran (3), Doan-An Trieu (4,5), Van-Hoang Le (3), and Ngoc-Loan Phan (3)

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High-order harmonic generation (HHG) has become a powerful tool for probing molecular structure and ultrafast electron dynamics with attosecond temporal resolution [1–4]. Within the strong-field regime, theoretical investigations are commonly performed by solving the time-dependent Schrödinger equation (TDSE) under the single-active-electron approximation which is a low-cost method is a common way for investigating these phenomena theorically [5, 6]. Although HHG is often dominated by the highest occupied molecular orbital (HOMO) [4], recent studies on HCN have shown that lower-lying molecular orbitals and multielectron interactions can also leave observable signatures in harmonic spectra at equilibrium geometries [7, 8]. However, how these orbital contributions evolve during the HCN–HNC isomerization process, where both nuclear and electronic structures undergo substantial changes, remains largely unexplored. In this work, we develop a machine-learning-based soft Coulomb effective potential model for the HCN–HNC isomerization pathway. The proposed model is trained to accurately describe the energies, dipoles and symmetries of deeper occupied molecular orbitals, along the entire reaction coordinate connecting HCN, HNC, and intermediate configurations. The model is constructed from electronic-structure data for representative geometries and is designed to preserve the essential multiorbital characteristics required for strong-field simulations.

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Presenter: Hoang-Trong D. Duong

O.8 – Oral, VCTP-51

How empty are the voids in the large-scale structure of the Universe?

Anton Baushev

BLTP

We find an analytical solution for the minimal matter density of a void, its central density. It turns out that the voids are not so empty: most of the voids have the central underdensity $\Delta_c \sim -50\%$ (which means that the matter density in their centers is only two times lower than in the Universe on average). For small voids (of radius $R_0 \simeq 5 - 10$ Mpc), the underdensity can

be significantly greater, but the number of voids decreases rapidly with increasing of $|\Delta_c|$ over 50%, and voids with $\Delta_c < -80\%$ are practically absent. The large voids ($R_0 \geq 40$ Mpc) always have $|\Delta_c| < 50\%$.

Presenter: Anton Baushev

O.9 – Oral, VCTP-51

Gravitational wave observables and soft factors from Wilson lines

Karan Fernandes (1), Feng-Li Lin (1) and Chris White (2)

(1) Department of Physics, National Taiwan Normal University, Taiwan

(2) School of Physical and Chemical Sciences, Queen Mary University of London, United Kingdom

We derive a Wilson line for gravitationally interacting theories using the Schwinger proper time formalism. A key feature of gravitational Wilson lines is that they can be systematically expanded in terms of multiple soft gravitons, derived from fluctuations about the asymptotic trajectories of the external particles. I will discuss our result for gravitational Wilson lines up to double soft graviton order. This will be shown to recover the known double soft graviton factor for scattering amplitudes, and a new universal double soft graviton factor at subleading order in the momentum expansion.

The Wilson lines can also be expressed in terms of radiative graviton modes to provide a dressing operator. I will discuss how this operator can be used to derive non-linear radiative observables from binary black hole interactions. In particular, I will discuss our result for the gravitational waveform and show that it recovers the non-linear memory effect sourced by low frequency emissions.

Presenter: Fernandes Karan

O.10 – Oral, VCTP-51

Pathways for primordial black holes to resolve the dark matter problem

Ngo Phuc Duc Loc

National Taiwan University

I will present scenarios for primordial black holes (PBHs) to resolve the dark matter (DM) problem. First, I will show how ultra-light PBHs can produce the observed DM abundance via Hawking evaporation while satisfying cosmological constraints. Second, I will show how heavy PBHs themselves could also be a natural DM candidate.

Presenter: Ngo Loc

O.11 – Oral, VCTP-51

Nonlinear transport in a one-dimensional superconducting wire within the time-dependent Ginzburg–Landau framework

Le Xuan The Tai, Nguyen Viet Hung, Bui Duc Tinh and Tran Ky Vi

Van Lang University

We investigate the nonequilibrium transport properties of a one-dimensional superconducting wire subjected to a uniform electric field within the framework of the time-dependent

Ginzburg–Landau (TDGL) theory. The model incorporates thermal fluctuations through a stochastic noise term satisfying the fluctuation–dissipation relation and is solved numerically using a nonlinear Crank–Nicolson finite-difference scheme combined with Picard iteration. The developed solver is employed to calculate the superconducting order parameter, current density, and electrical conductivity as functions of temperature and applied electric field. The numerical results show that both the superconducting order parameter and conductivity decrease with increasing temperature and field strength, consistent with theoretical expectations near the superconducting transition. In addition, the current–electric-field characteristics exhibit a pronounced nonlinear S-shaped behavior. Comparison between stochastic and deterministic simulations reveals that thermal fluctuations influence the quantitative features of the current response but are not the primary origin of the observed nonlinearity, which persists even in the absence of noise. These findings demonstrate that the proposed numerical framework provides a stable and efficient approach for studying nonlinear transport and fluctuation effects in low-dimensional superconducting systems.

Presenter: Lê xuân Thế Tài

O.12 – Oral, VCTP-51

Effects of weak electron-electron interactions on transport in a two-site charge Kondo circuit

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(2) The Abdus Salam International Centre for Theoretical Physics, Strada Costiera 11, I-34151, Trieste, Italy

We revisit the double charge Kondo circuit (DCKC), consisting of two charge Kondo circuits weakly coupled via a tunneling junction, as proposed in Phys. Rev. B **97**, 085403 (2018). We study transport in the presence of Luttinger-liquid correlations characterized by Luttinger parameters g_1 and g_2, assuming each subsystem realizes a single-channel Kondo setup. Using perturbation theory in the weak-backscattering regime, we analyze thermoelectric response and current fluctuations induced by small temperature and/or voltage biases. All observables exhibit Fermi-liquid-like temperature scaling with exponents determined by an effective Luttinger parameter $g_{eff} = 2g_1g_2/(g_1+g_2)$. Interaction asymmetry generates additional contributions to the thermoelectric coefficient and thermopower, a term proportional to $(1/g_1 - 1/g_2)$ that vanishes for $g_1 = g_2$. The thermopower is enhanced with increasing electron-electron interactions at the quantum point contacts (decreasing g_{eff}). In contrast, delta-T noise and shot noise are absent for identical CKCs but emerge with electron-electron interaction imbalance, exhibiting an approximately linear dependence on $g_1 - g_2$ and decreasing with increasing interaction strength (decreasing g_{eff}). These results establish thermoelectric transport and current fluctuations as sensitive probes of electron-electron interaction asymmetry in DCKCs.

Presenter: Nguyen Thi Kim Thanh

O.13 – Oral, VCTP-51

Noise and memory profiles of spin-chain multichannel Kondo model with image impurity boundaries

Vladimir P. Villegas

Mapua University

Multichannel Kondo effect can be realized using $J_1 - J_2$ Heisenberg chains subject to the image impurity boundary condition. In such systms, the XXZ anisotropy plays an important role on the impurity entropy, total impurity spin, and their scaling behaviors, such as the observation in a Luttinger liquid. By considering the impurity and the image as mean-field baths, one can study the spin-chain multichannel Kondo model with image impurity boundary condition as a non-Markovian open quantum system. Using the Heisenberg-Langevin formalism, it is shown that the impurity and the image cause noise and memory on two sites for both ends of each channel. Furthermore, the noise and memory are dependent on the anisotropy factor and their interaction with the other spins.

Presenter: Villegas Paat Vladimir

O.14 – Oral, VCTP-51

Sphalerons in the general two-Higgs-doublet model

Eibun Senaha

Van Lang University

Baryon-number-violating processes in the electroweak theory are mediated by the sphaleron, an unstable static solution of the field equations. In the Standard Model (SM), the sphaleron energy is determined primarily by the ratio of the Higgs quartic coupling to the SU(2) gauge coupling, or equivalently by the Higgs-boson-to-W-boson mass ratio. Beyond the SM, however, the sphaleron energy can deviate from the SM prediction even when the observed 125 GeV Higgs boson mass and the W-boson mass are fixed. A precise determination of the sphaleron energy is therefore essential for assessing the viability of electroweak baryogenesis. In this talk, we investigate the sphaleron solution in the general two-Higgs-doublet model (g2HDM), in which no discrete symmetry is imposed. Taking into account current theoretical and experimental constraints, we quantify the impact of the Z_2-breaking quartic couplings λ_6 and λ_7, which are absent in the conventional Z_2-symmetric 2HDM, on the sphaleron energy. We also discuss the resulting sphaleron decoupling condition relevant to electroweak baryogenesis.

Presenter: Senaha Eibun

O.15 – Oral, VCTP-51

Testing maximal Leggett–Garg inequality violation with two - detector accelerator - based neutrino experiments

Tran Van Ngoc (1), Cao Van Son (1) and Quach Khanh Duc (2)

(1) International Centre for Interdisciplinary Science and Education (ICISE)

(2) University of Science and Technology of Hanoi (USTH)

The Leggett–Garg Inequality (LGI) provides a powerful framework for testing macroscopic realism and quantum coherence through temporal correlations. Neutrino oscillations, which maintain quantum coherence over macroscopic distances, offer a unique laboratory for investigating these fundamental aspects of quantum mechanics. In this work, we present a systematic study of LGI violations in neutrino oscillations. By expressing the LGI parameter in terms of oscillation phases, we construct a phase-space representation of the violation landscape and identify the optimal baseline configuration $L_3 = 2L_2$, suggesting a two-detector configuration for accelerator-based experiments for testing maximal LGI violation. We further investigate the dependence of

the maximal LGI violation on the atmospheric mixing angle and find that the optimum occurs close to maximal atmospheric mixing. This observation highlights a unique feature of neutrino oscillations in testing the maximal violation of LGI. To assess experimental feasibility, we perform a study using Hyper-Kamiokande simulation data, incorporating realistic backgrounds and statistical uncertainties. Our results demonstrate that the predicted LGI violation remains robust under full three-flavor oscillations, across different θ_{23} octants, and in the presence of background contamination. These findings establish a quantitative framework for future LGI measurements in long-baseline neutrino experiments and highlight the potential of Hyper-Kamiokande to probe the foundations of quantum mechanics on macroscopic scales.

Presenter: Tran Van Ngoc

O.16 – Oral, VCTP-51

Physical state of axion in DFSZ model

V. H. Binh (1,2) and H. N. Long (3,4)

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Physical state of axion in the model is determined by diagonalizing the squared mass mixing matrix of CP-odd sector as well as applying Peccei - Quinn mechanism to determine PQ charges of particles that are used in general form of axion. In the model under consideration, PQ charge of the nontrivial singlet scalar and the mixing angle between PQ charges of neutral components of doublet scalars are parameters for other PQ charges of particles in the model. The anomaly couplings of axion is studied in comparison with other Beyond Standard Models which also contain axion arising from PQ symmetry spontaneous breaking. There is a new kind of triple-coupling arisen from kinetic term of scalars contributes to axion decay into a pair of photon, together with anomaly coupling.

Presenter: Vũ Hoà Bình

O.17 – Oral, VCTP-51

Exploring SnSe2 monolayer as a promising 2D material for the removal of heavy metals in wastewater

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Timely monitoring and removal of heavy metals from wastewater is actually critical considering that they cause severe issues for the environment and human health. In this work, SnSe2 monolayer is explored for the removal of heavy metals (HMs), including Arsenic (As), Cadmium (Cd), Chromium (Cr), Copper (Cu), Iron (Fe), Mercury (Hg), and Lead (Pb), from wastwater. SnSe2 monolayer is a nonmagnetic semiconductor two-dimensional (2D) material with a band gap of

0.77 eV. Except for Cd and Hg metals that are physisorbed , other heavy metals are chemically adsorbed on SnSe2 monolayer with adsorption energies between -4.80 and -2.15 eV. It is also found that Cr and Fe adsorption induces signi

cant magnetism with overall magnetic moments of 3.53 and 2.22B , respectively. In latter case, the half-metallicity is also obtained. Moreover, As, Cr, Cu, and Pb adsorption metallizes the monolayer, while the semiconductor nature is preserved after adsorbing Cd and Hg metals. The adsorption is considerably enhanced in aqueous conditions as a result of the metal stabilization induced by water molecules. The HM-Se chemical bond is predominantly ionic as consequence of the charge transfer from HM atoms to Se atom, which is con

rmed by the Bader charge analysis and linear electron localization function. In explicit solvent, heavy metals lose larger charge quantities than in vacuum, strengthening the electrostatic interactions. Our study demonstrates promising adsorption performance of SnSe2 monolayer towards trapping heavy metals in both gas phase and in aqueous conditions, such that this 2D material can be introduced as a promising candidate for the removal of heavy metals from wastewater.

Presenter: Hoat Do Minh

O.18 – Oral, VCTP-51

Quantum confinement effects on thermoelectric transport in nonuniform ultrathin films

Nguyen Trung Kien (1), Dinh Thi Hien (1), Pham Thi Hong (1), Nguyen Tran Thuat (1,2), Bach Huong Giang (1) and Nguyen Quoc Hung (1,3)

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Quantum confinement provides an effective route to enhance thermoelectric performance in thickness-limited two-dimensional materials. In this work, we theoretically investigate the influence of reduced thickness on the electronic transport and thermoelectric response of ultrathin material systems. By incorporating quantum confinement into the electronic density of states and transport calculations, we show that decreasing the film thickness can significantly modify the carrier distribution near the Fermi level, leading to an enhanced Seebeck coefficient and improved thermoelectric response. Importantly, the model is extended beyond the ideal uniform-thickness limit by considering spatially inhomogeneous thickness distributions, which more closely represent realistic thin-film fabrication conditions. The calculations demonstrate that the thermoelectric enhancement remains observable even in non-uniform systems, indicating that strict atomic-scale thickness uniformity is not an essential requirement for achieving the confinement-induced improvement. These results suggest that quantum confinement can be exploited as a practical strategy for optimizing thermoelectric properties in two-dimensional and ultrathin materials, while also providing theoretical guidance for experimentally accessible fabrication conditions.

Presenter: Nguyễn Trung Kiên

O.19 – Oral, VCTP-51

Toward a unified microscopic description of astrophysical capture reactions

Nguyen Le Anh, Nguyen Gia Huy, Dao Nhut Anh, Do Huy Tho and Hoang Thai An

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Microscopic descriptions of astrophysical capture reactions provide an important link between nuclear structure and stellar nucleosynthesis, while reducing the reliance on phenomenological models. Previous applications of the Skyrme Hartree-Fock (HF) framework have successfully described low-energy nucleon radiative capture reactions. In this work, this microscopic approach is extended beyond the nucleon limit to investigate, for the first time, a low-energy nucleus-capture reaction in the ^{3}He+α system.

The nucleon-α potential is derived self-consistently from the Skyrme interaction and folded with the ^{3}He density to construct the nucleus-nucleus interaction. Scaling parameters constrained by elastic-scattering phase shifts are then used consistently in the radiative-capture calculation. As a first application, the framework is employed to study the astrophysical $^3\mathrm{He}(\alpha,\gamma)^7\mathrm{Be}$ reaction, a key process in stellar hydrogen burning and Big Bang nucleosynthesis. The calculated phase shifts and elastic-scattering observables are reproduced satisfactorily, and the astrophysical S factor shows good agreement with available experimental data.

These results demonstrate that the Skyrme HF framework can provide a unified microscopic description of astrophysical capture reactions, extending its applicability from nucleon capture to nucleus capture with minimal empirical input.

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Presenter: Nguyen Le Anh

O.20 – Oral, VCTP-51

Nuclear shape coexistence and its impact on decay properties across the nuclear chart

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Nuclear shape coexistence, defined as the presence of competing intrinsic configurations such as spherical, prolate and oblate shapes at comparable excitation energies within a single nucleus, is now established as a widespread phenomenon across the nuclear chart, arising from the interplay of shell effects, pairing correlations and collective deformation mechanisms [1,2]. While its spectroscopic manifestations are well documented, the quantitative influence of shape coex-

istence on nuclear decay properties, particularly half-lives and branching ratios, has not been systematically explored, despite its relevance for nuclear-structure studies and astrophysical nucleosynthesis calculations [3].

We present a comprehensive investigation of the impact of shape coexistence on decay properties for approximately 1500 even-even nuclei spanning the range $8 \leq Z \leq 118$ and $8 \leq N \leq 184$. Potential energy surfaces are mapped using the macroscopic-microscopic Nilsson-Strutinsky method (NSM) together with NL3*, DD-ME2 and DD-PC1. Nuclei exhibiting near-degenerate minima within a small energy interval are identified as candidates for shape coexistence. For nuclei with experimentally known decay data from the NUBASE2020 evaluation [4], deformation-dependent established semi-empirical formulas for α, β^- and β^+/EC decay are applied, explicitly incorporating quadrupole deformations of both parent and daughter nuclei, motivated by earlier study [5]. Deformation inputs from multiple nuclear-structure models are combined using Bayesian model averaging to reduce systematic bias.

The results show that nuclear shape coexistence has a systematic impact on decay properties by modifying the decay Q-values and the structural overlap between parent and daughter nuclei. When more than one shape lies close in energy, decay pathways involving different shape configurations lead to noticeable variations in calculated half-lives and branching ratios. Calculations that consider only the lowest-energy shape generally reproduce the overall decay trends, but including shape-changing transitions often improves the agreement with experimental data, particularly in regions where competing shapes are separated by small energy differences. In such cases, the decay outcome depends on whether the transition connects similar or different shapes, leading to a redistribution among competing decay modes.

This study demonstrates that nuclear shape coexistence introduces quantitatively meaningful changes in decay Q-values, half-lives, and branching ratios [6]. Explicit inclusion of deformation effects is therefore necessary for a reliable description of nuclear decay and for providing more robust nuclear-physics inputs for astrophysical nucleosynthesis calculations.

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Presenter: Saxena Gaurav

O.21 – Oral, VCTP-51

Empirical systematics for spontaneous fission and alpha-decay half-lives of heavy and superheavy nuclei

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A systematic analysis of the relationship between spontaneous fission $T^{\rm SF}_{1/2}$ and α-decay $T^{\alpha}_{1/2}$

half-lives is performed for ground-state heavy and superheavy nuclei. The ratio of logarithmic half-lives exhibits a grid-like behavior with respect to proton Z and neutron N numbers and remains nearly constant along α-decay chains where the neutron excess $N - Z$ is fixed. This regularity leads to a three-parameter empirical formula linking $T^{\mathrm{SF}}_{1/2}$ directly to $T^{\alpha}_{1/2}$ and $N - Z$. In addition, a linear correlation between $\log_{10} T^{\mathrm{SF}}_{1/2}$ and the α-particle separation energy Q_α at fixed $N - Z$ is established, yielding a second formula. Both formulas reproduce experimental spontaneous fission half-lives with mean absolute deviations within one order of magnitude. They are applied to analyze the competition between α decay and spontaneous fission along α-decay chains originating from isotopes of elements 119 and 120. The existence of a fundamental relationship between spontaneous fission and α-decay processes is discussed.

Presenter: Moiseev Nikita

O.22 – Oral, VCTP-51

Low-energy enhancement in the gamma-Ray strength function

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The low-energy enhancement (LEE), also known as the upbend resonance (UBR), observed in the gamma-ray strength function has attracted considerable attention because of its significant impact on neutron-capture reactions and astrophysical nucleosynthesis. Despite extensive experimental evidence, its microscopic origin remains an open question. In this talk, we present a new microscopic description of the UBR based on the exact thermal pairing plus phonon-damping model. Our calculations demonstrate that the UBR emerges only at finite temperature and originates from non-collective particle-particle and hole-hole excitations. These results provide a microscopic explanation for the observed low-energy enhancement and offer strong theoretical evidence that the Brink-Axel hypothesis is violated in the very low-Eγ region.

Key words: gamma-ray strength function, Upbend resonance, Brink-Axel hypothesis, Exact pairing solution, Phonon Damping Model

Presenter: Le Tan Phuc

O.23 – Oral, VCTP-51

Efficient two-time lesser Green's function calculation via non-uniform pole expansions

Hoa Nghiem

Phenikaa University

Calculating the lesser Green's function $G^{<}(t, t')$ in non-equilibrium quantum impurity systems via the Keldysh formalism is linearly straightforward but computationally expensive. A real-time

grid faces a critical dilemma: it must be fine enough to capture fast quantum fluctuations and long enough to resolve the long-time limit, resulting in a heavy computational bottleneck. Transforming the problem into the energy domain, ω, utilizes the energy-time uncertainty relation but shifts the problem into a non-linear formulation with rapidly oscillatory $e^{i\omega t}$ kernels. This work demonstrates that these non-linear oscillations can be efficiently managed by replacing real-frequency integrals with convergent sums over Matsubara poles. Furthermore, we accelerate this convergence using the non-uniform Ozaki pole expansion, where the poles are clustered near low-energy regimes and sparsified at high-energy regimes. This approach enables accurate and long-time non-equilibrium simulations with minimized memory overhead.

Presenter: Nghiem Hoa

O.24 – Oral, VCTP-51

Unidirectional π-electron rotations for the helical-photo-dressed states in aromatic ring molecules

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Controlling the unidirectional rotation of π-electrons is a key challenge in the development of organic electronic and optoelectronic devices [1-4]. In our recent study [5, 6], we explored the generation of unidirectional π-electron rotations in both low- and high-symmetry molecules by utilizing helical photon-dressed states. These states were formed using circularly or elliptically polarized laser fields within a minimal three-state electronic model under the frozen-nuclei approximation. However, that approach did not address the preparation of appropriate initial conditions or the tailored light–matter interactions required to create photon-dressed states. To overcome this limitation, it is crucial to consider a process that prepares the photon-dressed states from the electronic ground state through optical pumping with pulsed lasers. In this work, we analytically design such pulsed lasers to induce helical photon-dressed states in aromatic rings, starting from the ground state. We further incorporate the nuclear vibrational effects within the adiabatic approximation, and apply those designed laser fields. Finally, we numerically demonstrate the generation of angular momenta associated with the photon-dressed states using the analytically designed laser fields. Here, we employ the toluene molecule as a typical aromatic ring molecule with low-symmetry.

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Presenter: Mineo Hirobumi

O.25 – Oral, VCTP-51

Compact indicator set of intrinsic molecular asymmetry in high-order harmonic generation from polar molecules

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High-order harmonic generation (HHG) is a powerful tool for probing molecular structure [1] and ultrafast electron dynamics [2]. For oriented polar molecules, the breaking of the spatial symmetry of the laser-target system leads to the simultaneous emission of both odd and even harmonics [3, 4], which encode the intrinsic asymmetry of the molecule [3-6]. However, quantitatively characterizing this asymmetry by connecting spectral measurements with microscopic emission dynamics on the sub-cycle timescale remains an open challenge [5, 6]. Specifically, existing retrieval approaches remain highly indirect and not self-contained, as they rely heavily on auxiliary pre-calculated structural inputs [4, 5] or operationally involved inverse numerical procedures [6]. In this work, we establish a complete set of indicators - namely, the odd-even HHG intensity and phase difference observed in the spectral - creating a direct and invertible mapping to the amplitude and phase of attosecond bursts in the time domain. This theoretical framework is validated by solving the time-dependent Schrödinger equation (TDSE) for the CO molecule, confirming that this set of indicators is an intrinsic signature of the molecular structure and is largely insensitive to laser parameters. Hence, this approach enables direct reconstruction of attosecond-burst asymmetries from experimentally accessible odd-even HHG observables.

Presenter: Tran Thanh

O.26 – Oral, VCTP-51

A multiwavelength ALMA view of gas and dust in binary protoplanetary system AS205: evidence of dust asymmetric distribution

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We present Atacama Large Millimeter/submillimeter Array observations of multiwavelength dust emissions at 3.1 and 1.3 mm, along with molecular line emissions of CO(2–1), CO(3–2), 13CO(3–2), and C18O(3–2) at spatial resolutions of 7–45 au toward the protoplanetary system AS 205. The dust emissions exhibit two distinct components of AS 205 N and AS 205 S, separated by 1. 3. While gas kinematics within the dust disk regions are dominated by Keplerian rotation, the more extended gas emission displays complex morphology and kinematics strongly affected by the binary gravitational interaction in the outer regions. The stellar masses of AS 205 N and AS 205 S are estimated at 0.78 ± 0.19 and 1.93 ± 0.86 M, respectively. Azimuthal variation is observed in the spectral index distribution of both disks. In AS 205 N, the spectral index minimum in the southwest is coincident with the peaks of CO(2–1), CO(3–2), and 13CO(3–2) integrated intensity and the relative position of its southern counterpart. On the other hand, the spectral index distribution in AS 205 S exhibits two prominent maxima, with the one in the northeast aligning with the peak of 13CO(3–2), and the peak in the south coinciding with local maxima in CO(2–1) and CO(3–2) azimuthal profiles. These results suggest a correlation between dust grain size and/or optical depth with the gas distributions. Dust trapping along the spiral arms possibly contributes to the spectral index minima in AS 205 N; however, the observed asymmetry across both disks suggests the involvement of additional mechanisms.

Presenter: Nguyen Thi Phuong

O.27 – Oral, VCTP-51

First predictions for triply polarized WWW cross sections production at the LHC at LO

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First results on triply polarized WWW cross sections at the LHC are presented. The Standard Model calculation is performed at leading order for the fully leptonic decay mode using inclusive kinematic cuts. For $W^-W^+W^+$, the triply-transverse fraction reaches about 51%, whereas the triply-longitudinal (LLL) fraction is minimal at 1.4%. Remarkably, this is even smaller than the interference contribution (+1.8%). Because the LLL fraction is heavily suppressed relative to the interference contribution and radiative corrections are not expected to substantially increase its share based on higher-order diboson data, isolating this polarized cross section at the LHC represents a formidable experimental challenge. Moreover, a new on-shell mapping for triboson processes is developed to enable these polarized cross-section calculations. Details of our results are avaiable in arXiv:2603.02917

Presenter: Le Van Cuong

O.28 – Oral, VCTP-51

Quasi-Dirac fermion: A source of neutrino mass and dark matter

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Neutral vectorlike fermion as inspired by unified theories might become quasi-Dirac states at TeV due to a violation in lepton-like symmetry. It is shown that such quasi-Dirac fermions can properly achieve radiative neutrino mass generation and dark matter stability. Indeed, the small splitting of quasi-Dirac masses, i.e. $\Delta M/M \ll 1$, suitably suppresses neutrino mass to be small in order to allow dark matter annihilation and detection to be appropriate to experiment as well as charged lepton flavor violation limit.

Presenter: Nguyễn Thị Nguyệt Nga

O.29 – Oral, VCTP-51

Role of van Hove singularity in moiré structures of twisted bilayer transition metal dichalcogenides

Son Trong Nguyen, Duy Hoang Nguyen and Hung The Dang

Faculty of Materials Science and Engineering, Phenikaa University

Recently, twisted structures of transition metal dichalcogenides have emerged as a novel testbed for strongly correlated systems. The moiré structures generated from the twisting reveal correlated flat bands around the Fermi level. Twist angles, displacement fields are some of the "knobs" that can be used to tune these low-energy flat bands to simulate familiar models, such as the Hubbard model, experimentally. In this theoretical work, we show that the van Hove singularity of the low-energy density of states of the twisted structure can be controlled by these "knobs", enabling the observation of different phenomena such as the ferromagnetism or non-Fermi liquid behaviors. By employing dynamical mean-field theory, we demonstrate these phenomena using the well-known Hubbard model in triangular lattice and investigate several different quantities such as optical conductivity, spin susceptibility, etc. that exhibit signature behaviors of each phenomenon, which can be useful to measure in experiments.

Presenter: Dang The Hung

O.30 – Oral, VCTP-51

From the first radiative capture reactions to the primordial deuterium abundance

Dao Nhut Anh, Nguyen Gia Huy, Hoang Thai An and Nguyen Le Anh

Department of Physics, Ho Chi Minh City University of Education, Ho Chi Minh City

The primordial deuterium abundance provides one of the most sensitive probes of Big Bang nucleosynthesis and the baryonic content of the Universe. In this work, the two earliest radiative capture reactions, $p(n,\gamma)d$ and $d(p,\gamma)^3$He, are investigated within a two-body potential framework based on the Malfliet–Tjon interaction. The nuclear model parameters are constrained by the thermal capture data of the $p(n,\gamma)d$ reaction and consistently applied to the calculation of the $d(p,\gamma)^3$He reaction rate. The resulting reaction rate is incorporated into a Big Bang nucleosynthesis network to evaluate the primordial deuterium abundance, yielding

$$\mathrm{D/H} = 2.479^{+0.350}_{-0.177} \times 10^{-5}.$$

The predicted value is consistent with observational constraints from metal-poor astrophysical systems, indicating that simple microscopic descriptions of low-energy radiative capture reactions can provide reliable nuclear inputs for cosmological studies.

Presenter: Dao Nhut Anh

O.31 – Oral, VCTP-51

General approach to the effective potentials in curved spacetime

V.A. Filippov, R.M. Iakhibbaev and D. M. Tolkachev

Bogoliubov Laboratory of Theoretical Physics, Joint Institute for Nuclear Research

We present a general approach to the effective potential for non-renormalizable general and SO(N) symmetric scalar theories in curved space-time. We discuss a method for finding all-loop corrections in the leading logarithmic approximation, which incorporates the non-minimal coupling with gravity within the linear curvature approximation. Using the Bogoliubov-Parasyuk theorem, we derive recurrence relations connecting different orders of loop correction contributions. Based on these relations, we obtain generalized renormalization group equations for the effective potential describing contributions on both flat and curved backgrounds. The developed approach is applicable to an arbitrary classical interaction potential. As an example, we analyze cosmological inflation models and show that the obtained effective potentials are directly applicable in the theory of cosmological inflation. Finally, we calculate the cosmological parameters for these models and compare them with the observational data.

Presenter: Filippov Aleksandrovich Vladislav

O.32 – Oral, VCTP-51

Proton-neutron pairing correlations in hot nuclei

Tran Vu Dong

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A generalized finite-temperature proton-neutron BCS (FT-pnBCS) framework is developed using the superoperator formalism, incorporating both isovector and isoscalar pairing channels. Calculations for the schematic equidistant multilevel model and realistic nuclei reveal a phase transition from a mixed superfluid to a pure proton-neutron (pn) superfluid phase, together with the emergence of pn pairing reentrance in hot even-even nuclei. We show that the formation of pn pairing correlations in hot nuclei is governed by a delicate interplay between thermal effects and like-nucleon pairing. Our findings highlight the crucial role of finite-temperature pn correlations in nuclear structure and astrophysics, as illustrated by a qualitative analysis of Fermi charge-exchange strength distributions in hot nuclei.

Presenter: Tran Vu Dong

O.33 – Oral, VCTP-51

Approximate solution of the Schrodinger equation with the Mie potential

Hieu T. Nguyen-Truong

Van Lang University

Solving the Schrödinger equation using the Mie potential, a generalized form of the widely-known Lennard-Jones potential, is crucial for both fundamental and applied research in fields such as quantum mechanics, molecular physics, and physical chemistry. However, this long-standing problem remains unresolved. Here, we present a generalized approximate solution to this problem.

Presenter: Nguyen-Truong T. Hieu

O.34 – Oral, VCTP-51

Anisotropic exciton in monolayer black phosphorus with exact center-of-mass separation

Dang-Khoa D.Le

HCMUE

Excitons play a fundamental role in determining the optical properties of two-dimensional semiconductor materials and have attracted considerable attention over the past decade. In this work, we develop a regulated perturbation theory for an anisotropic exciton in an external magnetic field based on an algebraic approach. The method is applied to calculate the energies and wave functions of magnetoexcitons in a monolayer black phosphorus, a prototypical anisotropic two-dimensional material. Our approach combines conventional perturbation theory with the Feranchuk–Komarov operator method and incorporates spatial scaling, the Levi-Civita transformation, and the introduction of a variational free parameter to improve the convergence of the perturbation expansion. The resulting formalism allows all matrix elements to be evaluated analytically and provides convergent solutions with controllable accuracy. Highly accurate exciton energies and wave functions are obtained, with energy values converged to six decimal places. For the zero-field case, the calculated results are in good agreement with available experimental data. The predictions presented for finite magnetic fields may serve as reliable benchmark results for future theoretical and experimental investigations of anisotropic excitonic systems.

Presenter: Le Do Dang Khoa

O.35 – Oral, VCTP-51

Controlling high-order harmonic peak shifts in two-color laser fields

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Precisely controlling the frequency of high-order harmonic generation (HHG) from interaction of matter with infrared (IR) pulses is crucial for driving and steering ultrafast physical and chemical processes [1]. To this end, although terahertz fields can be used to analytical control frequency of emitted harmonics, this method is challenging with expensive setup of terahertz and IR generation systems. In this work, we suggest using second-harmonic pulse of the IR, also called as 2ω pulse, to control the frequencies of emitted harmonics. By using strong-field approximation, the harmonic frequencies are predicted to be shifted peroidically with varying time delay between two pulses, and amplitude of this oscillation can be controlled by varying the strength of 2ω pulse. We validate our analytical predictions by numerically solving the three-dimensional time-dependent Schrödinger equation for a hydrogen atom in the two-color $\omega - 2\omega$ field using a self-developed computational code. The numerical results show a good agreement with the analytical predictions and evident for the independence of atomic parameters. These findings propose a practical tool for controlling the harmonic frequency to steer ultrafast physical and chemical processes.

Keywords: Strong-field physics, Ultrafast laser-matter interaction, High-order harmonic generation

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Presenter: Nguyễn Đinh Thanh Duy

O.36 – Oral, VCTP-51

Classification of phase transitions in hot nuclei

Le Thi Quynh Huong (1), Tran Quoc Viet (2,3), Le Tan Phuc (2,3), Tran Vu Dong (2,3), Hoang Anh Tuan Kiet (4), Balaram Dey (5), Nguyen Ngoc Anh (6) and Nguyen Quang Hung (2,3)

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Phase transitions in finite nuclei, particularly pairing and shape transitions, provide insight for advancing our understanding of fundamental physics, from the behavior of matter under extreme conditions to the nature of the strong force. However, classification of those transitions is always complex task due to the occurrence of several distinct phase transitions rather than a single one. In this work, phase transitions in hot $^{160–164}$Dy nuclei are classified using the distribution of zeros of the canonical ensemble (CE) partition function in the complex inverse temperature plane. Semi-empirical nuclear level densities (NLD), which are obtained by combining experimental data in the excitation-energy region below the neutron binding energy and the back-shifted Fermi gas model prediction for the high excitation-energy up to 250 MeV, are utilized to determine the CE partition function. Results obtained show that two phase transitions can appear in $^{160–164}$Dy isotopes, namely the pairing and shape phase transitions. The pairing phase transition is found to be of first-order and its critical temperature is ~ 0.5 MeV, while the shape phase transition is found to be also of first-order but it occurs at higher temperatures, i.e. around 2.2–2.5 MeV. A comparison between the present work and previous ones that involve the same classification scheme but employ purely theoretical NLD has shown a considerable inconsistency. However, our findings should be more conclusive due to various supports from previous theoretical and experimental studies [1].

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Presenter: Nguyen Quang Hung

O.37 – Oral, VCTP-51

Electromagnetic transitions of mesons in Covariant Confined Quark Model

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Electromagnetic decays of mesons play an important role in understanding the structure of hadronic states, testing the Standard Model (SM) predictions, and probing for New Physics beyond the SM. In this talk, I present recent results from our research group on this topic, including the radiative and Dalitz decays of bottom and charm mesons. The hadronic form factors required for these studies are calculated using the Covariant Confined Quark Model developed by our group. A brief discussion of the ATOMKI X(17) anomaly is also provided.

Presenter: Tran Chien-Thang

O.38 – Oral, VCTP-51

Variational quantum simulation of the Bose - Hubbard model

Ho Xuan Nhat (1), Tran Minh Duc (1), Pham Van Anh (1), Ho Khac Hieu (1), Nguyen Quang San (2), Dung Van Lu (1)

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The Bose–Hubbard model serves as a fundamental quantum model for studying strongly interacting bosonic systems, quantum phase transitions, and many-body correlation phenomena. However, the efficient encoding and representation of bosonic quantum states on quantum hardware remain significant challenges due to differences in quantum architectures and encoding strategies. In this work, the Bose–Hubbard model is investigated using the Variational Quantum Eigensolver (VQE) algorithm on two quantum computing architectures based on qubits and

qumodes. In terms of computational resources, qubit encoding requires a number of qubits proportional to n (with $n = \lfloor \log_2 D \rfloor$), whereas qumode encoding requires a number of modes equal to the number of lattice sites. The findings highlight the trade-off between the Hilbert-space compression capability of qubit-based encoding and the natural Fock-space representation offered by qumode-based encoding. These results provide useful guidance for selecting appropriate quantum architectures for the simulation of many-body bosonic systems.

Presenter: Dụng-Văn Lữ

O.39 – Oral, VCTP-51

Magnetically compressed hydrogen atom in spherical coordinates

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A magnetically compressed hydrogen atom has axial symmetry, meaning that a 3-dimensional boundary value problem for a fixed magnetic quantum number is reduced to a 2-dimensional boundary value problem for partial differential equations with non-separable variables in a spherical or cylindrical coordinate system. For small values of the radial variable, the Coulomb interaction predominates, while for large values, the potential energy of interaction with the magnetic field predominates. Accordingly, the energy eigenvalues are characterized by spherical quantum numbers at small magnetic fields and cylindrical quantum numbers at large magnetic fields. Therefore, solving the problem using the Galerkin method requires introducing a composite basis in both the spherical and cylindrical coordinate systems, as well as stitching them together, which is not a satisfactory procedure. A more general Kantorovich method for reducing a two-dimensional boundary-value problem to a second-order ODE system uses an orthogonal basis of oblate spheroidal functions as an expansion of the desired solution. These functions depend on the radial variable as a parameter, ensuring the correct asymptotic behavior of the solution to the original boundary-value problem. The boundary-value problem for the ODE system is solved using the finite element method. The performance of the computational scheme, implemented in Maple, which provides a user-friendly interface for developing algorithms for solving problems with non-separable variables, such as the Stark effect for a magnetically compressed Hydrogen atom in spherical coordinates with a complex-valued spectrum, is demonstrated by calculating the energy eigenvalues and eigenfunctions of the lower part of the spectrum.

Presenter: Luong Le Hai

O.40 – Oral, VCTP-51

Teraherzt-induced frequency shift of high - harmonic generation in transition metal dichalcogenide monolayers

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High-harmonic generation (HHG) in transition metal dichalcogenides (TMDCs) has emerged as a powerful tool for probing ultrafast electron dynamics, with microscopic properties directly encoded in the harmonic signals. Here, we investigate HHG in two-dimensional MoS_2 driven by an intense laser pulse in the presence of an additional Terahertz (THz) field. By solving the Semiconductor Bloch Equations (SBE), we find that the THz pulse induces a frequency shift in the HHG spectra, which depends on the THz field strength, harmonic energy and driving laser parameters. To elucidate the underlying mechanism, we apply a classical Strong Field Approximation (SFA) and find excellent qualitative agreement with the SBE results. The project is still going on with applying SFA to construct a simple analytical model to explain the shift law for wide range of harmonic energy and driving laser parameters. Our findings suggest a promising route toward coherent control of solid-state high harmonics in two-dimensional quantum materials.

Keywords: High-Order Harmonic Generation, Transition Metal Dichalcogenide Monolayers, THz Field, Strong-Field Approximation, High-harmonic frequency shift.

Presenter: Nguyen Dang Trong Thanh

O.41 – Oral, VCTP-51

Renormalization group study of the Aharony fixed point in dipolar magnets.

Georgii Kalagov

Joint Institute for Nuclear Research

We compute the critical exponents of three-dimensional magnets with strong dipole-dipole interactions using the functional renormalization group (FRG) within the local potential approximation including the wave function renormalization (LPA′). The system is governed by the Aharony fixed point, which is scale-invariant but lacks conformal invariance. Our nonperturbative FRG analysis identifies this fixed point and determines its scaling behavior. The resulting critical exponents are found to be close to those of the Heisenberg $O(3)$ universality class, as computed within the same FRG/LPA′ framework. This proximity confirms the distinct yet numerically similar nature of the two universality classes. [G. Kalagov, N. Lebedev, Nuclear Physics B 1027, 117474 (2026)]

Presenter: Kalagov Georgii

O.42 – Oral, VCTP-51

Ginzburg–Landau dynamics in dissipative nonlinear systems: superconductors, PT-symmetric photonics, and interfacial Bose–Einstein condensates

Tran Ky Vi (1,4,5), Bui Duc Tinh (2), Ngo Quang Duc (2), Chu Gia Bao (2), Le Xuan The Tai (4,5), Nguyen Viet Hung (1), Pham Van Hai (2), Tran Phan Thuy Linh (2) and Pham Duy Thanh (6)

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We present a unified theoretical report on nonlinear, nonequilibrium, and interfacial phenomena in modern quantum and photonic matter, viewed primarily through the perspective of Ginzburg–Landau-type field dynamics. The central focus is on two main directions: fluctuation-driven transport in low-dimensional superconductors and dissipative nonlinear dynamics in optical systems with gain and loss, including PT-symmetric photonic settings.

For two-dimensional superconductors, we employ the time-dependent Ginzburg–Landau equation with Langevin thermal noise and a self-consistent Gaussian (Hartree) approximation to describe renormalized resistive transitions under perpendicular magnetic fields, intrinsic S-shaped nonlinear I-V characteristics under electric-field drive, and transverse thermoelectric response through the coefficient α_{xy}. This framework provides a mesoscopic description of nonequilibrium superconducting fluctuations and their observable transport signatures in new-generation superconducting materials.

For nonlinear photonics, we discuss variational and non-conservative variational approaches for

open systems governed by nonlinear Schrödinger and Ginzburg–Landau-type equations. These methods yield reduced dynamical descriptions for dissipative solitons, vortex excitations, and PT-symmetric propagation regimes, highlighting the role of gain–loss balance and effective low-dimensional dynamics in non-Hermitian optical media.

As an interfacial extension of this general nonlinear-field viewpoint, we also briefly address binary Bose–Einstein condensates near an optical wall, where wetting and prewetting phenomena can be analyzed analytically. Taken together, these directions illustrate how Ginzburg–Landau-type thinking provides a coherent language for transport, dissipation, pattern formation, and interface physics across superconducting, photonic, and ultracold-matter platforms.

Presenter: Tran Ky Vi

O.43 – Oral, VCTP-51

Gravitational-waves from oscillons in a generalized exponential plateau potential

Peter Lott and Tuan Q. Do

Phenikaa Institute for Advanced Study

We study oscillon formation and gravitational wave production in a generalized exponential plateau inflationary potential. Using Floquet analysis, we identify parametric instability bands consistent with oscillon formation, and solve numerically for the oscillon profile, finding quasi-breather solutions with lifetimes $\tau_{\rm osc} m \simeq 10^3$–$6 \times 10^4$. Applying the poltergeist mechanism, we compute the induced gravitational wave spectrum and find a peak at $f_{\rm peak} \simeq 10^{11}$ Hz with amplitude $\Omega_{\rm GW,0} h^2 \simeq 10^{-9}$–$10^{-8}$ for the benchmark parameter $\beta_{\rm pot} = 5 \times 10^{-6}$, safely below the BBN bound. For $\beta_{\rm pot} = 5 \times 10^{-6}$, the signal exceeds the BBN bound for all considered oscillon energy fractions, constraining the parameter space of the model. The signal falls in the GHz regime, potentially accessible to future resonant cavity experiments. **Presenter: Lott Tell Peter**

O.44 – Oral, VCTP-51

Topological defects and gravitational waves

Adeela Afzal, Mansoor Ur Rehman , Qaisar Shafi and Amit Tiwari (NANOGrav Collaboration)

BLTP, JINR, Russia

Gravitational waves offer a powerful probe of the early universe, providing insights into its dynamics and fundamental physics. This talk will explore the stochastic gravitational wave background (SGWB) and its potential origins, including signals detected in the NANOGrav 15-year dataset. I will discuss the model building approach that can generate topological defects, such as cosmic strings, and contribute to the SGWB linking theory to observation. This talk aims to bridge theoretical insights with observational data.

Presenter: Afzal Adeela

O.45 – Oral, VCTP-51

Relating stellar and light curve parameters along the Asymptotic Giant Branch

Pham Tuyet Nhung, Do Thi Hoai and Pierre Darriulat

Vietnam National Space Center (VNSC/VAST)

Understanding the mechanisms responsible for pulsations in some AGB stars remains an open problem. While pulsation properties are primarily governed by the physics of the stellar interior, atmospheric processes have a strong impact on the appearance of the light curve. We investigate the extent to which the study of light curves may serve as an efficient tool for understanding the internal dynamics of pulsating AGB stars. Using well-measured light curves, we define parameters that characterize their features in greater detail than previously attempted and examine correlations between these parameters and stellar properties. Recent work has extended this approach beyond Mira variables to include semi-regular and irregular stars, providing evidence for two families of AGB stars following distinct evolutionary pathways and giving rise to different light-curve properties. The interpretation of these results is discussed in the context of current state-of-the-art knowledge. While stars belonging to the first family tend to have larger initial masses than those of the second, the properties of the circumstellar envelope also seem to play a role in determining which of the two families a star belongs to.

Presenter: Pham Thi Tuyet Nhung

O.46 – Oral, VCTP-51

Efficient tuning essential properties of semiconducting silicon carbide nanoribbons through rich p-type fluorination effects

Dang Phuc Dam (1), Pham Ngoc Thanh (2,3,4), Quoc Duy Ho (5), Huynh Khanh Van (1), Nguyen Hai Dang (6), Vo Khuong Dien (1), Nguyen Thanh Tien (1) and Duy Khanh Nguyen (7,8)

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Using comprehensive density functional theory (DFT) calculations, this study systematically investigates the structural, electronic, and magnetic properties of armchair silicon carbide nanoribbons (ASiCNRs) under various fluorine (F) adsorption concentrations and configurations. The underlying physical and chemical mechanisms are elucidated through detailed analyses of optimized geometries, adsorption energies, phonon spectra, one-dimensional electronic band structures, orbital-projected density of states (PDOSs), charge density distributions, crystal orbital Hamilton population (COHP), and spin density distributions. The results reveal that F atoms

preferentially adsorb at the top sites of Si atoms, forming energetically favorable and chemically robust F–Si bonds. Pristine ASiCNRs exhibit non-spin-polarized semiconducting behavior with a direct bandgap of 2.37 eV and maintain a planar hexagonal lattice confined along the ribbon direction. Upon fluorination, significant structural reconstruction occurs, leading to a buckled one-dimensional geometry driven by strong F–Si interactions. Depending on the fluorine concentration and adsorption distribution, the electronic and magnetic characteristics can be effectively tuned, giving rise to a wide range of states, including p-type non-spin-polarized semiconductors, p-type spin-polarized semiconductors, metals, and half-metals. The p-type doping mechanism originates from substantial charge transfer between the ASiCNR substrate and highly electronegative F adatoms, resulting in hole generation within the nanoribbon framework. These findings demonstrate that fluorination provides an effective strategy for engineering the electronic and magnetic properties of ASiCNRs, highlighting their considerable potential for next-generation nanoelectronic, optoelectronic, and spintronic applications.

Keywords: DFT calculations, silicon carbide nanoribbons, fluorine adsorptions, p-type doping, one-dimensional electronic structures, ferromagnetic semiconductors.

Presenter: Dang Phuc Dam

O.47 – Oral, VCTP-51

DFT study of volatile organic compound adsorption on metal oxide thin films

Le Nguyen Bao Thu (1,2) and Do Ngoc Son (1,2)

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Volatile organic compounds (VOCs) in human breath are gaining significant attention as potential biomarkers for cancer diagnosis. In this study, we employed density functional theory calculations within the Perdew–Burke–Ernzerhof generalized gradient approximation to investigate the adsorption of VOCs on metal oxide thin films. Structural analysis was used to determine the stability and geometry of the adsorption systems, while transport properties and sensing implications were evaluated through electrical conductivity, the Seebeck coefficient, and the temperature dependence of recovery time. The results reveal a weak, instantaneous adsorption of VOCs on the substrate.

Acknowledgement. This research was funded by Vietnam National University HoChiMinh City (VNU-HCM) under grant number A2025-20-02.

Presenter: Le Nguyen Bao Thu

O.48 – Oral, VCTP-51

Pressure-dependent structural and mechanical properties of Kaolin group minerals: a first-principles and molecular simulation study

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Kaolin-group clay minerals, including kaolinite, dickite, and nacrite, are important constituents of clay-rich geological formations and may be relevant to the mechanical integrity of caprocks used for underground H2 and CO2 storage [1]. However, their pressure-dependent structural and mechanical properties remain poorly constrained because experimental determination is still challenging. This study aims to address this limitation by combining two complementary computational approaches: first-principles density functional theory and classical atomistic simulations. Density functional theory calculations were performed using CASTEP [2]. The calculations employed the PBE generalized-gradient approximation, ultrasoft pseudopotentials, a plane-wave cutoff energy of 1000 eV, and Monkhorst–Pack k-point meshes selected to ensure total-energy convergence. Long-range dispersion interactions were accounted for using the D3 correction. Classical atomistic simulations were conducted using the General Utility Lattice Program (GULP) [3], in which interatomic interactions were described by Coulomb, Buckingham, Morse, harmonic bond-bending, and core–shell potentials. Polytype-specific potential parameters were obtained through relaxed fitting to experimental structural data. The results from both approaches are compared with available experimental and computational data to evaluate the reliability of the predicted pressure dependence of structural and mechanical properties of Kaolin group clays. This combined analysis provides molecular-scale insight into polytype-dependent layer stacking and interlayer interactions in controlling the structural and mechanical responses under static pressure.

Acknowledgements

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Presenter: Nguyen Minh Phi

P.1 – Poster, VCTP-51

Bayesian Parameter Estimation and Uncertainty Quantification in Radiative Charmonium Transitions

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We study radiative charmonium transitions within the Covariant Confined Quark Model (CCQM). Our predictions for the branching fractions agree well with experimental data. An important part of our analysis is the fitting process for the model free parameters and theoretical error estimation. In this poster, we describe the statistical determination of the model parameters entering the decay amplitudes. In particular, we extract two key parameters of the model: the charm quark mass (m_c) and the hadron size parameter (ρ). The parameter estimation is performed using Bayesian inference with the Nested Sampling algorithm, while uncertainties associated with particle masses and widths are incorporated through nuisance parameters. The theoretical predictions are fitted to the currently available experimental branching fractions of $J/\psi \to \eta_c\gamma$, $\chi_{c0} \to J/\psi\gamma$, and $\psi(2S) \to \chi_{c0}\gamma$. The resulting Bayesian credible intervals are compared with confidence intervals obtained from a profile likelihood analysis, showing good agreement between the two approaches. The posterior parameter samples are propagated through the model using Monte Carlo techniques to predict branching fractions for additional channels, including $h_c \to \eta_c\gamma$ and $\chi_{c1,c2} \to J/\psi\gamma$. We further analyze the relative contributions of different sources of uncertainty to the final predictions. The obtained results indicate that the CCQM can provide a consistent description of radiative charmonium decays while allowing a systematic treatment of theoretical uncertainties.

Presenter: Nguyen Nguyen Dang Khoa

P.2 – Poster, VCTP-51

Effects of temperature and SiO_2 content on the structure of lithium silicate glasses: A Molecular dynamics simulation study

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Molecular dynamics simulations were carried out to investigate the effects of temperature and composition on the structural characteristics of lithium silicate glasses with three representative compositions, denoted as LS1, LS2, and LS4. The simulations were performed over the temperature range of 300–973 K. The reliability of the simulated models was evaluated by comparing the calculated densities, radial distribution functions, and structure factors with available experimental data, showing good agreement. The results reveal that the Si–O network remains locally stable for all investigated compositions and temperatures. The Si–O bond length is approximately 1.55–1.60 Å, and the Si–O coordination number remains close to 4, confirming the persistence of SiO_4 tetrahedral units in the glass network. In contrast, the Li–O coordination environment is more broadly distributed, mainly involving LiO_4 and LiO_5 units, which reflects the role of Li^+ ions as network modifiers. Increasing SiO_2 content enhances the polymerization of the silicate network, as evidenced by the increase in O–Si coordination and the decrease in the

number of non-bridging oxygens per tetrahedron. Temperature mainly affects the medium-range structural order. With increasing temperature, the intensity of the first sharp diffraction peak decreases and its width increases, whereas its position remains nearly unchanged at $q \approx 1.75$–1.78 $\mathrm{\AA}^{-1}$. Meanwhile, the main peak located at $q \approx 2.7$ $\mathrm{\AA}^{-1}$ exhibits only minor changes, indicating that the short-range structure is much less sensitive to temperature. These findings demonstrate that composition primarily controls the network topology of lithium silicate glasses, while temperature mainly weakens the medium-range order without significantly altering the local Si–O structure.

Presenter: Pham Thi Lien

P.3 – Poster, VCTP-51

Fourier transformation for non-parametric CPT testing with neutrino oscillation data

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CPT invariance is a fundamental principle of quantum field theory, and its verification in the neutrino sector is essential since neutrinos have the smallest mass among leptons. Conventional analyses of neutrino oscillation data typically rely on model-dependent parameter fitting, which may introduce biases and potentially obscure subtle differences between neutrino and antineutrino behaviors. Here we propose a novel CPT-invariance testing using a non-parametric Fast Fourier Transform (FFT) approach. Our method can apply directly on the measurable ratio of the oscillated to unoscillated event rate spectra in the L/E domain, extracting phase position and amplitude of spectral peaks corresponding to Δm^2_{31} and leptonic mixing angles in the standard picture. Statistical uncertainties are rigorously handled through Monte Carlo sampling with Poisson fluctuations. A major focus of this work is validating the robustness of the frequency extraction algorithm under high-statistics conditions. We evaluate the algorithm's accuracy in handling propagated errors and discuss the expected sensitivity of this FFT-based technique. This method provides a robust, model-independent complementary tool for probing CPT violation in future precision neutrino experiments such as Hyper-Kamiokande in Japan and DUNE in the US

Presenter: Lê Cẩm Vi

P.4 – Poster, VCTP-51

Resolving Singularities in Sign-Changeable Interacting Dark Energy via Observational Constraints from Type Ia Supernovae

Dang Minh Nhut

Dalat University

Despite the remarkable phenomenological success of the standard ΛCDM cosmological model, it still exhibits many scientific gaps in both theoretical and observational aspects, particularly regarding the fine-tuning, cosmic coincidence, H_0 tension, and S_8 tension problems. Therefore, a new physical model beyond the ΛCDM paradigm is required. The Interacting Dark Energy (IDE) model, which assumes a non-gravitational interaction between dark energy (DE) and dark matter (DM), allows for the exchange of energy between them. Recent cosmological analyses indicate the possibility of a sign-changeable interaction, that is, the direction of energy transfer being reversed

during evolution. However, the linear parametrization based on the Taylor expansion, $b(z) = b_0 + b_1 z$, diverges and creates unphysical singularities in the early Universe. To resolve physical inconsistencies and ensure convergence at high redshifts, this study investigates the dynamics of the sign-changeable IDE model through the Chevallier-Polarski-Linder (CPL) and Jassal-Bagla-Padmanabhan (JBP) parametrizations, directly confronting them with the standard linear model. A numerical framework is established to combine the theoretical system of equations with a dataset of 580 Type Ia Supernovae from the Union2.1 compilation through an optimization algorithm, in order to estimate the density parameters and related dynamical quantities. The results confirm that the CPL and JBP parametrizations not only fit observational data in the late Universe but also preserve thermodynamic stability in the early Universe, thus providing a phenomenological mechanism significantly superior to the conventional linear approach.

Presenter: Dang Minh Nhut

P.5 – Poster, VCTP-51

First-principles elucidation of hydrogen insertion in Sr3Co3O8 in Grenier Phase

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Recently, oxygen-deficient transition-metal oxides with the Grenier-phase structure have attracted significant attention because they combine key structural and functional characteristics of both perovskite and brownmillerite oxides. This unique framework offers opportunities for tuning ionic transport, electronic properties, and topotactic phase transitions [1-3]. However, the atomic-scale mechanisms and electronic consequences of hydrogen insertion in Grenier-phase oxides remain poorly understood. In this work, we investigate the structural and electronic properties of $Sr_3Co_3O_8$ and its hydrogenated phases using first-principles density functional theory calculations. We find that the polar and antipolar phases are nearly degenerate in energy, suggesting that $Sr_3Co_3O_8$ exhibits a polar instability and may exhibit switchable structural distortions under external stimuli. Hydrogen insertion is thermodynamically favorable and proceeds through O–H bond formation, accompanied by significant charge redistribution and modifications of the Co–O bonding network. The resulting electronic-structure changes provide insights into the stabilization mechanism of the hydrogenated phase and the role of hydrogen in tuning the properties of Grenier-phase cobalt oxides. These findings will be presented and discussed at the conference. [1] J. Zhang et al. Nat. Mater. 23, 912-919 (2024) [2] Y Shin, J Liang, G. Yu, C. Leighton, G. Galli, ACS Appl. Mater. Interfaces 17, 15603-15612 (2025) [3] Y. Isoda, T. N.Pham, R. Aso, S. Nakamizo, T. Majima, S. Hosokawa, K. Nitta, Y. Morikawa, Y. Shimakawa, D. Kan, Nat Comm, 16, 56 (2025)

Presenter: Pham Ngoc Thanh

P.6 – Poster, VCTP-51

Thermodynamic properties and melting temperature of FCC Cu–Ni alloys under high pressure

Nguyen Thi Hong (1), Nguyen Hoai Thanh (2), Tran Le Ngoc Tho (1)

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In this study, the Debye model was developed to investigate the effect of high pressure on several characteristic thermodynamic properties and melting temperature of the face-centered cubic (FCC) Cu–Ni alloy, including the Debye frequency, Debye temperature, and Debye–Waller factor (DWF) and melting temperature. Based on the theory of lattice vibrations, expressions for the interatomic interaction potential in the FCC Cu–Ni alloy were constructed, forming the basis for describing the vibrational characteristics of the material system. From the established model, analytical expressions describing the volume (or pressure) dependence of the Debye frequency, Debye temperature, DWF and melting temperature were derived for Cu–Ni alloy across the entire pressure range under investigation. These analytical results were used to numerically calculate and analyze the variation of thermodynamic quantities with pressure. The results show that increasing pressure significantly affects the lattice vibrational characteristics of the alloy. Specifically, the Debye frequency and Debye temperature increase with increasing pressure due to the increased stiffness of the crystal lattice, while the DWF decreases, reflecting the reduction in the amplitude of atomic thermal vibrations under compression. The theoretical results were compared with available experimental and previously reported data, showing good agreement and confirming the reliability of the proposed model. This work provides a scientific basis for predicting lattice vibration properties, analyzing Extended X-ray Absorption Fine Structure (EXAFS) spectra, and designing Cu–Ni alloy for high-pressure applications.

Presenter: Nguyen Thi Hong

P.7 – Poster, VCTP-51

A Density Functional Theory Investigation into the Application Potential of an MBene Material Ti2B2 as an Anode Material for Sodium-Ion Batteries

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We represent here an investigation on an MBene material Ti2B2 as an anode material for sodium-ion batteries on the base of density functional theory (DFT) calculations. This material has been experimentally synthesized in two structural phases: hexagonal and orthorhombic [1, 2]. Our results indicate that the hexagonal phase is thermodynamically more stable than the orthorhombic phase, with an energy difference of 78 meV per formula unit. The electronic conductivity, ion conduction, and storage capacities of both phases were evaluated through detailed analysis of the electronic structures and the migration pathways of sodium ions on the material surfaces. Both structural phases exhibit a metallic band structure, ensuring excellent electronic conductivity. The effective masses of charge carriers in the hexagonal and orthorhombic phases are 1.42me and 2.06me, respectively. The lowest diffusion barriers for sodium ions in the hexag-

onal and orthorhombic phases are 7 meV and 19 meV, respectively, indicating rapid diffusion kinetics. Consequently, the hexagonal phase is significantly better than the orthorhombic phase in terms of both electronic and ionic conductivity. These differences are explained based on detailed analyses of the correlation between the electronic structure and the crystal lattice.

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Presenter: Phạm Tuấn Kiệt

P.8 – Poster, VCTP-51

Dual-site methylammonium-zinc co-doping enhances phase stability and tunable optoelectronic properties in α-CsPbI3 perovskites: a first-principles study

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All-inorganic cesium lead iodide (CsPbI3) perovskites are promising candidates for next-generation optoelectronic devices; however, their practical implementation is hindered by the poor phase stability of the photoactive α-phase. In this work, density functional theory calculations combined with M3GNet machine-learning-assisted structural optimization were employed to investigate the effects of A-site methylammonium (MA+) doping, B-site Zn2+ doping, and synergistic (MA-Zn) co-doping on the structural, mechanical, electronic, and optical properties of α-CsPbI3. The co-doped system exhibits the highest Goldschmidt tolerance factor (t = 0.834) and a strongly negative formation energy (-4.357 eV), indicating significantly enhanced thermodynamic stability relative to pristine CsPbI3. Phonon analysis further reveals that co-doping suppresses lattice instability while preserving the soft vibrational characteristics beneficial for carrier transport. Mechanical calculations confirm that all compositions satisfy the Born stability criteria and maintain ductile behavior despite progressive lattice softening upon doping. Electronic structure analysis demonstrates effective bandgap tunability from 1.253 to 1.730 eV depending on the dopant configuration, with the (MA-Zn) co-doped system exhibiting a direct bandgap of 1.594 eV, favorable for photovoltaic applications. Projected density-of-states analysis reveals that neither MA+ nor Zn2+ introduces detrimental mid-gap trap states near the band edges. Optical calculations show that Zn doping preserves strong visible-light absorption, whereas MA incorporation induces systematic blue shifts in the dielectric response and absorption spectra. Thus, the unified co-doping strategy provides a viable route for simultaneously improving phase stability and tailoring the optoelectronic properties of CsPbI3, offering atomistic insights for the rational design of stable perovskite-based photovoltaic and light-emitting devices.

Presenter: Nguyen Chi Ben

P.9 – Poster, VCTP-51

Reservoir-controlled topological triplet excitonic condensations

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We study nonequilibrium steady states of a two-dimensional electron-hole Hamiltonian with Rashba spin-orbit coupling, Zeeman splitting, Coulomb attraction, and band-selective tunnelling to independent fermionic reservoirs. Using self-consistent Hartree-Fock theory combined with steady-state quantum kinetic equations, we show that reservoir imbalance qualitatively reconstructs the topology of triplet excitonic condensates (ECs). At equilibrium, the emergence of the spin-down triplet EC converts the topological spin-up triplet EC into a topologically trivial coexistence phase. Away from equilibrium, the combined effect of bath chemical-potential imbalance and reservoir-coupling asymmetry stabilizes a topologically nontrivial coexistence of spin-up and spin-down triplet ECs. This topological sector shifts from negative to positive bath imbalance as the reservoir-coupling ratio is tuned through unity. Optical conductivity provides clear signatures through a two-peak longitudinal response and a chiral Hall signal. These results establish reservoirs as microscopic control fields for topological excitonic matter.

Presenter: Do Thi Hong Hai

P.10 – Poster, VCTP-51

Investigating the role of protein folding in G6PD deficiency

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G6PD deficiency is a widespread inherited disorder characterized by reduced activity of the enzyme glucose-6-phosphate dehydrogenase (G6PD), leading to hemolytic anemia. Apart from the enzyme's reduced thermosta-bility and diminished catalytic activity, there are indications that the deficiency can also result from impaired protein folding. In this work, we investigate the latter possibility by studying the folding of monomeric G6PD using the structure-based Go-like model. It is shown that G6PD is a three-state folder with an intermediate in which the N-terminal domain containing the NADP+ binding site is largely unfolded. The simulations also show that putative mutations at pathogenic mutation sites significantly slow down the folding process. The results support the hypothesis that the reduced enzymatic activity of certain G6PD mutants may be linked to impaired protein folding.

Presenter: Trinh Xuan Hoang

P.11 – Poster, VCTP-51

Theoretical predictions for triple Z boson production at the LHC

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In this work, a summary of the experimental and theoretical status of triple gauge boson pro-

duction at the LHC will be provided. Theoretical predictions for the specific case of triple Z boson production will then be presented.

Presenter: LE Duc Ninh

P.12 – Poster, VCTP-51

Metric Variation of the Energy-Momentum Tensor of a Perfect Fluid and Its Applications to Cosmology and Neutron Stars

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Previous studies have proposed specific forms for the matter Lagrangian L_m and the metric variation $\delta T_{\mu\nu}$ of a perfect fluid. However, we show in this work that these expressions are inconsistent with the standard energy-momentum tensor $T_{\mu\nu} = (\epsilon + P)u_\mu u_\nu - P g_{\mu\nu}$ under general conditions. As a result, a substantial body of work in cosmology and astrophysics based on these formulations requires careful re-evaluation. We derive an explicit expression for the metric variation $\delta T_{\mu\nu}$ by performing direct calculations on the standard perfect-fluid energy-momentum tensor, incorporating only the particle number conservation law. The obtained formula is completely independent of the choice of matter Lagrangian L_m. Applying this result to $f(R,T)$ gravity yields the precise form of the tensor $\Theta_{\mu\nu} = g^{\sigma\rho}\frac{\delta T_{\sigma\rho}}{\delta g^{\mu\nu}}$, which has long been a source of controversy in the literature. This expression remains valid for radiation as well, regardless of whether particle number conservation is imposed. A central finding of this study is that when the cosmic energy-momentum tensor contains only standard components obeying linear equations of state $P = \omega\epsilon$ with $\omega = 0$ (baryonic and cold dark matter), $\omega = 1/3$ (radiation), and $\omega = -1$ (cosmological constant), the conservation law $\nabla_\mu T^{\mu\nu} = 0$ holds for *arbitrary* functions $f(R,T)$. This contrasts sharply with earlier conclusions that restricted the allowed forms of $f(R,T)$. We further apply the derived $\Theta_{\mu\nu}$ to stellar interiors and obtain a family of $f(R,T)$ models that preserve energy-momentum conservation for a polytropic equation of state. A concrete model is constructed that remains consistent across both cosmological scales and high-density regimes inside neutron stars. Notably, the same set of parameters simultaneously alleviates the Hubble tension and accurately reproduces the observed mass-radius relation of neutron stars, including the maximum mass and corresponding radius.

Presenter: Pham Van Ky

P.13 – Poster, VCTP-51

Spectral signatures of the BCS–BEC crossover in mass - imbalanced Semimetal / Semiconductor Microcavities

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The spectral signatures of the Bardeen-Cooper-Schrieffer (BCS) - Bose-Einstein condensation (BEC) crossover in mass-imbalanced semiconductor and semimetal microcavities are investigated. In the framework of the unrestricted HartreeFock approximation, a two-band electron-hole model involving photon mode is analyzed by treating Coulomb attraction and light-matter coupling on equal footing. The single-particle spectral functions and the luminescence properties are then examined. In the semiconducting regime, a positive band gap stabilizes tightly bound excitons and yields predominantly BEC-type excitoniclike polaritonic condensates at low density, while increasing excitation density and reducing mass imbalance drives a continuous crossover toward BCS-type pairing with intermediate and photoniclike polaritonic character. In contrast, the semimetallic regime favors itinerant electron-hole pairing, with BCS-type condensates dominating and BEC excitoniclike coherence emerging only at sufficiently strong Coulomb interaction and large mass imbalance situations. The evolution of the single-particle and luminescence spectra provides clear spectroscopic signatures of these crossover phenomena, offering a unified framework for understanding and controlling polaritonic condensates in microcavity systems.

Presenter: Nguyen Thi Hau

P.14 – Poster, VCTP-51

Computational Design and Emergent Physical Characteristics of Novel 2D Janus Materials

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The advent of two-dimensional (2D) Janus materials has significantly broadened the scope of multifunctional low-dimensional systems. By breaking out-of-plane mirror symmetry, these structures unlock distinct phenomena absent from standard van der Waals counterparts. In this presentation, we detail a density functional theory (DFT) investigation into the structural engineering and emergent behaviors of several novel Janus monolayers. We demonstrate how intrinsic electric fields and geometric asymmetry drive remarkable features, notably giant Rashba spin splitting, enhanced piezoelectric response, and highly tunable band structures. Additionally, we evaluate carrier transport dynamics and the influence of phonon scattering to assess device viability. Ultimately, our results establish a robust theoretical foundation for realizing next-generation electronics and spintronics.

This research was funded by the Vietnam National Foundation for Science and Technology Development (NAFOSTED) under Grant No. 103.01-2024.14.

Presenter: Nguyen Ngoc Hieu

P.15 – Poster, VCTP-51

Enhancement of two-mode sum squeezing and quantum entanglement through two-photon addition and two-photon subtraction in Pair coherent states

Ho Sy Chuong, Le Minh Triet, Nguyen Thi Thu Thuy

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This work investigates the nonclassicality of the two-photon-added and two-photon-subtracted pair coherent state (TPA-TPS-PCS) through Hillery's two-mode sum squeezing and entanglement criteria. Our results show that TPA-TPS-PCS exhibits two-mode sum squeezing, whereas the original pair coherent state (PCS) does not. The degree of squeezing is enhanced with increasing degeneracy parameter (q). Furthermore, TPA-TPS-PCS displays stronger entanglement than PCS, with both the depth and the region of entanglement increasing for larger values of (q). These findings demonstrate that two-photon addition and two-photon subtraction can significantly enhance the nonclassicality of PCS by generating two-mode sum squeezing and strengthening entanglement resources in two-mode optical systems.

Presenter: Ho Sy Chuong

P.16 – Poster, VCTP-51

Material-Dependent Hot-Electron Energy Dissipation in GaAs-, GaSb-, and InAs-Based Asymmetric Gaussian Quantum Wells: Implications for Infrared and Terahertz Optoelectronics

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Material-dependent hot-electron energy dissipation in GaAs-, GaSb-, and InAs-based asymmetric Gaussian quantum wells is investigated through the hot-electron energy-loss rate (ELR), with particular asymmetric Gaussian confinement, which more closely represents practical quantum-well structures than idealized square-well models. The ELR is calculated within the electron temperature model by considering electron–LO phonon interaction under a quantizing magnetic field, while the effects of electron temperature, electric field, quantum-well depth, and quantum-well width are systematically examined. The results demonstrate that the ELR can be effectively controlled and tuned by adjusting the quantizing magnetic field, electron temperature, electric field, quantum-well depth, and quantum-well width, highlighting the high tunability of hot-electron energy dissipation in asymmetric Gaussian quantum wells. Distinct material-dependent ELR behaviors are observed among the GaAs-, GaSb-, and InAs-based structures owing to differences in their electronic properties, phonon characteristics, and electron–phonon interaction strengths. These findings provide valuable physical insight into carrier energy relaxation in low-dimensional semiconductor systems and have important implications for the design of infrared and terahertz optoelectronic devices based on quantum-confined nanostructures.

Presenter: Pham Tuan Vinh

P.17 – Poster, VCTP-51

Non-Gaussianity and nonclassicality of generalized superpositions of displaced Fock states

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In this work, we introduce a class of quantum states constructed as generalized superpositions of single-mode displaced Fock states (GSDFSs) with different photon numbers, displacement amplitudes, and relative phases. The non-Gaussianity of the states is investigated through the phase-space behavior of the Wigner function, while their nonclassical properties are examined using higher orders of Hillery squeezing and antibunching criteria. Furthermore, the degree of nonclassicality is quantified by the volume of the negative part of the Wigner function. The results show that the state parameters significantly influence the interference structure in phase space and the manifestation of nonclassical effects. For suitable parameter regimes, the states exhibit pronounced non-Gaussianity together with a high degree of nonclassicality. These findings provide further insight into the role of quantum interference arising from the superposition of single-mode displaced Fock states in generating and enhancing the nonclassical properties of non-Gaussian quantum states.

Presenter: Nguyen Thi Thu Thuy

P.18 – Poster, VCTP-51

Exploring Single-Molecule Magnets by Methods of Computational Quantum Chemistry

Anton Syurakshin

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Prominent physical properties of a broad family of single molecule magnets (SMM) based on the transition metal ions with the partially filled electronic 3d- orbital shell are characterized and their potential for practical applications is disclosed. Recent reviews [1,2] demonstrate numerous important scientific and application potentials of SMM for various quantum technologies. Among the major characteristic of SMM is the strength of intra-ion magnetic anisotropy $D(Sz)^2$, known also as zero field splitting (ZFS), that determines the barrier U_{eff} for SMM magnetization reversal. To evaluate the expected characteristic of a SMM such as the aforementioned ZFS, the low-energy subspace including the multi-electron eigenstates have to be obtained, together with their eigenenergies, by solving Schrodinger equation with a general all-electron Hamiltonian of the SMM. In our work this is done for mononuclear complexes such as metal-organic molecule, based on explicitly correlated (multiconfigurational) ab initio quantum- chemical calculations performed with the use of Firefly computer program [3]. Particular attention is paid to establishing the dependence of the ZFS value on the characteristics of the ligand field formed by the organic environment of the magnetic transition metal ion.

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Presenter: Syrakshin Anton

P.19 – Poster, VCTP-51

Estimating the magnitude of coherent ring current In π-conjugated aromatic molecules

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Photo-induced charge migration descibes the motion of an electron or a hole from one site to another within a molecule, and this process can be controlled by an external optical field. As a typical example of charge migration in π-conjugated aromatic molecules, coherent π-electron rotation can be generated by a laser pulse that excites a pair of degenerate excited states involved in the π-π^* transition from the ground state. Within the traditional Hückel model, π molecular orbitals are represented as linear combinations of pz atomic orbitals. The ring current induced by such rotational electron motion can generate a magnetic field strong enough to be detected experimentally. Therefore, the magnitude of ring current is one of the key observable quantities in the development of molecular switching devices based on organic molecules. In a previous theoretical study [J. Chem. Phys. 138, 074304 (2013)], the current magnitude has been evaluated along the bonds connecting neighboring atoms in a molecular ring, a quantity known as the coherent bond current. Here, the coherent bond current was calculated in π-conjugated aromatic systems by combining an analytical approach with ab-initio calculations, in which the bond current formula was derived using the Slater type pz atomic orbitals. However, the Slater type pz orbitals are not fully consistent with the Gaussian basis sets commonly employed in modern ab initio calculations. This motivates us to formulate the coherent bond current using Gaussian type pz orbitals in π-conjugated systems, such as benzene, toluene and coronene. The proposed formulation provides a more consistent framework for evaluating coherent bond currents in conjunction with Gaussian-based electronic structure calculations.

Presenter: Ho Quang Huy

P.20 – Poster, VCTP-51

In silico disease outbreak dynamics using stochastically-resetting 2D Ising and Blume-Capel models

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(3) Philippine Science High School-Main Campus;

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(5) University of the Philippines Manila

Two-dimensional lattice models are useful tools simulating dynamics of infectious diseases in a population. This study uses a stochastically-resetting Ising model to simulate a simple contagion, for which the spin-up denotes healthy individuals and vice versa. On the other hand, the spin-1

Blume-Capel model is run through algorithms as an alternative to the known suspected-infected-recovered model of epidemics. Both two-dimensional models at critical temperatures are subject to a four-part algorithm to represent waves of the outbreak, changes in an individual's state, spread or containment of the disease, and social restrictions. Results show a random final state for different cases. Furthermore, a higher number of initially infected individuals can cause more waves as indicated by the number of stochastic resets.

Presenter: Lamento-Villegas Barbarona Em-Em

P.21 – Poster, VCTP-51

Investigating physical properties of nano tungsten trioxide under the adsorption of liver cancer-related gases using density functional theory

Phan Thi Hong Hoa (1,2), Nguyen Luu Thanh Ngan (1,2), Nguyen Vu Dang Khoa (1,2), and Do Ngoc Son (1,2)

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Volatile organic compounds in exhaled breath open up a promising avenue for non-invasive early cancer diagnosis. Tungsten trioxide is a promising sensing material; however, no studies have been published to clarify its electronic and thermoelectric properties for detecting volatile organic compounds. By the density functional theory calculations and the Boltzmann transport equation, we clarified the properties of tungsten trioxide upon the adsorption of volatile organic compounds.

Acknowledgement. This research was funded by Vietnam National University Ho Chi Minh City (VNU-HCM) under grant number A2025-20-02.

Presenter: Phan Thi Hong Hoa

P.22 – Poster, VCTP-51

Synergistic multi-doping effect on thermal-electrical properties of $Ce_{0.8-x}$ $(La_{1/3}$ $Sm_{1/3}$ $Gd_{1/3})_{0.2}$ M_x O_{2-y} (M = Ca, Sr) electrolytes for intermediate temperature solid oxide fuel cells

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The simultaneous incorporation of rare-earth (La^{3+}, Sm^{3+}, and Gd^{3+}) and alkaline-earth (Ca^{2+} or Sr^{2+}) multi-dopants breaks the local lattice symmetry, suppresses the ordering of oxygen vacancies into defect clusters, and increases the unit-cell free volume, thereby leading to a marked improvement in ionic conductivity relative to single-doped ceria. The combined effects

of weakened interionic electrostatic attraction and a more flexible lattice structure enhance the thermal expansion coefficient to the range of 12.70–13.25 $\times 10^{-6}$ °C^{-1}. The non-linear dependence of vacancy activation energy and ionic conductivity on the multi-dopant concentration is governed by the competition between enhanced vacancy mobility resulting from the expanded free volume and elastic relaxation at low doping levels, and suppressed vacancy hopping caused by defect clustering and cation blocking at higher dopant concentrations. We find that $Ce_{0.75}(La_{1/3}Sm_{1/3}Gd_{1/3})_{0.20}Ca_{0.05}O_{1.85}$ and $Ce_{0.77}(La_{1/3}Sm_{1/3}Gd_{1/3})_{0.20}Ca_{0.03}O_{1.87}$ exhibit the lowest activation energy and the highest bulk ionic conductivity.

Presenter: Le Thu Lam

P.23 – Poster, VCTP-51

Unveiling Vacancy-Induced Magnetism in TiO2 via Electronic Structure Calculations

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We present a theoretical study on vacancy induced magnetism of anatase and rutile Titanium dioxide (TiO_2) based on Density Functional Theory (DFT) calculations. Perdew-Burke-Ernzerhof (PBE) and regularized-restored Strongly Constrained and Appropriately Normed (r^2SCAN) functionals with Hubbard Correction (DFT+U) were employed. While both the PBE and PBE+U functionals fail to predict the higher stability of the rutile phase over anatase, the r^2SCAN + U method correctly captures this relative stability. Regarding Ti-vacancy induced magnetism, PBE+U and r^2SCAN+U yield closely matching net magnetic moments for anatase, at 3.99 μ_B and 3.97 μ_B, respectively. However, for the rutile phase, the Ti-vacancy-induced magnetic moment predicted by PBE+U method, 0.73 μ_B is less than half of the value obtained with r^2SCAN + U method, 1.60 μ_B. For O-vacancy induced magnetism, while r^2SCAN + U method predicts zero net magnetic moment for both phases, PBE + U yields a non-magnetic state for anatase but a moment of 2.00 μ_B for rutile. The origins of magnetism and the discrepancies between the functional approximations are thoroughly elucidated through a detailed electronic structure analysis.

Presenter: Nguyen Duc Phong

P.24 – Poster, VCTP-51

Optimization of Light Collection in a Miniature Water Cherenkov Detector Using Geant4 Simulations

Hoang Nguyen

IFIRSE, ICISE Centre

Water Cherenkov detectors are widely used in particle and nuclear physics experiments for the detection of charged particles through Cherenkov radiation. Their performance strongly depends on optical photon transport and photon collection efficiency, making the optimization of the optical system a crucial aspect of detector design.In this work, a detailed Geant4 model

was developed to study light collection in a planned miniature water Cherenkov detector for cosmic-ray measurements. The proposed detector consists of a $10 \times 10 \times 10$ cm^3 acrylic water tank instrumented with 16 silicon photomultipliers (SiPMs), Tyvek reflectors, and a cosmic-ray muon coincidence trigger provided by two plastic scintillation counters positioned above and below the detector. The simulation accounts for Cherenkov photon production, optical photon transport, reflections from Tyvek surfaces, and photon collection at the SiPM array.Several optical design parameters were systematically investigated, including SiPM placement, acrylic thickness, Tyvek reflector configuration, and optical coupling conditions (air-gap vs. optical gel). Truth-level simulation data was utilized to evaluate photon collection efficiency, identify optical loss mechanisms, and separate water-generated Cherenkov photons from scintillation noise produced within the acrylic walls.The simulation demonstrates that optical gel coupling significantly suppresses total internal reflection (TIR) at the boundaries, increasing the pure photon yield by a factor of roughly 2.2 compared to the air-gap configuration. However, this index matching also introduces a trade-off, elevating the material noise fraction (acrylic scintillation) from $\sim 2.5\%$ to approximately 15.6%. Furthermore, positioning the Tyvek reflector on the outer surface of the tank enhances the overall photon yield by recovering light trapped in the acrylic walls. Crucially, timing analysis indicates that these acrylic-born photons introduce negligible time dispersion relative to the primary signal from water.These quantitative results provide key baselines for optimizing the detector design, highlighting the trade-offs between signal yield and noise, and support the development of compact SiPM-based water Cherenkov detectors for future applications.

Presenter: Nguyen Hoang

P.25 – Poster, VCTP-51

A computational framework for solving the few-body schrödinger equation with quantum interactions

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This work presents a high-performance computational framework designed to solve the few-body Schrödinger equation using the configuration interaction scheme. The many-body Hamiltonian is constructed in a Fock-state basis and solved via exact diagonalization. To overcome the curse of dimensionality, the developed program integrates configuration-space reduction techniques with parallel computing algorithms, significantly reducing computational costs and extending applicability beyond conventional limits. Characterized by a modular architecture, the framework seamlessly adapts to diverse particle species, physical models, and interaction potentials.

The program's accuracy and reliability are validated through benchmark calculations of low-dimensional confined systems, specifically 1D trapped bosons with delta-function interactions and fermions with regularized Coulomb potentials. This computational tool establishes a robust foundation for investigating both the stationary and dynamical properties of interacting quantum gases.

Presenter: Phan Quang Sơn

P.26 – Poster, VCTP-51

Microscopic description of Quarkyonic matter in neutron stars using the microscopic interaction

Ngo Hai Tan

Phenikaa University

Recent astrophysical observations of massive neutron stars and GW170817 require an equation of state (EOS) where the sound speed exceeds the conformal limit. While the Quarkyonic matter model naturally explains this behavior through a nucleon-quark crossover, it typically relies on simplified phenomenological potentials. In this work, we improve the dynamical Quarkyonic framework by integrating the microscopic, density-dependent CDM3Y6 interaction to describe the nucleon Fermi shell. By analyzing beta-equilibrated npeμ matter, we demonstrate that this realistic nuclear physics foundation naturally stiffens the EOS and provides radius predictions consistent with the latest observational constraints. Our findings underscore that incorporating realistic nucleon interactions is essential for accurately modeling the internal structure of hybrid stars.

Presenter: Ngo Hai Tan

P.27 – Poster, VCTP-51

Detecting Volatile Organic Compounds in Exhaled Breath: A Theoretical Perspective

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Exhaled breath analysis has emerged as a promising, non-invasive diagnostic tool for the early detection of metabolic disorders and respiratory diseases. Volatile organic compounds (VOCs) serve as critical biomarkers for conditions like diabetes and lung cancer. However, designing sensor materials with high sensitivity and absolute selectivity remains a significant hurdle due to the complex environment of human breath. This work establishes a fundamental theoretical framework to evaluate and predict the VOC-sensing performance of semiconductor materials. Acknowledgement. This research was funded by Vietnam National University HoChiMinh City (VNU-HCM) under grant number A2025-20-02.

Presenter: Do Ngoc Son

P.28 – Poster, VCTP-51

Defect and dopant engineering in silicene/MoS2 van der Waals heterostructures for next-generation gas sensing

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The development of next-generation environmental and industrial monitoring networks demands gas sensors that combine ultra-high sensitivity, chemical selectivity, and rapid recovery at room temperature. Two-dimensional van der Waals heterostructures are among the most promising candidates, yet their practical implementation is severely limited by the chemical inertness of basal planes and sluggish desorption kinetics. In this talk, we will present how atomic-scale design of Silicene/MoS2 heterostructures can address these long-standing challenges. Using density functional theory calculations, we reveal how controlled surface engineering, through atomic defect generation (VMo, VS, VMo2,. . .) and elemental co-doping (Au-B), modulates the electronic structure, adsorption strength, and interfacial charge transfer of the sensing platform. We systematically explore these defective and doped MoS2 capping layers, uncovering distinct chemisorption mechanisms, spintronic behaviors, and a dopant-driven semiconductor-to-metal transition that govern polysulfide-like anchoring and highly selective CO2 capture. These insights provide a direct link between atomic-level interactions and macroscopic sensor performance, guiding the rational design of advanced sensing materials with ultrafast recovery times (as low as 0.05 ns). The results highlight a unifying strategy to bridge computational materials design and practical gas sensing, paving the way toward sustainable, high-performance environmental monitoring networks.

Presenter: Duong Trong Nhan

P.29 – Poster, VCTP-51

A DFT study of acetone adsorption on the zinc oxide nanosheets

Nguyen Vu Dang Khoa (1,2), Nguyen Thi My Ngoc (1,2), Nguyen Luu Thanh Ngan (1,2), Phan Thi Hong Hoa (1,2), Pham Thanh Hai (1,2,3), Tran Phuong Dung (4,5), and Do Ngoc Son (1,2,)*

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Using density functional theory simulations, we theoretically investigate the acetone adsorption performance of pristine and doped zinc oxide (ZnO) nanosheets. Our results reveal that

the introduction of dopants significantly enhances the acetone-sensing capabilities of the ZnO nanosheets. Notably, acetone adsorption on the doped ZnO induces a dramatic shift of the Fermi level from the bandgap region into the conduction band, triggering a clear transition from a semiconducting to a metallic conducting state. This profound electronic modulation demonstrates the high potential of doped ZnO nanosheets for use in non-invasive, real-time breath acetone sensors for diabetic blood sugar monitoring.

Presenter: Nguyen Vu Dang Khoa

P.30 – Poster, VCTP-51

Enhancement of stability and electronic properties of ultra-high nickel cathodes by aluminium and boron codoping studied by combined density functional theory and neural network models.

Nguyen Vo Anh Duy (1, 2); Tran Van Thien (1, 3); Nguyen Huu Phuc (1); To Van Nguyen (4); Dang Minh Triet (1)

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(4) Le Quy Don Technical University

The rapid growth of electric vehicles and large-scale energy storage systems has intensified research on nickel-rich lithium-ion battery cathodes, prized for their high energy density, superior electrochemical performance, and reduced material costs. In this study, density functional theory (DFT) calculations are integrated with machine learning (ML) techniques using DeePMD-based neural network models to investigate the structural stability and electronic properties of Ni-rich cathode materials, including LiNi0.6Mn0.2Co0.2O2 (NMC622), LiNi0.8Mn0.1Co0.1O2 (NMC811), and LiNi0.9Co0.05Mn0.05O2 (NMC955). The neural network models successfully reproduce DFT-calculated energies and forces with R2 values exceeding 0.9, enabling accurate prediction of thermodynamic stability across wide temperature ranges. Increasing Ni content enhances electronic conductivity but reduces structural robustness due to intensified Ni–O hybridization. Co-doping NMC955 with aluminum and boron improves lattice stability, redistributes charge, and lowers the Li-ion diffusion barrier from 0.355 eV to 0.206 eV. Thus, Al–B codoping achieves a favorable balance between electronic and structural performance. This integrated DFT-ML framework offers an efficient pathway for the rational design of robust, high-energy Ni-rich cathodes for next-generation lithium-ion batteries.

Presenter: Duy Vo Anh Nguyen

P.31 – Poster, VCTP-51

Formic Acid Decomposition on Pd–Au Catalysts for Green Hydrogen Production

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Hydrogen is considered a promising clean energy carrier for sustainable energy development. Among hydrogen storage materials, formic acid (HCOOH) has attracted significant attention due to its high hydrogen content, safe storage, and easy transportation. In this study, the catalytic performance and reaction mechanism of formic acid decomposition on Pd–Au catalysts were investigated using Density Functional Theory (DFT) combined with Machine Learning Interatomic Potentials (MACE) and ML-NEB calculations. Various Pd–Au surface configurations were constructed and optimized to evaluate the adsorption behavior of HCOOH and reaction intermediates. Particular attention was paid to the two competing reaction pathways: the dehydrogenation pathway via HCOO* intermediates leading to H_2 and CO_2 formation, and the dehydration pathway via COOH* intermediates associated with CO production. Adsorption energies, activation barriers, and electronic structures were analyzed to clarify the role of Au doping in modifying the catalytic activity and selectivity of Pd surfaces. The results are expected to identify the most favorable pathway for hydrogen generation while suppressing CO formation, providing theoretical guidance for the design of efficient Pd–Au catalysts toward green hydrogen production.

Presenter: Huỳnh Thị Lan Trinh

P.32 – Poster, VCTP-51

Magnetic and transport properties of bilayer honeycomb lattice: Magnetization processes, magneto-caloric effect, and tunneling magneto-conductivity in CrI_3 thin films

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We investigate the magnetic, thermodynamic, magneto-caloric, and transport properties of a bilayer honeycomb spin lattice using both mean field theory and replica-exchange Monte Carlo simulations. In the absence of an external magnetic field, the bilayer system exhibits inter-layer antiferromagnetic (AF) ordering below the Néel temperature, which decreases with reducing inter-layer AF exchange coupling. Under an applied magnetic field, a field-driven first-order magnetization process (FOMP) is observed, characterized by a step-like magnetization curve and an abrupt transition to a fully polarized state at a critical field. The critical field is found to scale linearly with the inter-layer coupling strength, highlighting the key role of inter-layer magnetic interactions in determining the magnetic response. The thermodynamic behavior is further analyzed through the temperature dependence of magnetization, susceptibility, and specific heat. The magnetic entropy change exhibits a distinctive double-peak structure with opposite signs,

arising from the competition between AF inter-layer and ferromagnetic intra-layer interactions. This behavior reveals a complex magneto-caloric response associated with field-induced magnetic phase transitions. In addition, the field dependence of the tunneling magneto-conductivity is calculated and shows good agreement with available experimental observations in bilayer CrI_3 thin films. The results clarify the microscopic origin of FOMPs and their direct connection to tunneling magneto-transport phenomena in layered van der Waals magnets.

Presenter: Bach Huong Giang

P.33 – Poster, VCTP-51

Understanding the ferromagnetism in two-dimensional Hubbard model with application to twisted bilayer structures

Duy Hoang Nguyen, Son Trong Nguyen, Hung The Dang

Faculty of Materials Science and Engineering, Phenikaa University

Ferromagnetism is one of the most fundamental phenomena in condensed matter physics. Understanding the conditions for ferromagnetic order as well as designing materials exhibiting this physics is important because of the wide range of applications. In this work, we will review the conditions for ferromagnetism in the two-dimensional Hubbard model with square and triangular lattices, starting from the long-standing Stoner criterion to a more quantitative extension of this criterion for itinerant ferromagnetic order. In particular, we consider ferromagnetism in a special kind of triangular lattice that includes spin-valley locking effect, mimicking the flat bands of several twisted transition metal dichalcogenide structures. This work will shed more light into the ferromagnetism in these twisted structures, allowing for the design of materials that maximizes this effect.

Presenter: Nguyen Hoang Duy

P.34 – Poster, VCTP-51

Study of non-Fermi liquid behavior in the low-energy flat bands of twisted transition metal dichalcogenides

Son Trong Nguyen, Duy Hoang Nguyen, Hung The Dang

Faculty of Materials Science and Engineering, Phenikaa University

Fermi liquid is the de facto theory for strongly correlated systems. Therefore, finding materials exhibiting non-Fermi liquid behaviors is an important but non-trivial task for researchers in this field. In this work, we consider the two-dimensional Hubbard model in triangular lattice including spin-valley locking effect, which reflects the low-energy flat bands of twisted transitional metal dichalcogenide structures. By change the phase angle encoded in the model, which is related to the displacement field in the corresponding experiments of the twisted structures, we may enter the non-Fermi liquid regime, in which we study various physical quantities such as the mass enhancement, spin susceptibility using the dynamical mean-field theory. The study of these measurements for a wide range of the correlation strength provides more insights into the physics of the non-Fermi liquid vs. Fermi liquid behaviors that might be observed in the twisted structures of transition metal dichalcogenides.

Presenter: Nguyen Trong Son

P.35 – Poster, VCTP-51

Chiral Redistribution of Quantum Entanglement: Spectral Mechanisms and Delayed Correlation Transfer in a Rhombic Spin Network

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We investigate the dynamics of quantum entanglement in a rhombic spin-1/2 network with nearest-neighbor XY exchange, Dzyaloshinskii-Moriya (DM) interactions, and a diagonal cross coupling. Exploiting the symmetry of the single-excitation subspace, we obtain analytical expressions for the eigenstates and time-dependent wave amplitudes, which enable a detailed characterization of pairwise entanglement generation, redistribution, and propagation. The analysis reveals that the DM interaction does not simply enhance quantum correlations but reorganizes their distribution among competing channels. In particular, a pronounced suppression of the diagonal entanglement channel is accompanied by the activation of alternative pathways, leading to a redistribution of pairwise correlations across the network. This behavior is quantified through both the total negativity and a redistribution metric that measures the imbalance between dominant entanglement channels. Spectral analysis further shows that the strongest redistribution occurs near a level-crossing condition, where the eigenstate composition undergoes a significant rearrangement. Time-resolved cross-correlation analysis demonstrates characteristic delays between entanglement channels, indicating a sequential transfer of correlations through the network. These results identify a direct connection between spectral structure and correlation dynamics and suggest that chiral interactions provide an effective means of controlling the spatial and temporal organization of entanglement in finite spin systems.

Presenter: Tran Cong Phong

P.36 – Poster, VCTP-51

De Sitter vacuum on nucleated D-branes with stringy corrections

Cao Hoang Nam

Institute of Theoretical and Applied Research, Duy Tan University

We present four-dimensional de Sitter (dS) vacuum solutions on probe D-branes nucleating in a background, which is a U(1) charged black hole solution of IIB supergravity, including stringy corrections. A sufficiently high chemical potential induced by the wrapped D3-brane charge, inducing an instability in the system, is essential to lead to the nucleation of the probe D-branes. We show that stringy corrections can yield a dS vacuum on spherical D-branes consistent with the observations without fine-tuning.

Presenter: Cao Hoang Nam

P.37 – Poster, VCTP-51

Excited Exciton States and Hydrogenic Convergence in Anisotropic Two-Dimensional Materials

Le Hoang Viet, Le Do Dang Khoa, Le Van Hoang

Ho Chi Minh City University of Education

The excitonic energy spectrum in anisotropic two-dimensional monolayers has been extensively studied in recent years because of its fundamental and technological importance. Previous investigations have indicated that highly excited excitonic states tend to converge toward the spectrum of the two-dimensional hydrogen atom. Nevertheless, for anisotropic systems, the use of an effective Keldysh potential provides a computationally efficient framework for theoretical analysis. In this work, we examine the effective Coulomb potential and compare its results with those obtained from the Keldysh potential in the high-energy regime. Particular attention is devoted to the excited-state structure of excitons, aiming to clarify the applicability of the effective potential description in anisotropic two-dimensional materials.

Presenter: Le Hoang Viet

P.38 – Poster, VCTP-51

Transition metal dichalcogenides heterostructures for lung cancer diagnosis via alveolar gas analysis

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Early detection of lung cancer plays a decisive role in enhancing treatment efficacy and patient survival rates. Within this context, alveolar breath-sensing technology is recognized as a biomedical breakthrough, offering a non-invasive, safe, and highly cost-effective alternative to conventional clinical techniques. In this study, we design sensing films based on transition metal dichalcogenide heterostructures to precisely identify and screen volatile organic compounds acting as breath biomarkers. The primary advantage of these heterostructure systems over their pristine monolayer constituents lies in the formation of heterojunctions, which induce a robust built-in electric field that accelerates charge transfer kinetics upon interaction with target gas molecules. Utilizing density functional theory calculations, we elucidate the fundamental relationship between the geometric configurations, electronic structures, and gas-sensing characteristics of theses material systems. This work establishes a rigorous theoretical foundation, providing critical guidelines for the design, optimization, and fabrication of next-generation cancer-screening devices.

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Presenter: Ong Kim Le

P.39 – Poster, VCTP-51

Electronic and thermoelectric properties of WSe_2 under the adsorption of VOCs: First-principles study

Nguyen Luu Thanh Ngan (1,2), Nguyen Vu Dang Khoa (1,2), Nguyen Thi My Ngoc (1,2), Tran Phuong Dung (3,4), Huynh Tat Thanh (2,5), Pham Ngoc Thanh (2,5), and Do Ngoc Son (1,2,)*

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Detecting volatile organic compounds (VOCs) from exhaled breath linked to cancers could provide a non-invasive approach for early diagnosis. Transition metal dichalcogenides, a family of two-dimensional materials, are promising candidates for VOC sensors. sensors. We herein investigate the sensing properties of WSe_2 monolayers toward specific VOCs using van der Waals density functional theory calculations. We also elucidate the electronic properties of the substrates upon the adsorption of VOCs. We believe that these findings will contribute to the development of highly sensitive nano-sensors for the early detection of cancer-related VOCs, thereby enhancing diagnosis and facilitating early interventions that can significantly improve survival rates.

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Presenter: Nguyễn Lưu Thanh Ngân

P.40 – Poster, VCTP-51

Investigating the binding of agonists to the stability of μ-opioid receptor

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Opioid agonists expressing analgesia are usually followed by adverse reactions such as heart failure, respiratory depression, constipation, etc. Agonist binding to μ-opioid receptors (μOR) can activate two intracellular signaling pathways: (i) the G protein signal is responsible for alleviating pain; (ii) β-arrestin results in unwanted side effects. Here, we utilize recent advances in computational power and molecular dynamics (MD) simulations to analyze and evaluate the influences of unbiased (Morphine – M6G) and biased (TRV130) compounds of the G protein signal, on the structural stability and functions of the μOR receptor. We have identified that M6G with hydroxyl groups, forms hydrogen bonds and electrostatic interactions with key residues in the catalytic site of the μOR receptor, whereas TRV130 prefers binding by hydrophobic and van der Waals interaction types. The binding to M6G leads to the higher flexibility of the μOR's TM VII, which is known to activate the β-arrestin signal, while this TM VII is more stable in

the TRV130-μOR complex. Additionally, the allosteric pockets of the Sodium (Na+) ion are different in these μOR complexes. Taken together, these studies may provide new avenues for the design of biased opioids with appropriate efficacy.

Presenter: Lai T. T. Hien

P.41 – Poster, VCTP-51

Twin hypercharge

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It is shown that a duplication of the hypercharge, which is identical for the normal sector but different for the dark sector, may manifestly address neutrino mass and dark matter.

Presenter: Phung Van Dong

P.42 – Poster, VCTP-51

Tuning Noncollinear RKKY Interactions in Altermagnets via Adiabatic Electron–Phonon Coupling

Bui D. Hoi

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Altermagnets, characterized by vanishing net magnetization and momentum-dependent spin splitting, provide a promising platform for spintronic applications owing to their unconventional spin textures and tunable magnetic properties. In this work, we investigate the Ruderman–Kittel–Kasuya–Yosida (RKKY) interaction in two-dimensional Rashba d-wave altermagnets in the presence of adiabatic electron–phonon coupling and arbitrary Rashba spin–orbit coupling (RSOC). Employing a continuum model that incorporates altermagnetic order, Rashba spin–orbit interaction, and spin-dependent static-Holstein lattice distortions, we calculate the noncollinear RKKY exchange tensor using second-order perturbation theory combined with numerical momentum-space integration. Our results demonstrate that adiabatic lattice distortions provide an effective mechanism for controlling the strength, anisotropy, phase, and chirality of RKKY interactions. Increasing electron–phonon coupling generally suppresses long-range exchange coherence while inducing pronounced component-dependent phase shifts and sign reversals, particularly in the Dzyaloshinskii–Moriya and compass-like exchange terms. These effects enable transitions between ferromagnetic and antiferromagnetic alignments as well as reversals of clockwise and counterclockwise chiral magnetic configurations. Furthermore, the interplay among altermagnetic order, RSOC, electron–phonon coupling, and carrier doping gives rise to increasingly complex oscillatory behaviors of the exchange interaction. The present study identifies slow phonons as a versatile low-energy tuning parameter for engineering noncollinear magnetic interactions in altermagnets, offering a practical route toward controlling magnetic textures and chiral spin states in altermagnet-based spintronic heterostructures.

Presenter: Bui D. Hoi

P.43 – Poster, VCTP-51

First-Principles Study of the Electronic and Optical Properties of Oxygen Vacancy Defects in Bismuth Vanadate

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Bismuth vanadate (BiVO4) is a promising metal oxide semiconductor for photocatalytic and photoelectrochemical applications owing to its suitable band gap and strong visible-light absorption. Understanding the role of intrinsic defects, such as oxygen vacancies, is crucial for improving its photocatalytic performance. In this work, the effects of oxygen vacancies on the structural, electronic, and optical properties of bulk BiVO4 are investigated using Density Functional Theory (DFT) calculations. The oxygen-deficient BiVO4 models are constructed by removing an oxygen atom from the optimized bulk structure. The electronic properties are analyzed through band structure, density of states (DOS), and partial density of states (PDOS) calculations, while the optical properties are evaluated from the complex dielectric function, including the absorption coefficient, refractive index, reflectivity, and optical conductivity. This study aims to elucidate how oxygen vacancies influence the electronic structure and optical response of BiVO4. The findings are expected to provide theoretical insights into defect engineering and contribute to the development of high-performance photocatalytic and photoelectrochemical materials.

Presenter: Nguyen Le Bao Tran

P.44 – Poster, VCTP-51

The influence of confined phonon and electromagnetic wave on the Hall effect in asymmetric infinite semi-parabolic Quantum Wells

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The influence of confined phonons and electromagnetic waves on the Hall effect in asymmetric infinite semi-parabolic Quantum Wells (AISPQW) in the case of confined electron- acoustic phonon scattering is studied theoretically. Analytic expressions for the Hall coefficient are derived from the electron distribution function, which is established via the quantum kinetic equation method. The results show that the Hall coefficient depends not only on the temperature T, the magnetic field B, the electromagnetic wave frequency Ω and the confinement frequency ω_z, but also on the phonon confinement index. Numerical calculation results also show that both confined phonon and unconfined phonon appear Shubnikov-de Haas (SdH) oscillations with the amplitudes that decrease. The Hall coefficient values in the case of unconfined phonons are smaller than in the case of confined phonons at the same temperatures and magnetic fields, approximately 1.5 times. Notably, the Hall coefficient depends on the magnetic field at different temperatures; the higher the temperature, the smaller the coefficient. In addition, the structural parameters of the quantum well, such as the confinement frequency and the frequency of the electromagnetic wave, have a significant influence on the Hall coefficient as well as the SdH oscillations. When the confinement frequency is small, the SdH oscillation gradually becomes absent. Examining the dependence of the Hall coefficient on the electromagnetic wave frequency at different temperatures or confinement frequencies (ω_z), the SdH oscillation also becomes smaller as temperature increases and frequency ω_z increases. These results establish a theoretical

framework for controlling Shubnikov–de Haas (SdH) oscillations via the Hall coefficient and material structural properties in future experimental studies

Presenter: Nguyen Dinh Nam

P.45 – Poster, VCTP-51

Structure-informed α–nucleus optical potentials: from repulsive-core effects in α decay to deformed nonlocal (α, n) reactions

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The description of α–nucleus interactions provides a stringent test of microscopic nuclear dynamics, since both α decay and α-induced reactions are governed by barrier penetration in regions where density overlap, Pauli blocking, deformation, and exchange effects become important. In this talk, we present a unified semimicroscopic framework for the α–nucleus optical potential based on double-folding interactions supplemented by structure-dependent corrections. First, the role of a surface-type repulsive core in α decay of heavy and superheavy nuclei is discussed. The repulsive term, introduced to simulate Pauli blocking and finite nuclear incompressibility, removes the unphysical deep inner pocket of conventional double-folding potentials and reshapes the inner barrier relevant to WKB tunneling. The same framework is then extended to (α,n) reactions relevant to the γ process, where nuclear deformation is included through quadrupole and hexadecapole density components, and Pauli-type nonlocality is treated using a Perey–Buck Gaussian kernel. The results show that deformation lowers the effective Coulomb barrier and enhances sub-barrier transmission probabilities, while nonlocality further refines the radial wave function and improves the consistency of calculated cross sections. These findings indicate that short-range repulsion, deformation, and nonlocality are essential ingredients for a predictive, structure-informed α–nucleus optical potential connecting nuclear decay and astrophysical reaction dynamics.

Presenter: Nguyen Nhu Le

P.46 – Poster, VCTP-51

Study of diffusion in sodium silicate glasses by molecular dynamics simulation

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The diffusion process in sodium silicate glasses was investigated using molecular dynamics simulation. The result shows that unlike Si atoms, which remain within the same Si-O coordination cells during 150 ps, Na atoms frequently displace between different Na-O coordination cells (CC). By analyzing the set of CCs visited by Na atoms, the simulation identifies two displacement types resembling drift and activated hopping. We have established the expression for diffusion constant D, showing it is proportional F2d2/tCC where tCC, d2, and F2 represent the residence time in

CC, the mean square displacement per central CC, and the correlation factor, respectively. For systems at the same temperature, both D and the drift/hop ratio reduce with increasing SiO2 content. Conversely, for systems with the same SiO2 content, a decrease in temperature leads to a reduction in D but an increase in the drift/hop ratio.

Presenter: Nguyen Thi Thao

P.47 – Poster, VCTP-51

Frontal-Parietal Disruption in AD and FTD: A Multidimensional EEG Assessment via Symbolic Transfer Entropy

Le Duy Manh (1,2), Trinh Xuan Hoang (3), Man Minh Tan (1,2), Pham Thanh Dam (1,2), Dinh Thanh Binh (1,2), Nguyen Hoang Long (1,4), Ngo Thi Tam (1,4), Nguyen Thi Thuy (3)

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Tracking the breakdown of large-scale neural networks is vital for identifying cognitive decline, particularly along the frontal-parietal axis. This study evaluates an integrated electroencephalography (EEG) framework designed to map these regional disruptions, aiming to distinguish Alzheimer's disease (AD) and frontotemporal dementia (FTD) from healthy aging (HC).Resting-state recordings from 88 subjects (36 AD, 23 FTD, 29 HC) were sourced from public repository ds004504. Signals from channels Fz and Pz were modeled using Symbolic Transfer Entropy (Net Flow) alongside complementary spectral-temporal metrics. These parameters were projected into a unified biophysical manifold via Mahalanobis Distance.Statistical testing confirmed distinct group profiles ($p < 0.05$). Net Flow values dropped sequentially from HC to AD, revealing an asymmetrical collapse in directional frontal-parietal signaling. Concurrently, alpha-band slowing and temporal delays escalated, with FTD presenting intermediate degradation. The manifold optimization maximized group boundaries ($p = 2.95 \times 10^{-7}$). An SVM classifier separated HC from AD with 84.6% accuracy (AUC = 0.83). Ultimately, quantifying directional network failure via symbolic information theory serves as an effective, accessible biomarker for dementia classification.

Presenter: Le Duy Manh

P.48 – Poster, VCTP-51

Investigating the Structure of Two-Dimensional Penta-Silicene via Machine Learning and Classical MD

Nguyen Thanh Tien, Le Huu Nghia, and Pham Thi Bich Thao

College of Natural Sciences, Can Tho University, Can Tho City, Vietnam

In this work, we use MLIP from the DeepMD package and the classical Tersoff potential for SiC (Tersoff.SiC potential) to fully and accurately describe atomic interactions and apply them to molecular dynamics simulations of penta silicene sheet. The results show that the melting points (Tg) temperatures of the system in the canonical NVT and isobaric NPT sets are 632 K and 606 K, while the Tersoff.SiC has a high melting point. In addition, the radial distribution

function exhibits characteristic peaks at interatomic distances of 2.27 Å and 2.37 Å, while the Tersoff.SiC potential only describes the distance of 2.37 Å. Furthermore, penta silicene was simulated using on-the-fly machine learning for 10 ps to evaluate the system's structural stability. This study investigates the thermodynamic properties of two-dimensional penta silicene sheets with pentagonal structures using a high-precision, cost-effective method, contributing further evidence to support experimental synthesis and opening up potential future applications of this material. Machine Learning Interatomic Potentials (MLIPs) are a modern computational method that enables near-quantum-mechanical accuracy (DFT) while still describing large-scale systems in molecular dynamics (MD) simulations.

Presenter: Nguyen Thanh Tien

P.49 – Poster, VCTP-51

Significant variations of resonance energy transfer at magic angles

Nguyen Dung Chinh

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Using the Green-tensor formalism, we investigate the rate of resonance energy transfer (RET) between two two-level atoms or molecules, within the dipole approximation, in the presence of dispersing and absorbing macroscopic bodies. The RET rate in the near-field zone is analyzed as a function of the dipole orientation. Two types of waveguides are considered, including infinitely extended cylinders made of gold or intrinsic silicon. The contribution of surface plasmons is examined through the spontaneous emission (SE) rate of an excited atom. We show that, even in systems where surface plasmons do not exist, a remarkable enhancement of RET can still occur. We then discuss, both analytically and numerically, how magic angles emerge, why they strongly affect RET in the near field, and under what conditions their effect disappears. RET in the near-field regime in vacuum has been shown to follow an inverse-square distance dependence, which is associated with the contribution of the transverse component of the electromagnetic field.

Presenter: Nguyen Dung Chinh

P.50 – Poster, VCTP-51

Double exchange altermagnetism in the Lieb lattice

Nguyen Thi Hai Yen, Tran Minh Tien

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We investigate the emergence of altermagnetism in the two dimensional Lieb lattice by combining a double exchange framework with dynamical mean field theory (DMFT). The magnetic ground state configuration is obtained through energy minimization of localized spins coupled to itinerant electrons via Hund interaction. Our results demonstrate that the next nearest neighbor hopping integral plays a crucial role in breaking the lattice symmetry and stabilizing an altermagnetic phase. The calculated momentum resolved spectral functions exhibit a characteristic $d_{x^2-y^2}$-type spin splitting, providing a clear signature of altermagnetism despite the absence of net magnetization. These findings reveal how the interplay between lattice geometry, Hund coupling, and next nearest neighbor hopping promotes altermagnetic order in the Lieb lattice and offer insights into the realization of altermagnetism in itinerant magnetic systems.

Presenter: Nguyen Thi Hai Yen

P.51 – Poster, VCTP-51

Machine-Learning Molecular Dynamics Study of Wear Processes at Diamond – Iron Interfaces

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Diamond tools exhibit exceptional hardness and wear resistance; however, rapid tool degradation is observed during machining of ferrous materials, indicating the critical role of atomistic interactions at the Fe–C interface. In this study, the atomistic mechanisms governing diamond tool wear during iron cutting were investigated using machine-learning interatomic potential molecular dynamics (MLIP–MD) simulations. A highly accurate Fe–C machine-learning potential was employed to enable large-scale and long-time cutting simulations across multiple diamond tool orientations. The simulations reproduced experimentally reported orientation-dependent wear trends with qualitative and semi-quantitative agreement. The results show that wear initiates at the cutting edge, leading to rapid edge blunting and the formation of an intermediate surface between the rake and flank faces. Following this initial stage, wear propagates preferentially along stepped edge regions through successive carbon removal events. The wear rate is strongly influenced by the stability of the local edge structure. Stable edge configurations localize wear activity and suppress its propagation, whereas unstable edge configurations promote the formation of multiple active wear sites and accelerate material removal. Further analysis reveals that severe wear occurs only when an unfavorable orientation of edge C–C bonds relative to the interfacial Fe flow is coupled with strong edge-localized Fe motion. Neither factor alone is sufficient to explain the observed wear behavior. These findings provide atomistic insight into orientation-dependent diamond wear and identify the coupled effects of edge atomic structure and local interfacial flow as key factors controlling wear resistance during ferrous machining.

Presenter: Nguyen Trinh Bao Anh

P.52 – Poster, VCTP-51

Photon blockade in a system of two micro-cavities with nonlinear coupling kicked by periodic laser pulses

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We systematically investigate the quantum statistical properties and the mechanism crossover between conventional and unconventional photon blockade (CPB and UPB) in two nonlinearly coupled micro-cavities driven by periodic laser pulses. Using analytical derivations and numerical

simulations, we map the quantum phase profile over the driving detuning, nonlinear coefficient χ, and linear inter-cavity coupling strength β, all scaled by the cavity decay rate γ. In the strong nonlinearity regime ($\chi/\gamma \gg 1$), robust CPB occurs via energy-level anharmonicity. In the weak nonlinearity regime ($\chi/\gamma \ll 1$), UPB dominates through multi-path destructive interference within highly localized parameter regions. Crucially, the $(\beta/\gamma, \chi/\gamma)$ phase diagrams reveal a distinct boundary where the photon blockade completely collapses because the rising nonlinearity dismantles UPB phase-matching before CPB can be established. Furthermore, strong linear coupling induces normal-mode splitting, dynamically shifting blockade valleys and enabling multiphoton transitions to generate extreme super-bunching. This pulse-kicked system offers high tunability without requiring giant natural nonlinear materials, providing a feasible roadmap for high-performance quantum devices in scalable networks.

Presenter: Le Duc Vinh

P.53 – Poster, VCTP-51

Controlled Remote Implementation of Operators via Non-Maximal Hyperentanglement

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Controlled remote implementation of operators (CRIO) enables the remote execution of an unknown unitary operator on an unknown quantum state under the authorization of a distant controller. Such protocols are essential for secure and scalable distributed quantum computing. In this work, we extend our previous CRIO scheme based on maximally hyperentangled states [J. Phys. A: Math. Theor. 55, 225307 (2022)] to the more practical case of non-maximally hyperentangled resources. To enhance security, the parameters characterizing the quantum channel are assumed to be known only to the controller. We demonstrate that perfect implementation fidelity can still be achieved, although with a success probability determined by the degree of hyperentanglement. We further derive the average fidelity of the corresponding classical protocol and the average non-conditioned fidelity of the quantum protocol without the controller's participation. Finally, we quantify the advantage of the proposed scheme by evaluating its quantumness power and controller's power.

Presenter: Cao Thi Bich

P.54 – Poster, VCTP-51

Tunable Magneto-Optical Anisotropy in Nodal-Line Semimetals

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This study theoretically investigates the magneto-optical response in topological nodal-line semimetals (NLSMs), accounting for the effects of spin-orbit coupling (SOC), carrier doping, temperature, and magnetic fields. By incorporating a SOC-induced mass term into the effec-

tive Hamiltonian and employing the equation-of-motion formalism, we analyze the Landau level structure and calculate directional optical susceptibilities. Our findings reveal a pronounced anisotropy in the optical response, where the $\chi_{xx}(\Omega)$ component exhibits the strongest absorption compared to $\chi_{yy}(\Omega)$ and $\chi_{zz}(\Omega)$, reflecting intrinsic symmetry-driven selection rules. At low energies, intraband transitions dominate the spectrum with high intensity, while interband transitions display unique "half-peak" structures resulting from Pauli blocking in the doped regime. Furthermore, we demonstrate high tunability of the spectral features: increasing the magnetic field or electron density induces a significant blue shift, while SOC lifts spin degeneracy to produce symmetric peak splitting. These results establish a theoretical framework for the development of tunable infrared and terahertz optoelectronic devices using topological materials.

Presenter: Huynh V. Phuc

P.55 – Poster, VCTP-51

Microscopic signatures of quadrupole and hexadecapole softness in even-even nuclei

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Nuclear deformation is a fundamental manifestation of collective motion in atomic nuclei and provides important insights into shell structure and many-body correlations. While quadrupole collectivity is well established as a signature of deformation, recent experimental and theoretical developments have renewed interest in higher-order deformation modes. In this work, deformation softness in even-even nuclei is investigated within the self-consistent Skyrme HFBCS-QRPA framework through a systematic study of low-lying quadrupole ($\lambda = 2$) and hexadecapole ($\lambda = 4$) excitations. Enhanced transition strengths and the occurrence of QRPA collapse are employed as microscopic signatures of soft collective dynamics. A global survey identifies characteristic regions of enhanced collectivity and highlights the interplay between shell structure and pairing correlations underlying deformation softness. The results establish systematic links between collective excitations and deformation softness, providing a microscopic picture of shape evolution across the nuclear chart.

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Presenter: Hoang Thai An

P.56 – Poster, VCTP-51

Collective excitations in double-bilayer graphene: Spin polarization effects

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We investigate collective excitations in spin-polarized double-bilayer graphene within the random-phase approximation. Numerical results reveal two distinct plasmon branches, namely the optical and acoustic modes, originating from in-phase and out-of-phase charge oscillations between coupled bilayer graphene sheets. Spin polarization significantly modifies the dynamical screening properties, leading to noticeable changes in plasmon energies and damping rates. In addition,

dielectric screening and interlayer Coulomb coupling strongly affect the stability of the collective modes. These findings provide further insight into many-body effects in coupled graphene systems and may be useful for future graphene-based plasmonic applications.

Presenter: Đỗng Thị Kim Phượng

P.57 – Poster, VCTP-51

Two-dimensional graphene: Peltier coefficient with electron - optical phonon scattering under the influence of intense electromagnetic wave

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We present a theoretical study of the Peltier effect in two-dimensional graphene under influence of intense electromagnetic wave using the quantum kinetic equation method. Assuming electron-optical phonon scattering as the dominant scattering mechanism, analytical expressions for the kinetic transport tensors σ_{xx}, ζ_{xx} and the Peltier coefficient (PC) are derived, revealing their dependence on the external magnetic field, the frequency of the intense electromagnetic wave, and temperature. Numerical results show that the Peltier coefficient displays pronounced resonance peaks in its dependence on cyclotron energy and electromagnetic-wave frequency. These peaks emerge when the energies associated with Landau quantization, optical phonons, and the electromagnetic wave satisfy the magneto–phonon–photon resonance condition. For the cyclotron-energy dependence, resonance peaks involving photon emission shift toward lower energies, whereas those involving photon absorption shift toward higher energies. In contrast, resonance peaks involving only electron–phonon scattering remain fixed. Temperature modifies the peak amplitudes without significantly affecting their positions, and no resonance behavior is found in the temperature dependence of the Peltier coefficient. The present results may provide a theoretical basis for future experimental studies of thermoelectric transport in graphene subjected to intense electromagnetic radiation and quantizing magnetic fields. **Presenter: Nguyen Thu Huong**

P.58 – Poster, VCTP-51

Two-dimensional graphene: Magneto - optical phonon resonance in hall coefficient under terahertz radiation

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This work presents a theoretical investigation of magneto-optical phonon resonance in the Hall effect of two-dimensional graphene subjected to a terahertz laser field. The study is performed within the quantum kinetic equation formalism, considering electron–optical phonon scattering

as the dominant interaction mechanism. By solving the quantum kinetic equation for the electron distribution function, analytical expressions for the electrical conductivity tensor and the Hall coefficient are derived as functions of the external magnetic field, laser frequency, and radiation amplitude. Numerical calculations for graphene reveal pronounced magnetophonon resonance peaks in the dependence of the Hall coefficient on the cyclotron energy. These resonance peaks arise when the magneto-phonon-photon resonance condition is satisfied. Their positions are determined solely by the resonance condition and therefore remain unchanged with temperature, leading to an overlap of the resonance peaks obtained at different temperatures. In contrast, the resonance amplitude exhibits a clear temperature dependence. Furthermore, increasing the amplitude of the terahertz radiation results in a reduction of the Hall coefficient. The obtained results provide insights into the interplay among magnetic fields, optical phonons, and electromagnetic radiation in graphene, and may serve as a useful reference for future experimental studies of terahertz-driven transport phenomena.

Presenter: Nguyen Quang Son

P.59 – Poster, VCTP-51

Observation of the magnetic dipole scissors resonance in 182Ta(n,2γ) experiment

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The persistence of the magnetic dipole (M1) scissors resonance (SR) in odd-odd deformed nuclei is debated. To resolve this, we performed 182Ta(n,2γ) experiment using the thermal neutron beam of the Dalat Nuclear Research Reactor to measure the two-step γ-cascade (TSC) intensity distributions of 182Ta. Using the measured data and a locally scaled, multi-model evaluation framework, we deconvoluted the electric (E1) and magnetic (M1) dipole photon strength functions. Our results reveal a prominent SR peak near 2.5 MeV in 182Ta, confirming that the collective SR remains robust despite valence nucleon pairing. We demonstrate that previous studies using the Oslo method likely missed this feature due to signal convolution, where the M1 peak was masked by an dominant E1 background. In addition, our analysis constrains the three datasets available from the Oslo method to one that was normalized using the Hartree-Fock-Bogoliubov model.

Presenter: Nguyen Ngoc Anh

P.60 – Poster, VCTP-51

Spin–Valley Hall Transport in Jacutingaite under Finite Temperature Conditions

Do Muoi

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We theoretically investigate spin–Hall and valley–Hall transport in monolayer jacutingaite under off-resonant circularly polarized light and a perpendicular electric field using a low-energy massive Dirac model within linear response theory. At zero temperature, both conductivities exhibit quantized plateau structures, reflecting the topological nature of the band spectrum. The optical field effectively renormalizes the Dirac mass, enabling tunable transitions between different Hall regimes. While the spin–Hall effect arises from intrinsic spin–orbit coupling, the valley–Hall effect appears only when inversion symmetry is broken. At finite temperatures, thermal broadening smooths the plateau features and reduces their magnitude, though key topological signatures remain robust near charge neutrality. We also show that circularly polarized light alone cannot induce a finite valley–Hall response without inversion symmetry breaking. These results demonstrate that the interplay of optical driving, electric fields, and temperature provides an effective route to control spin and valley transport in jacutingaite, highlighting its potential for spintronic and valleytronic applications.

Presenter: Muoi Do

P.61 – Poster, VCTP-51

Thermodynamics of higher-dimensional Black Holes in dRGT Massive Gravity with Power Yang-Mills source

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We investigate the thermodynamic properties and phase structure of higher-dimensional black holes in the framework of de Rham–Gabadadze–Tolley (dRGT) massive gravity coupled to a power Yang–Mills field. By considering the cosmological constant as a thermodynamic pressure in the extended phase space, we derive the corresponding thermodynamic quantities, including the Hawking temperature, entropy, equation of state, and Gibbs free energy. We analyze the effects of the massive gravity parameters and the nonlinearity parameter of the power Yang–Mills field on the thermodynamic behavior and critical phenomena of the system.

Presenter: Phùng Huy Hiệu

P.62 – Poster, VCTP-51

Synthesis and structural stability investigation of Fe_3GeTe_2 van-der-Waals ferromagnet

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Fe_3GeTe_2 (FGT) is known as a layered van-der-Waals (vdW) ferromagnet that has recently attracted much interest of the scientific and technological community due to its intriguing magnetic properties and potential applications in spintronic devices. This work presents the synthesis of a bulk FGT sample using solid-state reactions. Powder X-ray diffraction (XRD) confirmed the as-prepared FGT crystallizing in the P63/mmc hexagonal structure. Its structural stability was

then examined under air exposure and mechanical milling. As a result, upon prolonged exposure to ambient air, the initially single-phase FGT gradually degraded, leading to the formation of secondary phases. Mechanical ball milling for durations ranging from one to 30 minutes also caused rapidly structural deconstruction and phase transformation, as evidenced by significant changes in the XRD patterns. Such results demonstrate that FGT is highly sensitive to both environmental and mechanical factors. To understand the origin of this behavior, density functional theory (DFT) calculations were performed. The calculated phonon spectra of FGT monolayers on metal substrates exhibit no negative frequencies, proving their intrinsic dynamical stability; free-standing FGT layers could be unstable. The discrepancy between the theoretical prediction and experimental observations suggests that the degradation of FGT is likely driven by extrinsic factors, such as oxidation, defect formation, strain accumulation, and mechanically induced structural disorder, which are not taken into account in the idealized DFT model. Our results highlight the importance of environmental and processing conditions in determining the practical stability of FGT, thereby providing valuable guidance for its handling, fabrication, and potential applications in next-generation electronic devices.

Presenter: Phan T. Long

P.63 – Poster, VCTP-51

A Capillary Bundle Model for Relative Permeability in Unsaturated Porous Media

Luong Duy Thanh and Nguyen Van Nghia

Thuyloi University

A physically-based model for relative permeability in partially saturated porous media is developed using the bundle-of-capillaries framework combined with a similarly skewed pore-size distribution. The proposed model relates permeability to pore-structure characteristics and water saturation. Numerical results indicate that relative permeability increases with effective water saturation but decreases as the pore-size distribution becomes increasingly skewed toward smaller pores. The model is validated against published experimental data, showing good agreement and performance comparable to that of the van Genuchten model. Overall, the proposed framework provides a simple and physically interpretable approach for analyzing fluid transport in partially saturated porous media.

Presenter: Nguyen Van Nghia

P.64 – Poster, VCTP-51

Simulation of the Talbot Effect in Nonlinear Binary Waveguide Arrays

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We numerically investigate the influence of Kerr-type nonlinearity on the Talbot effect in binary waveguide arrays (BWAs). The nonlinear Talbot effect is observed over a broad range of input intensities for transverse periods (N = 1) and (N = 2). For (N = 2), a sharp switching behavior emerges depending on the excitation of waveguides with lower or higher effective refractive indices under self-focusing or self-defocusing nonlinearity, respectively. In contrast, for (N = 3,

4,) and (6), nonlinearity suppresses the Talbot effect even at low input intensities.

Reference:

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Presenter: Tran Cong Minh

P.65 – Poster, VCTP-51

Two-component dark matter in an extended inert doublet model

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We investigate the multi-component dark matter problem within an extension of the inert doublet model stabilized by preserved discrete symmetries. This framework naturally accommodates co-existing stable fermionic and scalar fields as viable dark matter candidates. We comprehensively analyze the dark matter phenomenology of this multi-component system, detailing the unique annihilation and co-annihilation processes required to reproduce the measured dark matter relic abundance. We demonstrate that within an appropriate region of the parameter space, the model successfully yields the correct relic density while remaining fully compatible with current stringent limits from dark matter direct detection experiments.

Presenter: N.T.Duy

P.66 – Poster, VCTP-51

Interaction-Induced Noise Enhancement in a Single-Channel Charge Kondo Circuit

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We investigate fluctuations of charge and heat currents, together with their cross- correlations, in a single-channel charge Kondo circuit driven by either a voltage bias or a tempera- ture gradient across a weak link. To incorporate Coulomb interaction effects in a two-dimensional interacting electron gas, transport through the quantum point contact (QPC) is described within a Luttinger liquid (LL) framework characterized by the Luttinger parameter g. We show that the temperature dependence of the current noises deviates markedly from Fermi liquid predictions. In particular, the interplay between mesoscopic Coulomb blockade in the quantum dot and weak repulsive interactions in the LL leads to enhanced current fluctuations. We attribute this enhance- ment to the suppression of Kondo correlations by destructive quantum interference effects at the QPC, providing clear signatures of electron-electron interactions in the LL.

Presenter: Nguyen Hong Quang

P.67 – Poster, VCTP-51

Systematic Evaluation of ^{187}W Statistical Properties via Experimental Two-Step γ-Cascade Intensities

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Sparse experimental data for the nuclear level density (NLD) and the photon strength function (PSF) of the ^{187}W isotope require validation of theoretical models critical for fusion research and the production of medical isotopes. We performed a systematic evaluation of 390 model combinations, constrained by experimental two-step gamma-ray cascade (TSC) intensities from the ^{186}W$(n,\gamma)^{187}$W reaction and IAEA integral anchors (D_0, Γ_γ).

Our results demonstrate the superior predictive power of microscopic, temperature-dependent models. Hartree-Fock-Bogoliubov at finite temperature (HFBT) emerged as the most effective NLD model, while microscopic approaches, specifically Goriely's hybrid and temperature-dependent HFB with D1M Gogny force models, dominated the best performing $E1$ PSF ensemble. The methodology proved robust, successfully diagnosing an unexpected population of a neighboring $7/2^-$ state and identifying significant normalization disparities in existing (n,γ) cross-section databases. This work underscores the necessity of temperature-dependent microscopic treatments for accurately describing the statistical de-excitation of ^{187}W and provides a reliable framework for investigating other nuclei with incomplete statistical data.

Presenter: Phan Bao Quoc Hieu

P.68 – Poster, VCTP-51

Emergence of altermagnetism on the Lieb lattice with depleted local correlations

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We investigate the emergence of altermagnetism induced by the depletion of local correlations on the Lieb lattice. Specifically, we consider a scenario where local correlations at the corner sites of the Lieb lattice are depleted. To account for general non-collinear and non-coplanar magnetizations, we construct local rotations in spin space. Within dynamical mean-field theory, we find a double-diagonal strip magnetization pattern, where spins align ferromagnetically along individual diagonals but antiferromagnetically relative to adjacent diagonals.

Presenter: Tran Minh Tien

P.69 – Poster, VCTP-51

Entanglement and quantum teleportation with the generalized superposition

of two-mode coherent states SU(1, 1)

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In this paper, we investigated the entanglement properties of the generalized superposition of two-mode coherent states SU (1, 1) (STMCSSU) based on the linear entropy criterion. The results show that STMCSSU exhibits a high degree of entanglement and depends on the chosen input parameters. Furthermore, we used the STMCSSU as an entangled resource for the teleportation of a coherent state by using joint measurements of the quadrature amplitude. The results of the fidelity investigation show that the even of two-mode coherent states SU(1,1) is more suitable for quantum teleportation via quadrature-amplitude measurements. In addition, the teleportation fidelity varies appropriately with the input parameters.

Presenter: Truong Minh Duc

P.70 – Poster, VCTP-51

DFT-Calibrated Machine-Learning Screening of Off-Stoichiometric Na_xSbS_4 Solid Electrolytes

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Na_xSbS_4 is a representative sulfide solid electrolyte for all-solid-state sodium batteries, but the thermodynamic meaning of Na-deficient or Na-rich variants must be evaluated within the full Na–Sb–S phase field. In this work, we combine density functional theory (DFT) and machine-learning interatomic potentials to investigate the stability of tetragonal Na_xSbS_4 and off-stoichiometric Na_xSbS_4 structures. First, DFT calculations were used to construct a Na–Sb–S convex hull containing 103 entries. The tetragonal Na_3SbS_4 phase lies on the DFT hull with an energy above hull of 0 meV/atom, confirming it as a thermodynamically stable parent structure for further compositional screening. Starting from this host, 263 Na-deficient and Na-rich structures were generated and relaxed using CHGNet. These candidates were reduced to 25 representative Na_xSbS_4 variants for DFT verification. At the machine-learning screening level, 9 of 25 representatives lie on the CHGNet hull and 23 of 25 are within 25 meV/atom. However, DFT calculations completed for 24 representatives show that none of the off-stoichiometric variants reaches the ground-state hull; the lowest-energy case is Na_xSbS_4 with $E_{\mathrm{hull}} = 163.62$ meV/atom. The discrepancy between CHGNet and DFT is substantial, with a mean absolute error of 1239.29 meV/atom and a Spearman correlation of 0.164 for E_{hull}. Additional MatGL checks and geometry-sensitivity tests indicate that the main source of the discrepancy is not a simple single-point energy offset, but differences in relaxation pathways and geometric basins, especially for Na-rich structures. When machine-learning energies are evaluated on DFT-relaxed geometries, their correlation with DFT increases to nearly 0.99. These results show that machine learning is highly useful for expanding and prioritizing structural search spaces, but inter-model uncertainty checks, geometric audits, and DFT convex-hull calibration are essential before making phase-stability conclusions for off-stoichiometric solid electrolytes. **Presenter: Tran Van Thien**

P.71 – Poster, VCTP-51

Energy-Based Downfolding with One-Body MP2 for Molecular and Periodic Systems

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We present an ab initio downfolding framework based on orbital-optimized second-order Møller-Plesset perturbation theory (OBMP2) for constructing low-energy effective Hamiltonians. For molecular systems, dynamical correlation effects outside the active space are incorporated through an OBMP2-derived correlated potential, yielding compact Hamiltonians suitable for accurate many-body solvers. The approach is further generalized to periodic systems through k-point OBMP2 (kOBMP2), where downfolding is performed directly in Bloch space using an energy-based selection of target bands. The resulting effective Hamiltonians are transformed into localized Wannier representations and truncated in real space to generate finite lattice models. This unified framework provides an efficient route for reducing the complexity of correlated molecular and crystalline systems while retaining the essential low-energy physics required for advanced many-body calculations.

Presenter: Vũ Công Ngọc Thái

P.72 – Poster, VCTP-51

Microscopic alpha-nucleus potentials constrained by the Bohr-Sommerfeld quantization condition for alpha decay

Nguyen Gia Huy (1), Do Huy Tho (1), Mai Doan Quang Huy (1) and Nguyen Le Anh (1)

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Alpha (α) decay provides a sensitive probe of nuclear structure and remains one of the primary tools for studying heavy and superheavy nuclei. In this work, a systematic investigation of α decay is carried out using microscopic α-nucleus potentials constructed from Skyrme Hartree-Fock formalism within a folding framework. The resulting potentials are constrained by the Bohr-Sommerfeld quantization condition and employed within a semiclassical WKB framework to calculate α-decay half-lives over a broad range of even-even nuclei. The results suggest that the combination of microscopic Skyrme-based potentials and the Bohr-Sommerfeld constraint captures important aspects of the α-decay process. The present study represents a first step toward a more microscopic description of α decay and motivates further developments beyond the local mean-field framework.

References:

[1] N. Gia Huy, D. Huy Tho, M. D. Quang Huy and N. Le Anh, **Nuclear Physics A** 1069, 123352, 2026.

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Presenter: Nguyen Gia Huy

P.73 – Poster, VCTP-51

Enhanced Magneto-Optical and Transport Properties of InSb-, InAs-, and GaSb-Based Asymmetric Gaussian Quantum Wells under Confined Optical Phonons: Material-Dependent Behavior and Prospects for Infrared Photodetectors and Terahertz Optoelectronic Devices

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Magneto-optical and transport properties of InSb-, InAs-, and GaSb-based asymmetric Gaussian quantum wells under confined optical phonons are investigated within the framework of optically detected magnetophonon resonance (ODMPR). Using the projection operator method, analytical expressions for the magneto-optical absorption power are derived. Particular emphasis is placed on the comparison between confined and bulk optical phonons. The results show that confined optical phonons substantially enhance the magneto-optical absorption and transport characteristics while significantly increasing the ODMPR linewidth compared with bulk optical phonons. The enhancement exhibits strong material dependence owing to differences in the effective electron mass, phonon energy, and electron–phonon coupling strength among InSb, InAs, and GaSb quantum wells. Furthermore, the ODMPR linewidth provides valuable insight into the intensity of electron-phonon interactions, electron relaxation dynamics, and phonon-mediated scattering processes in these low-dimensional systems. The present findings demonstrate the important role of phonon confinement in tailoring the magneto-optical response of semiconductor quantum wells and suggest promising prospects for experimental and application studies of infrared photodetectors and terahertz optoelectronic devices.

Presenter: Nguyen Dinh Hien

P.74 – Poster, VCTP-51

Influence of laser wavelength on the cross - shaped structure in the nonsequential double ionization of noble gas atom

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In this study, we investigate the wavelength dependence of the cross-shaped structure in the nonsequential double ionization of noble gas atoms using the classical ensemble model. By introducing characteristic quantities associated with recollision dynamics, we analyze the microscopic mechanisms governing electron-electron correlation. The results reveal that the cross-shaped structure in the correlated two-electron momentum distribution persists across all noble gas atoms, originating from recollision-induced excitation with subsequent ionization. Furthermore, this structural feature gradually vanishes with increasing laser wavelength.

Presenter: Chau Bao Khoa

P.75 – Poster, VCTP-51

Structural and thermal stability of pentagonal PtN_2/PdN_2 heterostructures: Insights from machine learning interatomic potentials trained on first-principles data

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The integration of first-principles calculations (DFT), machine-learning interatomic potentials (MLIPs), and large-scale molecular dynamics (MD) simulations has emerged as a powerful approach for investigating the properties of advanced 2D materials. In this work, the monolayer of PdN_2 and PtN_2 are first based on DFT by electronic structures, phonon dispersions, and thermal stability. Based on the DFT-generated dataset, the MLIP models were assessed using the root mean square error (RMSE) of atomic energies and forces. The energy/force RMSE values were 8.71×10^{-4} eV atom^{-1} and 8.14×10^{-2} eV Å^{-1} for PdN_2, 6.11×10^{-4} eV atom^{-1} and 4.35×10^{-2} eV Å^{-1} for PtN_2, and 4.14×10^{-4} eV atom^{-1} and 4.02×10^{-2} eV Å^{-1} for the PdN_2/PtN_2 heterostructure, respectively. The reliability of the trained potentials is further validated through a comparative analysis of phonon spectra obtained from DFT and PhonoLAMMPS calculations. Large-scale MD simulations are performed using NPT and NVE ensembles to optimize the structures and investigate their thermal behavior. The resulting radial distribution functions (RDFs) reveal a strong consistency with the equilibrium atomic configurations predicted by DFT. The proposed multiscale DFT–MLIP–MD approach opens new opportunities for the accelerated design and large-scale simulation of next-generation functional materials.

Presenter: Mai Ngoc Qui

P.76 – Poster, VCTP-51

A New Set of Combining Rules for the Mie (λ, 6) Potential for Predicting Thermophysical Properties of Fluid Mixtures

Nguyen Van Phuoc, Thanh Doanh Le, Van Hoa Nguyen, Suresh Alapati, Stéphanie Delage Santacreu, Guillaume Galliéro, and Hai Hoang

Trường ĐH Tôn Đức Thắng

Accurate prediction of thermophysical properties of fluid mixtures is essential for chemical engineering, petroleum engineering, separation processes, and supercritical-fluid applications [1]. Molecular simulation provides a powerful route for predicting such properties when experimental data are limited or difficult to obtain [2]. Among molecular models, force fields based on the Mie (λ, 6) potential have attracted increasing interest because they offer greater flexibility than the Lennard-Jones potential by explicitly tuning the repulsive exponent. These models have been successfully applied to pure fluids and mixtures, especially within coarse-grained molecular simulation frameworks [3,4]. However, the predictive capability of Mie-based force fields for mixtures strongly depends on the accuracy of unlike interaction parameters, which are usually estimated from pure-component parameters using combining rules. In this work, a new set of combining rules is proposed for the Mie (λ, 6) potential. The derivation is based on a distortion model for the repulsive contribution and a geometric mean approximation for the attractive contribution [5], in conjunction with first-order mathematical approximations. The resulting

expressions provide the unlike repulsive exponent, collision diameter, and potential well depth directly from pure-component Mie parameters, without introducing additional adjustable binary parameters. The proposed combining rules were evaluated for a broad range of systems, from simple monoatomic to more complex molecular mixtures, using Monte Carlo simulations. Their predictive performance was assessed using several thermodynamic properties that are sensitive to unlike interactions, including Henry's law constants, pressure–composition phase diagrams, and excess molar volumes. For mixtures whose components have comparable Mie parameters, the new rules yield predictions similar to those obtained with existing combining rules. However, for highly asymmetric systems, they provide substantially better agreement with experimental data. These results indicate that the proposed rules offer a more reliable and transferable approach for predicting thermophysical properties of fluid mixtures without requiring additional binary parameter fitting. Keywords: Mie (λ, 6) potential; combining rules; molecular simulation; phase equilibrium; Henry's law constant; excess molar volume. Keywords: Mie (λ, 6) potential; combining rules; molecular simulation; phase equilibrium; Henry's law constant; excess molar volume.

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Presenter: Nguyen Van Phuoc

P.77 – Poster, VCTP-51

Structures and Dynamics of α-Synuclein in Different States: A Molecular Dynamics Study

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Parkinson's disease (PD) is a slowly progressive movement disorder resulting from the loss of dopaminergic neurons in the substantia nigra, a small area of cells in the mid-brain. Both genetic and environmental factors play a huge role in causing this illness. Several evidence link α-synuclein (α-Syn), a small highly conserved presynaptic protein with unknown function, to both familial and sporadic PD. In fact, rare familial cases of PD are associated with missense point mutation in α-Synuclein, or with overexpression of the wild-type protein due to its gene

duplication both in vivo and in vitro and are associated with accelerated progression of PD. Experimental studies have shown that C-terminal truncation stabilizes the fibrillar state of α-Syn, whereas graphene-based nanomaterials can modulate or even inhibit its aggregation. In this work, we employed all-atom replica-exchange and conventional molecular dynamics simulations to investigate α-Syn in multiple structural and oligomeric states, including truncated and full-length forms. Furthermore, coarse-grained molecular dynamics was used to characterize the oligomerization pathway, enabling us to track oligomer lifetimes and intermediate species relevant to early aggregation. Together, these simulations provide a comprehensive view of how structural variants and nanoscale environments influence the conformational landscape and aggregation propensity of α-Syn.

Presenter: Tran Thi Minh Thu

P.78 – Poster, VCTP-51

A Hierarchical Binding Mechanism Governs the SARS-CoV-2 N Protein-G3BP1 Interaction: A Computational Insight

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The sequestration of host G3BP1/2 by the SARS-CoV-2 nucleocapsid (N) protein is vital for viral antagonism of the cellular stress response. While N-terminal residues 14–17 are critical for this interaction, the atomistic determinants defining viral variant affinities remain ambiguous. Integrating umbrella sampling and molecular dynamics simulations, we elucidate a hierarchical binding mechanism wherein a primary electrostatic anchor (Asp22) is locked by a secondary hydrophobic interface (Phe17). Our calculations reveal that the F17A mutation exerts a significantly more detrimental effect on binding than the Omicron P13L mutation or the direct removal of the electrostatic anchor (D22A). Crucially, F17A induces an allosteric collapse: the loss of the hydrophobic contact triggers backbone rearrangements that displace the critical Asp22 anchor. In contrast, D22A selectively abrogates the electrostatic interaction while preserving the hydrophobic core, resulting in a less severe affinity loss. These findings identify Phe17 as a structural linchpin allosterically controlling the primary electrostatic interaction, providing a detailed rationale for the mutational landscape of this viral-host interface

Presenter: Nguyễn Hoàng Linh

P.79 – Poster, VCTP-51

Temperature-dependent EXAFS parameters of wurtzite CdSe derived from a classical correlated Einstein model

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The temperature-dependent extended X-ray absorption fine structure (EXAFS) parameters of wurtzite CdSe are investigated using a correlated Einstein model combined with an anharmonic effective potential based on a classical statistical approach. The effective potential is constructed to incorporate the ionic nature of the Cd–Se interaction and the local coordination geometry of the wurtzite structure. Analytical expressions for the effective potential, correlated Einstein frequency, Einstein temperature, and the first four EXAFS cumulants are obtained as functions of temperature. Numerical results reveal the effects of temperature on the local pair distribution and anharmonicity of the Cd–Se bond. Comparison with available experimental EXAFS data over the temperature range 18–300 K is used to evaluate the applicability of the present model. The present approach provides an efficient framework for describing local anharmonic vibrations and EXAFS cumulants in ionic wurtzite crystals.

Presenter: Tong Sy Tien

P.80 – Poster, VCTP-51

Gravitational waves from CP domain wall collapse and electron EDM in a complex singlet model with dimension-five Yukawa interactions

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We study the interplay between gravitational waves (GWs) from domain wall collapse and the electron electric dipole moment (EDM) in a complex singlet extension of the standard model with dimension-five Yukawa interactions. In this framework, the scalar potential admits CP-related degenerate vacua, leading to the formation of CP domain walls. While the resulting GW signal provides a probe of the vacuum structure of the singlet scalar sector, it does not by itself constitute a CP-violating observable. Once the singlet scalar is coupled to standard model fermions, CP-violating phases become observable through EDMs. We analyze whether current and future EDM experiments can probe the parameter region where the GW signal is detectable by SKA and THEIA. We find that the current electron EDM bound already constrains part of the parameter space, while future sensitivities at the level of 10^{-31}–$10^{-32}\,e\,\mathrm{cm}$ can probe regions overlapping with the GW-detectable domain. Our results highlight the complementarity between GW and EDM observables in probing the singlet scalar sector, providing a coherent picture of its vacuum structure and CP properties.

Presenter: Pham The Hieu

P.81 – Poster, VCTP-51

A new effecient scan tool of the NMSSM parameter space: NMSSMScanner

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Extensions of the Standard Model are required to explain new physics phenomena, such as Dark Matter, the Baryon Asymmetry of the Universe, and neutrino masses. These extensions are typically accompanied by a number of new particles and additional parameters. While the introduction of such particles and parameters can explain the observed phenomena, they also affect observables that have been measured with high precision in experiments. To identify viable regions of parameter space that are relevant for experimental searches, efficient scanning tools are essential. Such tools must consistently incorporate all relevant theoretical and experimental constraints. We present here a newly developed framework, called NMSSMScanner, which interfaces BSMArt, NMSSMCALC, HiggsTools, HPAIR, SusHi, RelExt, PYTHIA, and SModelS. As an illustration of its capabilities, we use NMSSMScanner to determine the maximal viable di-Higgs production cross sections in the NMSSM.

Presenter: Dao Thi Nhung

P.82 – Poster, VCTP-51

One-loop gauge boson contributions to decays $h \to e_a e_b$ in the general gauge R_ξ

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Trường Đại học Văn Lang, Đại học Sư phạm Hà Nội 2, Đại học An Giang

Analytic formulas to express one-loop contributions to lepton flavor violating decays of the Standard Model-like Higgs boson $h \to e_a e_b$ are calculated in the general gauge R_ξ for the general seesaw version of the Standard Model. The calculation is performed using the Passarino-Veltman functions, which include various well-known relations useful for analytic transformations. This calculation also requires precise forms of the couplings of the Goldstone boson of $W^\pm$, which are model-dependent. We demonstrate analytically that the final result is gauge-independent, namely, the free unphysical parameter ξ of the R_ξ gauge vanishes completely. Moreover, the resulting decay amplitude is consistent with those previously calculated in different gauges, including the unitary gauge.

Presenter: Trịnh Thị Hồng

P.83 – Poster, VCTP-51

Power-law Bianchi type I inflation with multiple vector fields

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We investigate anisotropic cosmic inflation within a supergravity-motivated Bianchi type I model featuring a scalar field non-minimally coupled to three orthogonal vector fields. We identify four

types of power-law solutions, classified by the number of persisting vector fields, and determine their quantitative and qualitative stability regions. Notably, vector fields with larger coupling constants persist during cosmic expansion, while those with smaller couplings dilute. Finally, we show that cosmic anisotropy depends directly on the number of surviving vector fields.

Presenter: Nguyen Hoang Duy

P.84 – Poster, VCTP-51

Topological edge states in one-dimensional off-diagonal mosaic lattices

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We investigate topological edge states in one-dimensional off-diagonal mosaic lattices, where nearest-neighbor hopping amplitudes are periodically modulated. Analytically, we derive a simple expression for the energies of discrete edge states, extending the Su–Schrieffer–Heeger model to multi-band systems. Numerical calculations reveal that these states remain robustly localized and exhibit distinctive nodal structures. Their existence is found to depend sensitively on the edge termination, particularly on the arrangement of strong and weak bonds at the lattice boundaries. Our results uncover a rich interplay between topology and periodic modulation, providing a versatile framework for designing multi-gap topological phases and facilitating their realization in synthetic quantum and photonic platforms. Keywords: Mosaic lattice model, extended SSH model, topological edge states, bulk-boundary correspondence. References: [1]. Y. Wang et al., Phys. Rev. Lett. 125,196604 (2020). [2]. B. P. Nguyen et al., Phys. Rev. B 106, 134204 (2022). [3]. B. P. Nguyen and K. Kim, Results Phys. 77, 108433 (2025).

Presenter: Nguyen Ba Phi

P.85 – Poster, VCTP-51

LFV decays in a 3-3-1 model with singlet leptoquark

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Motivated by a recent study of a 3-3-1 model supplemented by a singlet scalar leptoquark, which was shown to account for the muon anomalous magnetic moment and the charged lepton flavor-violating decay $\mu \to e\gamma$, we demonstrate that this framework can simultaneously accommodate the latest experimental results on $(g-2)_\mu$ and provide viable predictions for charged lepton flavor-violating processes, as well as lepton flavor-violating decays of the SM-like Higgs boson and the Z gauge boson. Our numerical analysis identifies the regions of parameter space consistent

with current experimental constraints, highlighting in particular the strong correlations between the branching ratios of charged lepton flavor-violating processes and the anomalous magnetic moments of charged leptons.

Presenter: Nguyen Hua Thanh Nha

P.86 – Poster, VCTP-51

Design of polaron confinement by Ta doping in rutile TiO_2 for colossal permittivity

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Polarons in Nb-doped TiO_2 have attracted significant interest due to their hopping behavior, which contributes to the colossal permittivity observed at low temperatures. However, polaron hopping and its impact on permittivity of TiO_2 doped with other pentavalent elements has not yet been systematically investigated. In this work, we employ density functional theory (DFT), combined with chemical bond analysis, to investigate the behavior of polarons in Ta-doped TiO_2, and their influence on the permittivity. We find that the polaron in Ta-doped TiO_2 preferentially localizes at the second-nearest Ti site relative to the Ta dopant along the [001] direction. This behavior contrasts with that of V- and Nb-doped TiO_2, where the polaron is most stable at the dopant site and the first-nearest Ti neighbor of the dopant, respectively. The polaron in Ta-doped TiO_2 predominantly hops between Ti sites located between Ta dopants, rather than passing through the dopant itself, in contrast to Nb-doped TiO_2. This behavior suggests a higher permittivity in Ta-doped TiO_2 at low temperatures. At high doping concentrations, we also find that Ta dopants exhibit a tendency to stay spatially separated rather than forming a cluster. This arrangement is expected to promote extended polaron hopping pathways, thereby contributing to an increase in permittivity.

Presenter: Dinh Ngoc Dung

P.87 – Poster, VCTP-51

The structural stability of monomeric Glucose-6-phosphate dehydrogenase and its relationship to G6PD deficiency

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G6PD deficiency, an enzymopathy associated with glucose-6-phosphate dehydrogenase (G6PD), is caused by genetic mutations that reduce the enzyme activity, resulting in hemolytic anemia. Biochemical studies have shown that G6PD deficiency in various variants is associated with

reduced thermal stability, reduced catalytic activity, or both. In this study, we investigate the structural stability of the wild-type G6PD monomer at a physiological temperature using molecular dynamics simulations, in the absence and in the presence of its G6P and NADP+ ligands. We find that the G6P ligand has a low affinity for the G6PD monomer, which may result from fluctuations in the size of its binding pocket. This finding helps explain the catalytic inactivity of monomeric G6PD. The binding of NADP+ ligands is found to enhance the structural stability of the protein and the G6P-binding pocket. Our analysis also shows that, with a statistically significant confidence, class I mutations occur preferentially at residues that are more flexible than randomly selected residues, whereas class II mutations tend to occur at residues that are less flexible than randomly selected ones. This result reflects the distinct structural roles of the G6PD mutation sites and further supports the relationship between enzyme activity and thermal stability.

Presenter: Nguyen Thi Thuy Nhung

P.88 – Poster, VCTP-51

Tracking the HCN isomerization process by HHG spectra simulations

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High-order harmonic generation (HHG) is a highly nonlinear optical process that transforms intense laser light into shorter wavelengths. Serving as an ultrafast atomic camera, HHG enables us to image molecular orbitals as well as investigate vibrational-rotational dynamics and chemical reactions. Furthermore, HHG spectroscopy is a versatile tool applicable to diverse states of matter, including atoms, molecules, solids, and liquids. This work investigates HHG spectra along the intrinsic reaction coordinate of hydrogen cyanide (HCN) isomerization via a three-step model implemented in the Strong Laser Interaction Model Package (SLIMP). Geometry optimization, energy, and harmonic frequency calculations were conducted at the MP2/6-311+G(d,p) level of theory using the Gaussian 16 package. These simulations aim to trace the HCN isomerization pathway and extract key orbital information from the generated spectra.

Presenter: Hai Thi Huynh

P.89 – Poster, VCTP-51

Doubly holography for understanding the dynamics of entanglement entropy

Trần Ngọc Hưng

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We review recent developments in the study of the black hole information paradox using doubly holographic models (DHMs). By introducing an additional brane embedded in the AdS bulk, DHMs allow black holes to be coupled to thermal baths, enabling the emergence of Page curves and entanglement islands. This framework has provided significant insights into the unitarity of black hole evaporation. In particular, the entanglement entropy initially increases and then saturates after the Page time due to the appearance of an island on the brane. Furthermore,

applications of DHMs to charged black holes have revealed new critical parameters and phase transitions, as well as the influence of charge on the Page time and the entanglement structure.

Presenter: Tran Ngoc Hung

P.90 – Poster, VCTP-51

Floquet band engineering in graphene from perturbative to extreme driving: a multi-photon driven-Dirac observability map

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Floquet engineering is a method of controlling the dynamic electronic structure of quantum mat- ter, the regime of which has been experimentally verified in graphene, although mostly to small driving. We consider in this paper single-layer graphene, which is pumped with high-order multi- photon driven Dirac Floquet strong linearly and circularly polarized mid-infrared light. The gap between the one-photon hybridization is reappeared in the perturbative regime and its development is continued into the nonperturbative limit. Here the higher-order n =2 and n=3 Floquet signals, sharp spectralweight redistribution, and nonmonotonic strong-field gap renormalization can be found. We demonstrate that the nodal direction which is symmetry-protected remains strong in all resolved photon sectors in the driven-Dirac model when the driving is linearly polarized. We obtain a gap induced by light which is identical at the Dirac point on both sides in circular polarization which is consistent with a Haldane-like Floquet mass term. To quantify observability, we apply phenomeno- logical widening and chart the range of linewidths over which higher-order Floquet effects can be spectroscopically resolved. We find a model phase diagram of the onset of strong-field Floquet behavior in graphene. They also indicate the signals that are strong, those that are restricted by coherence and those that require more models detailed to be compared directly in the laboratory.

Presenter: Nguyen Duc Long

P.91 – Poster, VCTP-51

Magnetocaloric effect in the skyrmion material Cu_2OSeO_3

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Polycrystalline Cu_2OSeO_3 with the cubic structure has been prepared by solid-state reactions. Magnetization measurements indicate its magnetic ordering established at temperatures below T_C of 59 K. At low fields $H < 500$ Oe, zero-field-cooled and field-cooled M(T) curves show a sharp peak at 57 K associated with the skyrmion phase, and the splitting between them, which become invisible at higher fields. Both Maxwell's relations and mean-field theory have been used to calculate the magnetic-entropy change. The results indicate the maximum magnetic-entropy change near T_C, which is about 5.7 J/kgK for a field variation of 140 kOe. For the first time, direct measurements of the adiabatic-temperature change (delT) for Cu_2OSeO_3 have been carried out, indicating its significant variation in value. At temperatures around T_C, delT

reaches about 2.6 K for the field H = 140 kOe. At the same field, the relative cooling power and working range for refrigeration applications are about 222 J/kg and 40 K, respectively. Additional analyses of magnetocaloric-effect-related exponents under high applied fields, we have found that Cu_2OSeO_3 exhibits short-range magnetic ordering, which is ascribed to a coexistence of ferromagnetic and antiferromagnetic interactions between Cu ions at different sublattices.

Presenter: Hoang Nam Nhat

P.92 – Poster, VCTP-51

Machine-Learning Hamiltonian Approach to Electronic Structures and Moiré Physics in Twisted Transition Metal Dichalcogenides

Thi Phuong Thao Nguyen and Emi Minamitani

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Twisted transition metal dichalcogenides (TMDs) have emerged as a promising platform for investigating moiré quantum phenomena due to their intrinsic semiconducting band gaps, strong spin-orbit coupling (SOC), and valley-dependent electronic properties [1]. However, first-principles calculations of large moiré supercells remain computationally demanding, particularly when considering SOC, heterostructures, and structural perturbations. In this work, we apply a machine-learning-based Hamiltonian model using graph neural network (GNN) techniques [2] to efficiently investigate the electronic properties of twisted TMD systems with near-density-functional-theory (DFT) accuracy. ViThe Hamiltonian model is trained on a dataset of bilayer structures with varying interlayer translations and separations and subsequently applied to twisted bilayer MoS_2, WSe_2, and their heterobilayers. Benchmark comparisons demonstrate excellent agreement between the GNN Hamiltonian and DFT calculations. By systematically varying the twist angle, we identify the emergence of moiré-induced flat bands in twisted bilayer MoS_2, with ultraflat bands appearing at small twist angles around 3.5^{deg}, accompanied by strong spatial localization of electronic states. Furthermore, we investigate the role of spin-orbit coupling and show that SOC-induced valley splitting is substantially larger in W-based systems than in Mo-based systems and becomes strongly suppressed in low-energy moiré bands at small twist angles. In twisted MoS_2/WSe_2 heterobilayers, we find that the electronic structure is qualitatively distinct from that of twisted homobilayers. The intrinsic band offset between MoS_2 and WSe_2 induces strong layer polarization of the low-energy electronic states, while the lattice mismatch introduces strain as an additional tuning parameter for moiré electronic properties. As a result, the heterobilayer exhibits a reduced band gap and enhanced tunability compared with the corresponding homobilayer systems. Our results demonstrate that machine-learning Hamiltonians provide an efficient and accurate framework for exploring the interplay among moiré physics, spin-orbit coupling, layer polarization, and structural degrees of freedom in large-scale twisted TMD systems, opening new opportunities for studying correlated and topological phenomena in moiré quantum materials.

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Presenter: Nguyễn Thị Phương Thảo

P.93 – Poster, VCTP-51

Optoelectronic properties of WSe 2 monolayer with local deformation

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We investigate the optoelectronic properties of monolayer WSe 2 under local out-of-plane deformation using first-principles calculations. Local deformation is introduced by lifting a selected W atom by 0.2-2.0 Å, with a W vacancy considered as the limiting case. Density functional theory calculations, including spin-orbit coupling, show that pristine WSe 2 is the most stable structure with a direct band gap of 1.283 eV. Increasing deformation progressively reduces structural stability and narrows the band gap from 1.264 to 0.094 eV, while the W-vacancy structure exhibits a slightly larger gap of 0.112 eV. The electronic structure also shows band flattening, valley reordering, and the emergence of localized near- gap states. These findings demonstrate that local out-of-plane deformation provides an effective approach for tuning the electronic structure of monolayer WSe 2 , offering opportunities to control carrier localization in two-dimensional optoelectronic materials.

Presenter: Nguyen Hoang Hieu

P.94 – Poster, VCTP-51

Investigation of phase transitions in hot $^{166-170}$Er nuclei

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The phase transitions in hot $^{166-170}$Er nuclei are investigated within the canonical ensemble framework using the Distribution of Zeros (DOZ) approach. The partition functions are constructed from experimental nuclear level densities at low excitation energies combined with the Back-Shifted Fermi Gas (BSFG) model at high excitation energies. The distribution of complex-temperature zeros is analyzed to identify and classify phase transitions occurring in these finite nuclear systems. Two major phase transitions are observed. The first corresponds to the breaking of nucleon Cooper pairs at temperatures around $T_c \simeq 0.5$–0.7 MeV, while the second is associated with a shape transition from a deformed to a nearly spherical configuration at $T_c \simeq 2.0$–2.6 MeV. The results are compared with previous studies of neighboring rare-earth nuclei and provide further insight into the thermodynamic behavior of finite nuclear system [1].

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Presenter: Le Thi Quynh Huong

P.95 – Poster, VCTP-51

Two-Mode Photon-Added Displaced Fock States: Non - Gaussianity and Nonclassical Properties

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In this work, we propose a new class of quantum states obtained by adding photons to both modes of two-mode displaced Fock states, referred to as two-mode photon-added displaced Fock states (TMPADFSs). The non-Gaussian and nonclassical properties of the proposed states are investigated using the Wigner function, two-mode squeezing, and higher-order two-mode antibunching. The degree of nonclassicality is characterised by the Wigner-function negativity and its negative volume, while squeezing and antibunching are analysed to clarify the role of photon addition in enhancing the nonclassical properties of the states. The results show that the proposed states exhibit strong non-Gaussianity together with pronounced nonclassical effects, including squeezing and higher-order antibunching. Compared with the original two-mode displaced Fock states, photon addition significantly increases the Wigner-function negativity and negative volume, while enhancing the squeezing effects and antibunching. These findings demonstrate that combining photon addition and displacement operations provides an effective approach to enhancing the non-Gaussianity and nonclassical properties of two-mode quantum states.

Keywords: two-mode photon-added displaced Fock states; Two-mode displaced Fock states; Non-Gaussianity; Nonclassicality; Wigner function; Higher-order squeezing; Higher-order antibunching.

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Electron dynamics in nonsequential triple ionization of neon atoms: Laser-wavelength dependence

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In this study, we employ the full classical ensemble model to enhance the computational simulation of nonsequential triple ionization (NSTI) in Ne atoms induced by a strong laser field. By tracing the electron trajectories, we uncover the underlying mechanisms of NSTI, which involve a combination of recollision and sequential ionization. Specifically, electrons ionized by the laser field can return to recollide with the parent ion, either directly ionizing the remaining bound electrons or exciting them to be ionized after a characteristic time delay. Crucially, we investigate how the laser wavelength impacts the dynamics of this NSTI process. Our results demonstrate that with laser fields of identical intensity, varying the wavelength significantly alters the ionization dynamics and shifts the relative contributions of the underlying mechanisms.

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