Program & Abstracts

45th Vietnam Conference on Theoretical Physics

HỘI NGHỊ VẬT LÝ LÝ THUYẾT VIỆT NAM LẦN THỨ 45

Vĩnh Yên

12-14 October, 2020

Program & Abstracts

45th Vietnam Conference on Theoretical Physics

Sông Hồng Resort
189 Lam Sơn, Vĩnh Yên
Vĩnh Phúc, Việt Nam

12-14 October, 2020

Contents

Welcome Message

It is a great pleasure to welcome you in the *45th Vietnam Conference on Theoretical Physics* (VCTP-45) in Vinh Yen.

The VCTP-45 is organized by the Institute of Physic, Vietnam Academy of Science and Technology (IOP-VAST) under the auspices of the Vietnam Theoretical Physics Society (VTPS).

The VCTP, formerly known as NCTP, has been an annual activity of VTPS since 1976. The VCTP is aimed to be an international conference for physicists in Vietnam, in the region and worldwide. Our mission is to foster scientific exchanges and to promote a high-standard level of research and education in Vietnam and in South East Asia.

This year, the VCTP conference will be participated by 148 participants. 9 invited talks, 25 oral and 99 poster contributions will be presented. Due to the Covid-19 pandemic, about one third of the participants will join via video conferencing method.

We wish you enjoy the scientific atmosphere at the conference with both offline and online methods.

The Organizing Committee

Committees

Organizer

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

Honorary Chair

- Nguyen Van Hieu (Vietnam Academy of Science and Technology)

Chair

- Bach Thanh Cong (VNU University of Science, Hanoi)

Organizing Committee

- Trinh Xuan Hoang (Institute of Physics, VAST), Chair
- Dinh Nguyen Dinh (Institute of Physics, VAST)
- Tran Minh Tien (Institute of Physics, VAST)

Program Committee

- Hoang Anh Tuan (Institute of Physics, VAST), Chair
- Le Van Hoang (Ho Chi Minh City Pedagogical University)
- Phung Van Dong (Phenikaa University)
- Nguyen The Toan (VNU University of Science, Hanoi)
- Vu Ngoc Tuoc (Hanoi University of Science and Technology)

Secretariat

- Duong Thi Man (Institute of Physics, VAST)

Sponsor

- International Centre of Physics (ICP), Institute of Physics, Vietnam Academy of Science and Technology —*The Category 2 Centre under the auspices of UNESCO*

General Information

Conference venue

The VCTP-45 conference takes place in:

Song Hong Resort
189 Lam Son street
Vinh Yen city, Vinh Phuc province, Viet Nam

Instructions for offline/online participation

Offline participation

- Offline participation takes place at the conference site.
- Oral presenters present their talks as in a normal conference, except that the presentations will be broadcast via video conferencing for online participants.
- Poster presenters present the posters as in a normal conference, but they must also upload the PDF files of their posters to the conference website before the conference dates for online viewing.

Online participation

- Online participation takes place in Zoom/Microsoft Meeting/Google Meet platforms.
- The link for each session will be posted on the program page of the conference website.

- All online presenters must join the online session before the session starts.
- The online sessions are coordinated by session chairs.
- Poster presenters must upload the PDF files of their posters to the conference website before the conference dates.
- Poster presenters will be asked by the poster session chair to show up online to answer questions of other participants.

Instructions for speakers

The duration of an invited talk is 30 minutes. This includes 25 minutes for the presentation itself and 5 minutes for Q&A. The duration of a regular presentation is 20 minutes. This includes 17 minutes for presentation itself and 3 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. Please hang your poster on the poster standee with a correct presentation code as given in the abstract book. At least, the corresponding author of the poster should be present during 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.

Meeting rooms

All sessions on Monday (all day) and Tuesday morning will take place in Nhà Thủ Đô Hall. On Tuesday afternoon, the conference will be in Sông Lô Room. Please follow the directions at the conference site.

Lunches

Lunches are provided for offline participants at the conference site. Lunch coupons are included in your name badge holder. Extra coupons (limited in number) may be purchased for accompanied family members at the registration desk.

Gala dinner

All participants are invited to gala dinner:

Time: Monday, 12 October 2020, from 18:30 PM
Place: Sông Lô Room, Song Hong Resort.

For your accompanied family members to attend the gala dinner, please buy tickets from the conference secretary.

VTPS Meeting

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

Time: 17:10 PM - 18:00 PM, Monday, 12 October 2020.
Place: Nhà Thủ Đô Hall, Song Hong Resort.

VTPS Young Research Award

An announcement of the recipients of the 2020 VTPS Young Research Award will be given at the opening session of the VCTP-45 conference.

Program timetable

Time	Monday, 12 October	Tuesday, 13 October	Wednesday, 14 October
	Offline Meeting	**Offline Meeting**	**Online Meeting**
08:30 – 10:00	Opening (8:50) *(Chair: Bach Thanh Cong)* Dao Vong Duc (O.1) Do Quoc Tuan (O.2) Photo Session	Poster Session 1 *(Chair: Hoang Anh Tuan)*	Poster Session 2 *(Chair: Vu Ngoc Tuoc)*
10:00 – 10:30	Coffee break	Coffee break	Coffee break
10:30 – 12:00	Nguyen Thi Hong Van (I.1) Tran Van Ngoc (O.3) Eibun Sehana (O.4) Cao Hoang Nam (O.5) *(Chair: Dao Vong Duc)*	Nguyen Thi Kim Thanh (I.4) Do Van-Nam (O.10) Phan Dang Thao Nguyen (O.11) Phung T. V. Bac (O.12) *(Chair: Nguyen Quang Bau)*	Shingo Takeuchi (I.8) Kazuhito Mizuyama (O.16) Le Duc Ninh (O.17) Trinh Thi Ngoc Gia (O.18) *(Chair: Nguyen Quang Hung)*
12:00 – 14:00	Lunch	Lunch	Lunch
14:00 – 15:30	Nguyen Truong Hieu (I.2) Nguyen Nhu Dat (O.6) Ho Quoc Duy (O.7) *(Chair: Nguyen Toan Thang)*	Le Thi Cam Tu (I.5) Hirobumi Mineo (I.6) Tran Xuan Truong (I.7) *(Chair: Le Van Hoang)*	Nguyen Ai Viet (I.9) Tran Viet Nhan Hao (O.19) Nguyen Ngoc Anh (O.20) Tran Minh Duc (O.21) *(Chair: Le Duc Ninh)*
15:30 – 16:00	Coffee break	Coffee break	Coffee break
16:00 – 17:30	Phan Duc Anh (I.3) Emmanuel Plan (O.8) Lai Thi Thu Hien (O.9) *(Chair: Trinh Xuan Hoang)*	Nguyen Quang Hung (O.13) Le Tan Phuc (O.14) Tran Thi Thai (O.15) *(Chair: Phung Van Dong)*	Phan Ngoc Loan (O.22) Pham The Song (O.23) Luong Thi Theu (O.24) Do Ngoc Son (O.25) *(Chair: Nguyen Hong Quang)*
	VTPS Meeting Gala dinner		Closing

Program

Monday, 12 October 2020

Opening Session
Chair: Bach Thanh Cong, Trinh Xuan Hoang

08:50 - 09:00 Opening

09:00 - 09:10 Announcement of 2020 VTPS Young Research Award Recipients

Oral Session 1: *Particle Physics and Cosmology*
Chair: Bach Thanh Cong

09:10 - 09:30 O.1 – Oral
Extradimensions as the Originality for Gauge Interactions
Dao Vong Duc (Institute of Physics, VAST)

09:30 - 09:50 O.2 – Oral
Five-dimensional black hole solutions of scalar-vector Kalb-Ramond model
Do Tuan (PIAS, Phenikaa University)

09:50 - 10:00 Photo Session

10:00 - 10:30 Coffee break

Oral Session 2: *Particle Physics and Cosmology*
Chair: Dao Vong Duc

10:30 - 11:00 I.1 – Invited
An indication of matter-antimatter symmetry violation in neutrinos with the T2K experiment
Nguyen Thi Hong Van (Institute of Physics, Vietnam Academy of Science and Technology)

11:00 - 11:20 O.3 – Oral
Potential of discovering CP violation and mass hierarchy with T2K-II, NOvA and JUNO experiments
Trần Văn Ngọc (IFIRSE, ICISE)

11:20 - 11:40 O.4 – Oral
Sphaleron decoupling condition with a magnetic mass
Eibun Senaha (TDTU-AIMaS)

11:40 - 12:00 O.5 – Oral
p-wave holographic superconductor in massive gravity
Cao Hoang Nam (Phenikaa University)

12:00 - 14:00 Lunch

Oral Session 3: *Condensed Matter Physics*
Chair: Nguyen Toan Thang

14:00 - 14:30 I.2 – Invited
Low-energy electron inelastic mean free paths in materials
Nguyen-Truong Hieu (Ton Duc Thang University)

14:30 - 14:50 O.6 – Oral
Effect of Dielectric Constant Mismatch on Plasmons in Cylindrical Semiconductor Quantum Wires
Nguyen Nhu Dat (Duy Tan University)

14:50 - 15:10 O.7 – Oral
Defects Studies in beta-Ga2O3 Using an Optimized Hybrid Functional
Ho Quoc Duy (Can Tho University of Technology)

15:30 - 16:00 Coffee break

Oral Session 4: *Soft Matter and Biological Physics*
Chair: Trinh Xuan Hoang

16:00 - 16:30 I.3 – Invited *(online presentation)*
Theoretical models for molecular dynamics of amorphous drugs, polymers, and glass-forming liquids under various conditions
Phan Duc Anh (Phenikaa University)

16:30 - 16:50 O.8 – Oral
Active matter in a viscoelastic environment
Emmanuel Lance Christopher VI M. Plan (Duy Tan University)

16:50 - 17:10 O.9 – Oral
hTSPO monomeric structural model in complex with the PK11195 ligand studied by molecular dynamics simulations
Lai Thi Thu Hien (Hanoi University of Science)

17:10 - 18:00 VTPS Meeting

18:30 - 20:30 Gala dinner

Tuesday, 13 October 2020

Poster Session 1
Chair: Hoang Anh Tuan

08:30 - 10:00 P.1 – Poster

Fast Estimation of the Blood-Brain Barrier Permeability by Pulling a Ligand through a Lipid Membrane

Nguyen Quoc Thai (Dong Thap University)

08:30 - 10:00 P.2 – Poster

Competition between heating and cooling effects on an optomechanical oscillator by a squeezed light

Nguyen Duy Vy (Laboratory of Applied Physics, Ton Duc Thang University)

08:30 - 10:00 P.3 – Poster

Exact mode shapes of T-shaped and overhang-shaped microcantilevers

Le Tri Dat (AIMaS, Ton Duc Thang University)

08:30 - 10:00 P.4 – Poster

Interfacial characteristics, Schottky contact and optical performance of Graphene/Ga2SSe van der Waals heterostructure: Strain engineering and electric field tunable

Nguyen V. Chuong (Le Quy Don Technical University)

08:30 - 10:00 P.5 – Poster

Chaoticity and mixing in a dilute suspension of rods

Emmanuel Lance Christopher VI M. Plan (Duy Tan University)

08:30 - 10:00 P.6 – Poster

Gas adsorption on Sc2CO2 monolayer from first-principles calculations

Phạm Dinh Khang (Military Institute of Mechanical Engineering)

08:30 - 10:00 P.7 – Poster

Multicomponent dark matter in noncommutative B-L gauge theory

Le Xuan Thuy (Faculty of Basic Science, Vinh Long University of Technology Education)

08:30 - 10:00 P.8 – Poster

The influence of confined acoustic phonon on the quantum Peltier effect in doped semiconductor superlattice in the presence of electromagnetic wave

Nguyễn Thị Lâm Quỳnh (VNU University of Science)

08:30 - 10:00 P.9 – Poster

The melting curve of gold up to 500 kbar

Phạm Duy Tân (Research Department, Tank Armour Command)

08:30 - 10:00 P.10 – Poster

Thermodynamic properties of Cu3Au alloy

Phạm Duy Tân (Research Department, Tank Armour Command)

08:30 - 10:00 P.11 – Poster

Effects of hydrophobic and electrostatic interactions of the ribosomal exit tunnel on the escape and folding of nascent proteins

Bui Phuong Thuy (Duy Tan University)

08:30 - 10:00 P.12 – Poster

Structural and mechanical properties in densified (AlN)0.85(Si3N4)0.15 ceramics: A molecular dynamics simulation study

Le Van Vinh (Phenikaa University)

08:30 - 10:00 P.13 – Poster

Investigation of S-shaped heat capacity in hot nuclei

Le Thi Quynh Huong (University of Khanh Hoa)

08:30 - 10:00 P.14 – Poster

The influence of confined acoustic phonon on the quantum Ettingshausen effect in cylindrical quantum wire with a infinite potential in presence of Strong electromagnetic Wave

Nguyễn Thị Nguyệt Ánh (VNU University of Science)

08:30 - 10:00 P.15 – Poster

Effect of ionic potential in a model of magnetic topological insulators

Nguyễn Hồng Sơn (Trường Đại học Công đoàn)

08:30 - 10:00 P.16 – Poster

A DFT Study of Some VOCs Adsorption on the Pristine Graphene

Phung T. V. Bac (VNU Vietnam Japan University)

08:30 - 10:00 P.17 – Poster

Longitudinal excitations of the Heisenberg model: a functional integral approach

Nguyen Van Hinh (Hanoi University of Industry)

08:30 - 10:00 P.18 – Poster

Molecular dynamics simulation of the structure and mechanical properties of CuNi alloy

Nguyen Thi Thao (Hanoi National University of Education)

08:30 - 10:00 P.19 – Poster

Study on anharmonic effects in the material with the cubic crystal structure by an analytic statistical moment method.

Cao Huy Phương (Hung Vuong University)

08:30 - 10:00 P.20 – Poster

Investigate the recollision dynamics in the nonsequential double ionization induced by an orthogonal two-color laser field

Pham Nguyen Thanh Vinh (Ho Chi Minh City University of Education)

08:30 - 10:00 P.21 – Poster

Derivation of the magnetic induction vector for a rectangular permanent magnet

Pham Nguyen Thanh Vinh (Ho Chi Minh City University of Education)

08:30 - 10:00 P.22 – Poster

Impact of magnetic dopants on magnetic and topological phases in magnetic

topological insulators
Trần Minh Tiến (Institute of Physics)

08:30 - 10:00 P.23 – Poster
Surface plasmon resonance of plasmonic polymers
Do Thi Nga (Institute of Physics, VAST)

08:30 - 10:00 P.24 – Poster
Morphologies and strengths of magnetic fields in LkHα-101
Nguyen Thi Bich Ngoc (Department of Astrophysics, Vietnam National Space Center, VAST)

08:30 - 10:00 P.25 – Poster
Spin excitations in the Kitaev-Heisenberg model on the square lattice
Pham Thi Thanh Nga (Thuyloi University)

08:30 - 10:00 P.26 – Poster
Magnetic competition in magnetic topological kagome systems
Trần Minh Tiến (Institute of Physics)

08:30 - 10:00 P.27 – Poster
Effect of electric fields on the electronic structures of zigzag buckling silicene nanoribbons
Pham Nguyen Huu Hanh (Can Tho University)

08:30 - 10:00 P.28 – Poster
Asymmetric matter from B-L symmetry breaking
Dương Văn Lợi (Đại học Phenikaa)

08:30 - 10:00 P.29 – Poster
Electronic and magnetic properties of HfO2 and HfMnO2: First priniciples prediction
Hoat Do Minh (Advanced Institute of Materials Science, Ton Duc Thang University)

08:30 - 10:00 P.30 – Poster
Tomography of partially aligned molecules
Tran Cong Minh (Ho Chi Minh City University of Education)

08:30 - 10:00 P.31 – Poster
Understanding the electronic band structures of single-layer and bilayer graphene nanoribbons: An intensive comparison
Nguyen Lam Thuy Duong (Can Tho University)

08:30 - 10:00 P.32 – Poster
Size effect on melting of silicene nanoribbons by molecular dynamics simulation
Huỳnh Anh Huy (Can Tho University)

08:30 - 10:00 P.33 – Poster

Melting point of silicene nanoribbons affected by pressure
Huỳnh Anh Huy (Can Tho University)

08:30 - 10:00 P.34 – Poster
The decay of the Standard model-like Higgs boson $h \to Z\gamma$ in the 3-4-1 model
Nguyen Thi Tham (Hanoi Pedagogical University No2)

08:30 - 10:00 P.35 – Poster
The optical absorption coefficients and the refractive index changes in MoTe2 monolayer
Huynh V. Phuc (Dong Thap University)

08:30 - 10:00 P.36 – Poster
Correlated phases in three-component Falicov-Kimball model
Nguyễn Hồng Sơn (Trường Đại học Công đoàn)

08:30 - 10:00 P.37 – Poster
Resolving the octant of leptonic mixing angle θ_{23} with Hyper-Kamiokande experiment.
Phan To Quyen (IFIRSE, ICISE)

08:30 - 10:00 P.38 – Poster
Canonical seesaw implication for two-component dark matter
Phung Van Dong (Phenikaa University)

08:30 - 10:00 P.39 – Poster
Device Physics and Design of InAs Line-Tunneling Field-Effect Transistors with Laterally Doped Pocket
Nguyễn Đăng Chiến (Dalat University)

08:30 - 10:00 P.40 – Poster
Transport and localization of waves in complex random potential with power-law correlations: A numerical study
Nguyen Ba Phi (Mientrung University of Civil Engineering)

08:30 - 10:00 P.41 – Poster
The distribution of counterions in a hexagonal DNA lattice within mean field theory
Nguyen Thi Thu Hang (Vietnam Atomic Energy Institute)

08:30 - 10:00 P.42 – Poster
The effect of parameters on interaction of two two-level atoms with a single-mode field in a squeezing-enhanced superposition of coherent state
Le Thi Hong Thanh (Quang Nam University)

08:30 - 10:00 P.43 – Poster
Nonclasical properties and quantum teleportation of the superposition of two-mode photon-added pair coherent state
Ho Sy Chuong (Dong Nai University)

08:30 - 10:00 P.44 – Poster

Investigation of radiative process $\tau \to \mu\gamma$ in the simple 3-3-1 model

Nguyen Tuan Duy (Institute of Physics)

08:30 - 10:00 P.45 – Poster

Optimizing of InGaAsSb/GaSb Layer for Infrared Optoelectronics Devices

Nguyen Tien Dai (Duy Tan University)

08:30 - 10:00 P.46 – Poster

Comparison of the contribution of the photon's vector and scalar Kaluza-Klein partners in the neutron lifetime

Pham Tien Du (Thuyloi University)

08:30 - 10:00 P.47 – Poster

Improvement of quantum teleportation and controlled quantum teleportation via photon-added trio coherent state

Tran Quang Dat (University of Transport and Communications - Campus in Ho Chi Minh City)

08:30 - 10:00 P.48 – Poster

Metal-insulator transitions of fermionic mixtures with mass imbalance in disordered optical lattice

Hoang Anh Tuan (Viện Vật lý)

08:30 - 10:00 P.49 – Poster

Iron-tin-based nanocomposite anodes for sodium-ion batteries

Nguyen Tuan Loi (Institute of Fundamental and Applied Sciences, Duy Tan University)

08:30 - 10:00 P.50 – Poster

Phase diagrams of Falikov-Kimball model with Gaussian distribution for impurities and box distribution for Coulomb disorder

Nguyen Thi Hai Yen (Institute of Physics)

08:30 - 10:00 P.51 – Poster

Effect of electron-impurity scattering on the magneto-optical absorption property in MoS_2 monolayer

Le Thi Thu Phuong (Hue University of Education)

08:30 - 10:00 P.52 – Poster

Studying the spread of epidemics by matrix logistic map

Chu Thuy Anh (Institute of Physics)

08:30 - 10:00 P.53 – Poster

Non-Equilibrium Molecular Dynamics Simulations of Self-Diffusion Coefficient at Infinite Dilution: Applications to Fractionation of Noble Gases

Lục Hán Tường (IFAS)

08:30 - 10:00 P.54 – Poster

Elemental and Isotopic Fractionation of Noble Gases by Molecular Diffusion

Nguyễn Phúc (Trường Đại Học Khoa học Tự nhiên - Đại học Quốc gia Tphcm)

08:30 - 10:00 P.55 – Poster
Probing degrees of orientation of polar molecules
Nguyen Huynh Kim Ngan (Ho Chi Minh City University of Education)

08:30 - 10:00 P.56 – Poster
The effect of vacancies on the electronic properties of bilayer graphene nanoribbons
Nguyen Thi Kim Quyen (Can Tho University)

08:30 - 10:00 P.57 – Poster
Rectangular Quantum Wire with an Infinite potential GaAs/AlGaAs: Quantum theory of Acoustomagnetoelectric effect in the presence of Electromagnetic wave
Nguyễn Quyết Thắng (Hanoi University of Science)

08:30 - 10:00 P.58 – Poster
A Toy Model for Prediction of Pandemics
Nguyễn Văn Hoa (HCMUE)

08:30 - 10:00 P.59 – Poster
Aggregation of microorganisms on engineered topographic surfaces: a simulation study
Trinh Xuan Hoang (Institute of Physics, VAST)

08:30 - 10:00 P.60 – Poster
Counterion distribution near macroions, a field-theoretical treatments up to two-loop order
Tran Thanh Tuyen (Vietnam National University)

08:30 - 10:00 P.61 – Poster
On the Quatron State in Parabolic Quantum Dots
Nguyen Hong Quang (Viện Vật lý)

08:30 - 10:00 P.62 – Poster
Total decay rate of $\mu \to e\gamma$ in a model with electroweak scale right-handed neutrino
Dinh Nguyen Dinh (Institute of Physics, VAST)

10:00 - 10:30 Coffee break

Oral Session 5: *Condensed Matter Physics*
Chair: Nguyen Quang Bau

10:30 - 11:00 I.4 – Invited
Thermoelectric transport in a three channel charge Kondo circuit
Nguyen Thi Kim Thanh (Institute of Physics, Vietnam Academy of Science and Technology)

11:00 - 11:20 O.10 – Oral

Real-approach for the electronic calculation of twisted bilayer graphene: The neutrino oscillation-like dynamics of electrons

Do Van-Nam (Phenikaa Institute for Advanced Study (PIAS))

11:20 - 11:40 O.11 – Oral

The correlation between transition of the energy bands and the optical absorption spectrum in bilayer armchair graphene nanoribbons

Phan Dang Thao Nguyen (Can Tho University)

11:40 - 12:00 O.12 – Oral

Adsorption of Toxic Gases on Pristine Graphene, Graphene/h-BN and Graphene/α-SiO2 Heterostructures: Density Functional Theory Calculations

Phung T. V. Bac (VNU Vietnam Japan University)

12:00 - 14:00 Lunch

Oral Session 6: *Molecular Physics and Quantum Optics*
Chair: Le Van Hoang

14:00 - 14:30 I.5 – Invited *(online presentation)*

Effect of dynamic core-electron polarization on harmonic process of linear molecules

Le Thi Cam Tu (Ton Duc Thang University)

14:30 - 15:00 I.6 – Invited

Theoretical study of dynamic Stark-induced pi-electron rotations in low symmetry aromatic ring molecules beyond the frozen nuclear approximation

Hirobumi Mineo (Ton Duc Thang University)

15:00 - 15:30 I.7 – Invited

Waveguide Arrays: from Discrete Optics to Quantum Field Theory

Tran Xuan Truong (Le Quy Don Technical University)

15:30 - 16:00 Coffee break

Oral Session 7: *Nuclear and Astro- Physics*
Chair: Phung Van Dong

16:00 - 16:20 O.13 – Oral

A fully microscopic model of total level density in spherical nuclei: an example of ^{60}Ni nucleus

Nguyễn Quang Hưng (Institute of Fundamental and Applied Sciences, Duy Tan University)

16:20 - 16:40 O.14 – Oral

Role of pairing correlation in the radiative strength function

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

16:40 - 17:00 O.15 – Oral

Morpho-kinematics of the molecular gas in a quasar host galaxy at redshift z=0.654

Tran Thi Thai (Vietnam National Space Center, VAST)

Wednesday, 14 October 2020

Poster Session 2
Chair: Vu Ngoc Tuoc

08:30 - 10:00 P.63 – Poster *(online presentation)*

A discrete differential evolution for fuel loading optimization of the DNRR reactor and comparison with genetic algorithm

Phan Thi Thuy Giang (Institute of Fundamental and Applied Sciences, Duy Tan University)

08:30 - 10:00 P.64 – Poster *(online presentation)*

Thermodynamics and control systems theory: Application to non-equilibrium single-phase or multi-phase processes

Hoang Ngoc Ha (Duy Tan University)

08:30 - 10:00 P.65 – Poster *(online presentation)*

Transmembrane Amyloid β-Peptide Structures: In Silico Study

Ngo Son Tung (Laboratory of Theoretical and Computational Biophysics, Ton Duc Thang University, Vietnam)

08:30 - 10:00 P.66 – Poster *(online presentation)*

Diverse Structural and Electronic Properties of Si-Doped Graphene

On Van Vo (Thu Dau Mot University)

08:30 - 10:00 P.67 – Poster *(online presentation)*

Thermoelectric and magnetic properties of gadolinium doped bismuth telluride: first-principles investigation

Tran Van Quang (Department of Physics, University of Transport and Communications, Hanoi, Vietnam)

08:30 - 10:00 P.68 – Poster *(online presentation)*

Simulation for CO2 capture and permanent underground geological storage

Phan Van Cuong (Nha Trang University)

08:30 - 10:00 P.69 – Poster *(online presentation)*

Adsorption of Gas Molecules on Sawtooth Penta-Graphene Nanoribbon

Nguyen Thanh Tien (Can Tho University)

08:30 - 10:00 P.70 – Poster *(online presentation)*

Study on structural and elastic properties of interstitial alloy FeSi with B2 structure under pressure

Nguyen Minh Hoa (Hue University of Medicine and Pharmacy)

08:30 - 10:00 P.71 – Poster *(online presentation)*

Feature-Rich Magnetic and Electronic Properties of Halogen-Doped Silicene
On Van Vo (Thu Dau Mot University)

08:30 - 10:00 P.72 – Poster *(online presentation)*
Effects of pH of the precipitation environment on SiO2 synthesis from rice husk ash
Nga Huynh Nguyen Thi (Thu Dau Mot University)

08:30 - 10:00 P.73 – Poster *(online presentation)*
Exact electron-muon elastic scattering in QED at next-to-leading order: Soft-photon contribution
Le Duc Truyen (IFIRSE, ICISE)

08:30 - 10:00 P.74 – Poster *(online presentation)*
Isotropic Strain Effect on 2D Charge Density Wave Materials NbX2 (X = S, Se)
Lương Thị Thêu (Hanoi Pedagogical University)

08:30 - 10:00 P.75 – Poster *(online presentation)*
Effect of dynamic core-electron polarization on odd-even high-order harmonic generation from CO molecule
Nguyen Thi Hien (Department of Physics, Tay Nguyen University)

08:30 - 10:00 P.76 – Poster *(online presentation)*
Transition-Metal Dichalcogenides MoX2 (X=Te, Se) under Biaxial Strain
Nguyễn Hoàng Hưng (VNU Viet Nam Japan University)

08:30 - 10:00 P.77 – Poster *(online presentation)*
DFT Study on Crystal and Electronic Structures of Potential Cathode Material $Na_2Ni_3(SO_4)_4$
Trần Thiện Lân (Hue University of Education)

08:30 - 10:00 P.78 – Poster *(online presentation)*
A connection between domain structure and dynamical properties of liquid silica under pressure
Giap Thi Thuy Trang (Thainguyen University of Education)

08:30 - 10:00 P.79 – Poster *(online presentation)*
Enhancement of the electric current in high-Tc superconductor interacting with an artificial pinning arrayan
Nguyen Minh Hoa (Hue University of Medicine and Pharmacy)

08:30 - 10:00 P.80 – Poster *(online presentation)*
Exciton Creation and Annihilation Mechanism in Monolayer WSe2 under Tensile and Compressive Strains
Tran Thi Nhan (Hanoi University of Industry)

08:30 - 10:00 P.81 – Poster *(online presentation)*
The possibility of supersolid phase in the hard-core boson model on the triangular lattice

Nguyen Oanh (Electric Power University)

08:30 - 10:00 P.82 – Poster *(online presentation)*
First-principles insight into the structural, electronic and optical properties of cadmium selenium nanocrystals
Đỗ Quang Tâm (Hue University of Medicine and Pharmacy)

08:30 - 10:00 P.83 – Poster *(online presentation)*
Reconstruction of the highest-occupied molecular orbital
Truong Quan Hao (Ho Chi Minh city University of Education)

08:30 - 10:00 P.84 – Poster *(online presentation)*
The optical Stark effect of excitons in InGaAs/InAlAs prolate ellipsoidal quantum dots
Le Thi Ngoc Bao (Hue University of Sciences)

08:30 - 10:00 P.85 – Poster *(online presentation)*
Phenomenology study of the lepton sector in an S_3 flavor symmetry with inverse seesaw mechanism
Nguyễn Thanh Phong (Can Tho University)

08:30 - 10:00 P.86 – Poster *(online presentation)*
Casimir effect in a single weakly interacting Bose gas at zero-temperature with Neumann boundary condition
Song Thế Phạm (Trường đại học Tây Bắc)

08:30 - 10:00 P.87 – Poster *(online presentation)*
Gelation of Anisotropic Colloids with Short-Range Attraction
Tran Van Thien (Can Tho University)

08:30 - 10:00 P.88 – Poster *(online presentation)*
Numerical determination of the soft Coulomb in considering the nonsequential double ionization process
Truong Dang Hoai Thu (Ho Chi Minh city University of Education)

08:30 - 10:00 P.89 – Poster *(online presentation)*
Controlled teleportation between a continuous-variable state and a discrete-variable state using hybrid entanglement under decoherence effects
Cao Thi Bich (Institute of Physics, Ha Noi)

08:30 - 10:00 P.90 – Poster *(online presentation)*
Parity violation by gravity in QCD as Discretize Kaluza-Klein theory
Nguyễn Văn Đạt (Trường Đại học KHTN, ĐHQG Hà Nội)

08:30 - 10:00 P.91 – Poster *(online presentation)*
The correlation function dependence on temperature in EXAFS spectra. Application for Cu-Ag alloys
Nguyen Ba Duc (Tan Trao University)

08:30 - 10:00 P.92 – Poster *(online presentation)*

Electronic properties of the pentagonal silicon dicarbide nanoribbons
Nguyen Thanh Tien (Can Tho University)

08:30 - 10:00 P.93 – Poster *(online presentation)*
Two-dimensional clusters of colloidal tetramers via droplet emulsion templating
Pham Van Hai (Hanoi National University of Education)

08:30 - 10:00 P.94 – Poster *(online presentation)*
Neutron bubble in ^{54}Ca nucleus
Le Ngoc Uyen (Ho Chi Minh City University of Education)

08:30 - 10:00 P.95 – Poster *(online presentation)*
Discrete SHADE method for in-core fuel management of VVER-1000 reactor
Tran Viet Phu (Institute for Nuclear Science and Technology - VINATOM)

08:30 - 10:00 P.96 – Poster *(online presentation)*
Otpical properties of slidding bilayer graphene
Tran Ky Vi (Hanoi National University of Education)

08:30 - 10:00 P.97 – Poster *(online presentation)*
Opto-electronic property of Nitrogen doped graphene quantum dots
Nguyen Vo Anh Duy (Can Tho University)

08:30 - 10:00 P.98 – Poster *(online presentation)*
Structural, Electronic and Mechanical Properties of Few-layer Porous Nanosheet from spheroidal cage-like ZnO polymorph
Vu Ngoc Tuoc (Hanoi University of Science and Technology)

08:30 - 10:00 P.99 – Poster *(online presentation)*
Investigate the dependence of multiple recollision on laser wavelength in the nonsequential double ionization process
Truong Dang Hoai Thu (Ho Chi Minh city University of Education)

08:30 - 10:00 P.100 – Poster
Molecules on β_{12} borophene: chemical bonding analysis and van der Waals density functional assessment
Dinh Van An (VNU Vietnam Japan University)

08:30 - 10:00 P.101 – Poster
Novel orthorhombic Tavorite-like material for lithium ion batteries: DFT investigation
Dinh Van An (VNU Vietnam Japan University)

10:00 - 10:30 Coffee break

Oral Session 8: *Particle and Nuclear Physics*
Chair: Nguyen Quang Hung

10:30 - 11:00 I.8 – Invited *(online presentation)*
Hawking Flux of Black Hole with nonlinear soft-hairs

Shingo Takeuchi (Phenikaa University)

11:00 - 11:20 O.16 – Oral *(online presentation)*
Fano effect caused by the pairing on neutron-nucleus elastic scattering
Kazuhito Mizuyama (Duy Tan University)

11:20 - 11:40 O.17 – Oral *(online presentation)*
Vector boson scattering to diphoton at the LHC
Le Duc Ninh (IFIRSE, ICISE)

11:40 - 12:00 O.18 – Oral *(online presentation)*
Probing atmospheric electric fields under thunderstorm conditions by using radio emission from extensive air showers
Trinh Thi Ngoc Gia (Physics Education Department, School of Education, Can Tho University)

12:00 - 14:00 Lunch

Oral Session 9: *Particle and Nuclear Physics, Quantum Information*
Chair: Le Duc Ninh

14:00 - 14:30 I.9 – Invited *(online presentation)*
Photon-fermion Kaluza-Klein partners in bilayer systems
Ai-Viet Nguyen (Information Technology Institute, Vietnam National University)

14:30 - 14:50 O.19 – Oral *(online presentation)*
Effects of velocity-dependent and spin-orbit term of Skyrme interaction on neutron elastic scattering observables
Trần Viết Nhân Hào (Khoa Vật Lý, Trường Đại học Sư Phạm, Đại học Huế)

14:50 - 15:10 O.20 – Oral *(online presentation)*
Experimental study on the nuclear level scheme in Vietnam: examples of ^{153}Sm and ^{172}Yb
Nguyen Ngoc Anh (Dalat Nuclear Research Institute)

15:10 - 15:30 O.21 – Oral *(online presentation)*
Interaction-free measurement in IBM quantum computers
Tran Minh Duc (Hanoi University of Science)

15:30 - 16:00 Coffee break

Oral Session 10: *Molecular Physics, Condensed Matter Physics*
Chair: Nguyen Hong Quang

16:00 - 16:20 O.22 – Oral *(online presentation)*
Wavelength dependence of high-order harmonic yields of Rydberg atom
Phan Ngoc-Loan (Ho Chi Minh City University of Education)

16:20 - 16:40 O.23 – Oral *(online presentation)*
Density of condensates of two-component Bose-Einstein condensates restricted

between two planar walls
Song Thế Phạm (Trường đại học Tây Bắc)

16:40 - 17:00 O.24 – Oral *(online presentation)*
Band Dispersion and Exciton Creation and Annihilation under Isotropic Strain in Monolayer WS2
Lương Thị Thêu (Hanoi Pedagogical University)

17:00 - 17:20 O.25 – Oral *(online presentation)*
DFT study of water monomer adsorption on Nitrogen and Boron doped graphene
Ngoc Son Do (Ho Chi Minh City University of Technology)

17:20 - 17:30 Closing

Abstracts

I.1 – Invited, VCTP-45

An indication of matter-antimatter symmetry violation in neutrinos with the T2K experiment

Nguyen Thi Hong Van

Institute of Physics, Vietnam Academy of Science and Technology

The Universe is made up almost of matter but not of antimatter. This matter-antimatter asymmetry is a mystery of science since the laws of physics are essentially symmetrical. Under the language of particle physics, this asymmetry is called CP violation where "C" stands for "Charge-conjugation" symmetry and "P" stands for "Parity reversal" symmetry. Violation of the CP symmetry was observed for the first time in 1964 in the quark sector, however, this CP violation is too small in order to explain the imbalance of matter-antimatter in the Universe. Therefore, a CP violation in the lepton sector, which so far has not yet been observed, is expected to be a potential source for the asymmetry of matter-antimatter in the Universe. Recently, the T2K (Tokai to Kamioka), a long baseline (anti-) neutrino oscillations experiment located in Japan, has published in "Nature" their recent result showing an indication of CP violation in neutrinos. It is shown that the probability for a muon neutrino to become an electron neutrino is different from that of muon antineutrino to become an electron antineutrino, leading to a possible CP violation at 95% confidence level. On behalf of the T2K collaboration, I will present this result together with an overview of the T2K experiment and especially the participation of Vietnam in this experiment.

Presenter: Nguyen Thi Hong Van

I.2 – Invited, VCTP-45

Low-energy electron inelastic mean free paths in materials

Hieu T. Nguyen-Truong

Ton Duc Thang University

The electron inelastic mean free path (IMFP) is an important quantity for studying electron transport in condensed matter and for various types of electron spectroscopy/microscopy. For decades, experimental techniques and theoretical models have been developed to determine this quantity. However, the determination of low-energy IMFPs is still a challenge. Recently, we have presented a theoretical approach to this problem [1]. Accordingly, we determine the IMFPs for energies below 100 eV within the dielectric formalism and the time-dependent density functional theory. Our calculated IMFPs for elemental solids [2] and monolayer graphene [3] agree well with experimental data. In this talk, we present an overview of the recent progress in this field

and report our latest results. We show that the presented approach is general and reliable not only for bulk materials but also for two-dimensional materials.

References: [1] H. T. Nguyen-Truong, Appl. Phys. Lett. 108, 172901 (2016). [2] H. T. Nguyen-Truong, J. Phys. Condens. Matter 29, 215501 (2017). [3] H. T. Nguyen-Truong, B. Da, L. Yang, Z. Ding, H. Yoshikawa, and S. Tanuma, Appl. Phys. Lett. 117, 33103 (2020).

Presenter: Nguyen-Truong Hieu

I.3 – Invited, VCTP-45

Theoretical models for molecular dynamics of amorphous drugs, polymers, and glass-forming liquids under various conditions

Anh D. Phan

Phenikaa University

Although crystalline drugs dominate drug market, amorphous drugs have recently been studied worldwide since a significant enhancement of solubility and bioavailability in comparison with their crystalline counterparts. In this work, we formulate theoretical approaches to investigate the molecular mobility, dynamic fragility, and glass transition temperature (T_g) of amorphous drugs and materials under different cooling rates, compression, and confinement effects. The molecular dynamics and T_g have a strong correlation with the melting point, physical stability, and solubility of amorphous drugs. We can determine the molecular dynamics via the structural relaxation time calculated by a model of hard-sphere fluid and a thermal mapping to convert from the effective fluid density to temperature of real materials. Under compression/stress and confinement conditions, the speeding-up and slowing-down of molecular mobility in various structures are strongly dependent on each particular case. The physical picture has been quantitatively and qualitatively explained the glassy transition of polymers and glass-forming liquids. The timescale from my calculations ranges from 1 picosecond to several years, which is far beyond the computational capability of current supercomputers (up to 107 picoseconds) in the world. Numerical results allow not only comparing with experimental data, but also qualitatively predicting appropriate storage and manufacturing conditions for various amorphous materials.

Presenter: Phan Duc Anh

I.4 – Invited, VCTP-45

Thermoelectric transport in a three channel charge Kondo circuit

T. K. T. Nguyen (1) and M. N. Kiselev (2)

(1) Institute of Physics, Vietnam Academy of Science and Technology, 10 Dao Tan, Hanoi, Vietnam (2) The Abdus Salam International Centre for Theoretical Physics, Strada Costiera 11, I-34151, Trieste, Italy

In this talk I will present our theoretical work about the thermoelectric transport through a circuit implementation of the three-channel charge Kondo model quantum simulator [Z. Iftikhar et al., Science 360, 1315 (2018)]. The universal temperature scaling law of the Seebeck coefficient is computed perturbatively approaching the non-Fermi liquid strong coupling fixed point using abelian bosonization technique. The predicted $T^{1/3} \log T$ scaling behaviour of the thermoelectric power sheds a light on the properties of Z_3 emerging parafermions and gives an access to exploring pre-fractionalized zero modes in the quantum transport experiments. We discuss

a generalization of approach for investigating a multi-channel Kondo problem with emergent Z_N to Z_M crossovers between "weak" non-Fermi liquid regimes corresponding to different low-temperature fixed points.

Reference: T. K. T. Nguyen and M. N. Kiselev, Phys. Rev. Lett. 125, 026801 (2020)

Presenter: Nguyen Thi Kim Thanh

I.5 – Invited, VCTP-45

Effect of dynamic core-electron polarization on harmonic process of linear molecules

Cam-Tu Le (1,2)

(1) Atomic Molecular and Optical Physics Research Group, Advanced Institute of Materials Science, Ton Duc Thang University; (2) Faculty of Applied Sciences, Ton Duc Thang University

This talk gives a review of dynamic core-electron polarization (DCEP) effect on the harmonic process of linear molecules. High-order harmonic generation (HHG) which is one of nonlinear phenomena occurring when atoms/molecules subjected to intense ultrashort lasers [1] has become a powerful tool to probe and control molecular dynamics. In principle, the strong-field processes can be obtained from directly solving the time-dependent Schrodinger equation (TDSE). However, in practical, this method is usually handled by using some schemes such as single-active electron approximation to apply for more-than-two-electron systems. In this framework, we investigate the influence of the DCEP [2], which is induced by the driving laser, on the HHG stimulated from linear molecules, such as CO – polar molecule and CO2 – nonpolar molecule. With the few-cycle pulses, the results show that DCEP plays an essential role for the polar molecule CO, it makes the results meet the agreement with experimental and other theoretical results. By investigating the time-dependent ionization rate, we explain completely the DCEP mechanism: it affects the harmonic intensity through the ionization at a specific instant, rather than throughout the whole pulse propagation as understood. Furthermore, based on the instantaneous ionization rate, one can predict the influence of DCEP on the harmonic intensity of polar molecules [3]. Meanwhile, for nonpolar molecules such as CO2 , the DCEP can affect the harmonic process through a different mechanism – suppressing the distortion of the laser field on the highest occupied molecular orbital (HOMO) during the recombination phase, thus partially recovering the HOMO symmetry [4]. Consequently, this shifts and sharpens the minima in the HHG spectra, which arise from the two-center interference [5]. Furthermore, the influence of DCEP can manifest in case of multicycle pulses in which the DCEP affects the ratio of even-to-odd harmonic intensity emitted from CO due to the degree of symmetry breaking of the molecule-laser system [6].

References: [1] A. McPherson et al., J. Opt. Soc. Am. B 4, 595 (1987). [2] B. Zhang, J. Yuan, and Z. Zhao, Phys. Rev. Lett. 111, 163001 (2013). [3] C.-T. Le, V.-H. Hoang, L.-P. Tran, and V.-H. Le, Phys. Rev. A 97, 043405 (2018). [4] C.-T. Le, D.-D. Vu, C. Ngo, and V.-H. Le, Phys. Rev. A 100, 053418 (2019). [5] M. Lein, N. Hay, R. Velotta, J. P. Marangos, and P. L. Knight, Phys. Rev. Lett. 88, 183903 (2002). [6] N.-L. Phan, C.-T. Le, V.-H. Hoang, V.-H. Le, Phys. Chem. Chem. Phys. 21, 24177 (2019).

Presenter: Le Thi Cam Tu

I.6 – Invited, VCTP-45

Theoretical study of dynamic Stark-induced pi-electron rotations in low sym-

metry aromatic ring molecules beyond the frozen nuclear approximation

Hirobumi Mineo

Ton Duc Thang University, AIMaS

Effects of vibrational modes on dynamic Stark-induced pi-electron rotations in low-symmetry aromatic ring molecules were theoretically studied under the adiabatic approximation. The lowest vibronic states in the two electronic excited states are set to be degenerate by using two UV lasers. The parameters of the two lasers (frequencies, intensities) were determined under the condition in which the lowest two vibronic states are in equal energy with each other. The resultant degenerate state is called dynamic Stark-induced degenerate vibronic state (DSIDVS), which is an essential key to generate coherent pi-electron angular momentum of aromatic ring molecules taking into account vibrational degrees of freedom. Closed forms of vibronic state wavefunctions are derived by solving the time-dependent Schrödinger equations analytically. Here the number of the vibronic excited states were restricted to extract the essential role of vibrational mode on pi-electron rotations. In this work we adopt toluene molecule, which is one of the typical aromatic ring molecules with lower symmetry.

Presenter: Hirobumi Mineo

I.7 – Invited, VCTP-45

Waveguide Arrays: from Discrete Optics to Quantum Field Theory

Tran Xuan Truong

Le Quy Don Technical University

The waveguide array (WA) is a perfect system to study many interesting discrete classic optical phenomena, such as discrete diffraction, discrete solitons [1], the generation of diffractive resonant radiation from discrete solitons [2], and supercontinuum generation in both the frequency and wave number [3]. In applications, logic functions such as AND and NOT, and time gating function can be realized in WAs. Amazingly, some fundamental nonrelativistic quantum mechanics effects rooted in the Schrödinger equation, such as Zener tunneling and Bloch oscillations [4], have been intensively investigated through their photonic analogs in WAs. More remarkably, the binary waveguide array (BWA) – a special class of WAs – is a wonderful system to simulate fundamental relativistic quantum mechanics effects rooted in the Dirac equation in quantum field theory, such as Zitterbewegung [5], Dirac solitons (DSs) [6–10], and the topological Jackiw–Rebbi (JR) states [11–14]. The JR states are well known for predicting the charge fractionalization phenomenon, which is basic in the fractional quantum Hall effect [15]. The JR state solutions are also well known for the topological nature and can be interpreted as a precursor to topological insulators, which have attracted a lot of interest recently. Another extraordinary fundamental relativistic quantum mechanics effect called Klein tunneling (KT) has also been simulated in BWAs [16]. The KT effect was predicted by Oscar Klein in 1929 with suggestion that relativistic fermions can tunnel through a repulsive potential step, whose height is greater than the particle energy, without the exponential damping conventionally ruled by the Schrödinger equation. In short, in this presentation I would like to show the achievements in exploiting this amazing platform of WAs from both classical and quantum points of view.

References: [1] D. N. Christodoulides, F. Lederer, and Y. Silberberg, Nature 424, 817 (2003). [2] Tr. X. Tran and F. Biancalana, Phys. Rev. Lett. 110, 113903 (2013). [3] Tr. X. Tran, D. C. Duong, and F. Biancalana, Phys. Rev. A 89, 013826 (2014). [4] T. Pertsch, P. Dannberg, W. Elflein, A. Bräuer, and F. Lederer, Phys. Rev. Lett. 83, 4752 (1999). [5] F. Dreisow, M.

Heinrich, R. Keil, A. Tünnermann, S. Nolt, S. Longhi, and A. Szameit, Phys. Rev. Lett. 105, 143902 (2010). [6] Tr. X. Tran, S. Longhi, and F. Biancalana, Ann. Phys. 340, 179 (2014). [7] Tr. X. Tran and D. C. Duong, Ann. Phys. 361, 501 (2015). [8] Tr. X. Tran, X. N. Nguyen, and F. Biancalana, Phys. Rev. A 91, 023814 (2015). [9] Tr. X. Tran and D. C. Duong, Chaos 28, 013112 (2018). [10] Tr. X. Tran, J. Opt. Soc. Am. B 36, 2001 (2019). [11] Tr. X. Tran and F. Biancalana, Phys. Rev. A 96, 013831 (2017). [12] Tr. X. Tran, H. M. Nguyen, and D. C. Duong, Phys. Rev. A 100, 053849 (2019). [13] Tr. X. Tran, J. Opt. Soc. Am. B 36, 2559 (2019). [14] R. Jackiw and C. Rebbi, Phys. Rev. D 13, 3398 (1976). [15] R. B. Laughlin, "Nobel lecture: fractional quantization," Rev. Mod. Phys. 71, 863 (1999). [16] Tr. X. Tran, J. Opt. Soc. Am. B 37, 1811 (2020).

Presenter: Tran Xuan Truong

I.8 – Invited, VCTP-45

Hawking Flux of Black Hole with nonlinear soft-hairs

Shingo Takeuchi

Phenikaa University

I will report the Hawking flux from a black hole with soft hair by the anomaly cancellation method . My analysis takes into account the supertranslation hair to the quadratic order unlike the earlier studies considering the black hole with linear supertranslation hair, which yields the angular dependent horizon. As a result, highly nontrivial kinetic-mixings appear among the spherical Kaluza-Klein modes of the (1+1)d near-horizon reduced theory, which obscures the traditional derivation of the Hawking flux. However, after a series of field re-definitions, we can disentangle the mode-mixings into canonical normal modes, but the reduced metrics for these normal modes are mode-dependent. Despite of this, the resultant Hawking flux turns out to be mode-independent and remains the same as the Schwarzschild's one.

Presenter: Shingo Takeuchi

I.9 – Invited, VCTP-45

Photon-fermion Kaluza-Klein partners in bilayer systems

Ai-Viet Nguyen

Information Technology Institute, Vietnam National University

A geometric description of bilayer systems is formulated as a space-time manifold extended by a discrete dimension of two discrete points. The interlayer interactions are taken into consideration as a consequence of the discrete derivation and Kaluza-Klein partners. The scalar Kaluza-Klein partner has a quartic potential, which gives a mass to the vector Kaluza-Klein partner of the photon via an Abelian Higgs mechanism. The discrete dimension also leads to a non-diagonal mass matrix for the fermions. Its diagonalization by a mixing angle results in a mass splitting formula of fermion's Kaluza-Klein partners and their couplings to the photon sector.

Presenter: Ai-Viet Nguyen

O.1 – Oral, VCTP-45

Extradimensions as the Originality for Gauge Interactions

Dao Vong Duc

Institute of Physics, VAST

The mechanism for mass and charge creation from Extradimensions proposed in our previously published works [DV Duc et al. Int. J. Theor. Phys. 54, 1071 (2015); Int. J. Theor. Phys. 55, 959(2016); Mod. Phys. Lett. A 33, N1 (2019) 1950130] is generalized for the case of non-abelian gauge interactions. Illustration example is presented for unifying existing flavour and colour quarks with respect to electromagnetic and strong interactions, as well as unifying three existing lepton generations. On the base of the derived charge-mass sum rules we would predict the existence of some hidden tachyon quarks with fractional charges,as well as some hidden tachyon leptons, neutral or negative charged.

Presenter: Dao Vong Duc

O.2 – Oral, VCTP-45

Five-dimensional black hole solutions of scalar-vector Kalb-Ramond model

Tuan Q. Do

Phenikaa Institute for Advanced Study, Phenikaa University, Hanoi 12116, Vietnam

We have found spherically symmetric black hole solutions to a five-dimensional scalar-vector Kalb-Ramond model. In this talk, therefore, we would like to present basic details of these obtained black holes.

Presenter: Do Tuan

O.3 – Oral, VCTP-45

Potential of discovering CP violation and mass hierarchy with T2K-II, NOvA and JUNO experiments

Tran Van Ngoc (1), Cao Van Son (2), Ankur Nath (3), Nguyen Thi Hong Van (4), Phan To Quyen (1), Francis Ng K (3)

(1) Institute For Interdisciplinary Research in Science and Education, Quy Nhon, Vietnam; (2) High Energy Accelerator Research Organization (KEK), Tsukuba, Ibaraki, Japan; (3) Tezpur University, Assam, India; (4) Institute of Physics (IOP), VAST, Hanoi, Vietnam

CP violation in lepton sector and mass hierarchy are two among unsolved questions in neutrino physics. In this presentation, we will explore a potential to discover CP violation and mass hierarchy with a joint analysis of T2K-II, NOvA and JUNO experiments. T2K (located in Japan) and NOvA (located in USA) are two world-leading accelerator-based long baseline neutrino oscillation experiments. T2K-II is an extension of the T2K experiment which can provide a strong evidence for CP violation. NOvA is significantly sensitive to both CP violation and mass hierarchy. JUNO, a medium baseline reactor neutrino experiment which is under construction in China, is able to have 3 σ or higher sensitivity to the mass hierarchy and can achieve better than 1% precision on solar parameters with its proposed running in six years. A combined analysis of T2K-II, NOvA and JUNO at the end of their runs can completely establish the neutrino mass hierarchy and indicate CP violation in the lepton sector at more than 4σ if $\delta_{CP} \ -\pi/2$.

Presenter: Trần Văn Ngọc

O.4 – Oral, VCTP-45

Sphaleron decoupling condition with a magnetic mass

Koichi Funakubo (1), Eibun Senaha (2)

(1) Saga University; (2) Ton Duc Thang University

We elucidate a magnetic mass effect on a sphaleron energy that is crucial for baryon number preservation needed for successful electroweak baryogenesis. It is found that the sphaleron energy increases in response to the magnetic mass. As an application, we study the sphaleron energy and electroweak phase transition with the magnetic mass in a two-Higgs-doublet model. Although the magnetic mass can screen the gauge boson loops, it relaxes a baryon number preservation criterion more effectively, broadening the baryogenesis-possible region. Our findings would be universal in any new physics models as long as the gauge sector is common to the standard model.

Presenter: Eibun Senaha

O.5 – Oral, VCTP-45

p-wave holographic superconductor in massive gravity

Cao Hoang Nam (1),Tran Ngoc Hung (2), Tran Dinh Tham (3)

(1) Phenikaa University; (2) Institute of Physics, Vietnam Academy of Science and Technology; (3) Pham Van Dong University

In this representation, we provide the analytical investigation of p-wave holographic superconductor in massive gravity in the probe limit. We obtain the analytical expressions for the critical temperature, the value of the condensate operator, and the difference of the free energy between the superconductor and normal phases. It is found that the behavior of these quantities in the presence of the mass of graviton to be dependent almost on the sign of the massive gravity couplings. The critical temperature becomes (lower)higher and the condensate value gets (larger)smaller with (decreasing)increasing the massive gravity couplings or increasing the mass of graviton with the sufficiently (negative)positive massive gravity couplings. This fact corresponds to that the superconductor phase is (more)less thermodynamically favored.

Presenter: Cao Hoang Nam

O.6 – Oral, VCTP-45

Effect of Dielectric Constant Mismatch on Plasmons in Cylindrical Semiconductor Quantum Wires

Nguyen Nhu Dat

Institute of Theoretical and Applied Research, Duy Tan University

The dielectric response function of the electron system in a cylindrical semiconductor quantum wire is derived within the random phase approximation by using the linear response theory in the quantum limit when the only lowest electron subband is assumed to be occupied. The plasmon dispersion is obtained as a root of the dielectric function in which the mismatch of dielectric constants of the wire material and the barrier one is taken into account.

Presenter: Nguyen Nhu Dat

O.7 – Oral, VCTP-45

Defects Studies in beta-Ga2O3 Using an Optimized Hybrid Functional

Quoc Duy Ho

Can Tho University of Technology

Monoclinic gallium oxide (beta-Ga2O3) has recently attracted a lot of attention due to its unique properties. Beta-Ga2O3 is a wide band gap semiconductor, a lot of deep defect levels can be present in the gap state. Although, recently, on beta-Ga2O3 more scientific results have been published, due to the appearance of new experimental technologies, there is still little known about beta-Ga2O3. Density functional theory (DFT) with hybrid exchange, so-called hybrid functional (HSE), with two parameters (α and μ) can be tuned to reproduce the experimental band gap and fulfill the generalized Koopman's theorem. Peter Deak, Quoc Duy Ho et al. [Phys.Rev. B 95, 075208 (2017)] has tuned both α and μ and found that the hybrid functional with the parameters $\alpha = 0.26$ and $\mu = 0.00$ is the optimal HSE for beta-Ga2O3 defects studies. This optimized hybrid functional, HSE(0.26,0.00), satisfies the generalized Koopman's theorem and can reproduce the whole GW band structure accurately. In this research, HSE(0.26,0.00) is utilized to study transition levels, origins of luminescence and hyperfine interaction of defects in beta-Ga2O3.

Presenter: Ho Quoc Duy

O.8 – Oral, VCTP-45

Active matter in a viscoelastic environment

Emmanuel Lance Christopher VI M. Plan (1), Julia M. Yeomans (2), Amin Doostmohammadi (3)

(1) Institute of Theoretical and Applied Research, Duy Tan University, Hanoi 100000, Viet Nam, (2) The Rudolf Peierls Centre for Theoretical Physics, Department of Physics, University of Oxford, Clarendon Laboratory, Oxford OX1 3PU, United Kingdom (3) The Niels Bohr Institute, University of Copenhagen, Blegdamsvej 17, 2100 Copenhagen, Denmark

Active matter systems such as eukaryotic cells and bacteria continuously transform chemical energy to motion. Hence living systems exert active stresses on the complex environments in which they reside. One recurring aspect of this complexity is the viscoelasticity of the medium surrounding living systems: bacteria secrete their own viscoelastic extracellular matrix, and cells constantly deform, proliferate, and self-propel within viscoelastic networks of collagen. It is therefore imperative to understand how active matter modifies, and gets modified by, viscoelastic fluids. Here we present a two-phase model of active nematic matter that dynamically interacts with a passive viscoelastic polymeric phase and perform numerical simulations in two dimensions to illustrate its applicability. Motivated by recent experiments we first study the suppression of cell division by a viscoelastic medium surrounding the cell. We further show that the self-propulsion of a model keratocyte cell is modified by the polymer relaxation of the surrounding viscoelastic fluid in a nonuniform manner and find that increasing polymer viscosity effectively suppresses the cell motility. Last, we explore the hampering impact of the viscoelastic medium on the generic hydrodynamic instabilities of active nematics by simulating the dynamics of an active stripe within a polymeric fluid. The model presented here can provide a framework for investigating more complex dynamics such as the interaction of multicellular growing systems with viscoelastic environments.

Presenter: Emmanuel Lance Christopher VI M. Plan

O.9 – Oral, VCTP-45

hTSPO monomeric structural model in complex with the PK11195 ligand studied by molecular dynamics simulations

*Hien T. T. Lai (1), Giulia Rossetti (2,3,4), Alejandro Giorgetti (2, 5), Paolo Carloni (2, 6), Toan T. Nguyen (1, *), Agata Kranjc (2, *),*

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The translocator protein 18kDa (TSPO) normally present in mitochondria in all human tissues was found to be overexpressed in cancer and at the sites of neuroinflammation processes in cerebral ischemia, Alzheimer 's, Parkinson's and Huntington's diseases and multiple sclerosis. Due to the up-regulated expression it represents an important biomarker to identify the location of neuronal damage and tumor tissue development. The TSPO radiolabeled ligands are used in positron emission tomography (PET) for imaging of inflammatory sites. One of the most commonly used TSPO ligands for studying diagnostics and therapeutics is the 1-(2-chlorophenyl)-N-methyl-N-(1-methylpropyl)-3-isoquinolinecarboxamide (PK11195) ligand. Despite large number of studies the cellular role of the TSPO is not yet clear and many questions about its structure-function relationships persist. We have built the human TSPO (hTSPO) structural model, since its 3D structure is unknown. With the MD simulations we studied its structural properties in the apo form and when it is in complex with the PK11195 ligand. Our results are in line with the experimental studies: the PK11195 ligand stabilizes the TSPO fold, the most possible way for PK11195 ligand binding is through the membrane and between the TSPO transmembrane helices I and II. We discuss about the interactions between the PK11195 and the hTSPO structural model. Our results add to the knowledge about the structural properties of the TSPO protein and can be of help in search for new diagnostic or therapeutic ligands.

Presenter: Lai Thi Thu Hien

O.10 – Oral, VCTP-45

Real-approach for the electronic calculation of twisted bilayer graphene: The neutrino oscillation-like dynamics of electrons

Van-Nam Do

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Stacking two-dimensional materials is a novel method based on the lego principle for creating new van der Waals heterostructures with well-controlled properties. However, it usually results in a system of reduced symmetry compared to the two constituent lattices. As the translational symmetry of the hetero-lattices is broken, the electronic calculations based on the time-independent Schrodinger/Kohn-Sham equation combined withh the Bloch theorem are no longer applicable. In this talk, I will show that methods based on the time-dependent Schrodinger equation in real space are a powerful alternative to treat the problem. Applied to the case of twisted bilayer graphene I will show the dynamics of electrons in the real lattice of generic configurations using the tight-binding description. I will show that the interlayer electronic coupling induces the interchange transfer of waves between the two graphene layers, resulting a picture similar to that

of neutrino oscillations.

Presenter: Do Van-Nam

O.11 – Oral, VCTP-45

The correlation between transition of the energy bands and the optical absorption spectrum in bilayer armchair graphene nanoribbons

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In this work, we investigated the effect of external electric fields including a transverse electric field generated by side gates and a vertical electric field generated by top/back gates on the optical absorption spectra of AB-stacked bilayer armchair graphene nanoribbons (BAGNRs). By using a tight-binding model in combination with the gradient approximation, we first studied the energy band and the density of states (DOS), then absorption spectra A(ω). Our results demonstrated that (i) the low-frequency optical absorption spectra displays rich peaks and they vanish at $\omega = 0$; (ii) the number of the absorption peaks, the frequency and the intensity of peaks are strongly associated with the ribbon width and the magnitude of the electric fields. With the wider ribbon width M, more the absorption peaks are created and the lower threshold absorption frequency is observed. More importantly, unlike in the case without electric fields, the AB-stacked systems in the presence of a modulated electric field have lower threshold absorption frequency, more absorption peaks, and weaker spectral intensity; (iii) In semi-metallic structures, vertical fields impact more effectively than transverse fields in terms of opening larger band gap by analyzing the change of frequency of the first peak in the absorption spectrum. (iv) When the increase of electric field, the prominent peaks of the edge-dependent selection rules are lowered, and the sub-peaks satisfying the extra selection rules come to exist. With the obtained results, we expect to contribute to a more comprehensive understanding of the optical properties as well as the electronic structure of BAGNRs. Furthermore, the modulation of the band gap can lead to many interesting and attractive properties to bilayer graphene, that could be applied for various electronic and optical-electronic device applications.

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Presenter: Phan Dang Thao Nguyen

O.12 – Oral, VCTP-45

Adsorption of Toxic Gases on Pristine Graphene, Graphene/h-BN and Graphene/α-SiO2 Heterostructures: Density Functional Theory Calculations

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In this study, the adsorption properties of five toxic gases in the atmosphere CO2, CO, NH3,

NO, NO2 onto the surface of pristine graphene and graphene on substrates of h-BN and α-SiO2 are studied systematically using the density functional theory (DFT). All considered gases are physically adsorbed on graphene-based surface. With reference to the adsorption characteristics and electronic properties of considered toxic gases on different substrates, α-SiO2 has been predicted as the good substrate to enhance the selectivity for NO, NO2 gas sensing compared to h-BN substrate. The band structures and density of states (DOS) analysis results show that the interaction between h-BN and alpha-SiO2 with π and π^* states of the C atoms in graphene breaks the symmetry of graphene and small band gap occurs at the Dirac cone. New bands originating from different substrates modify the band structure of pristine graphene and open a band gap of 0.05 eV in Graphene/h-BN and 1.75 eV in Graphene /α-SiO2, respectively. These changes in band gap from zero in pristine graphene to 1.75 eV in Graphene/α-SiO2 suggests the potential use of Graphene/α-SiO2 for gas sensing applications. During adsorption, the considered toxic gases CO2, CO, NH3, NO, NO2 cause a change in the electronic structure of graphene. By DOS analysis of adsorption systems, we found that the highest occupied molecular orbitals (HOMO) of these gas molecules shift backward the Fermi level, suggesting the charge donation tendency of gas molecules to the graphene on substrates. The enhancement of sensitivity and selectivity of graphene-based gas sensing materials by introducing different substrates as h-BN or α-SiO2 are discussed in detail..

Presenter: Phung T. V. Bac

O.13 – Oral, VCTP-45

A fully microscopic model of total level density in spherical nuclei: an example of ^{60}Ni nucleus

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A fully microscopic model for the description of nuclear level density (NLD) in spherical nuclei is proposed. The model is derived by combining the partition function of the exact pairing solution plus the independent-particle model at finite temperature (EP+IPM) [1] with that obtained by using the collective vibrational states calculated from the self-consistent Hartree-Fock mean field with MSk3 interaction plus the exact pairing and random-phase approximation (SC-HFEPRPA) [2]. For the first time, two important factors are taken into account in a fully microscopic way, namely the spin cut-off and vibrational enhancement factors are, respectively, calculated using the statistical thermodynamics and partition function of the SC-HFEPRPA without any fitting parameters. The numerical test for a spherical ^{60}Ni nucleus, the only nucleus whose experimental NLD data are presently available from 0 to about 23 MeV of excitation energy, shows that the collective vibrational enhancement is mostly dominated by the quadrupole and octupole excitations. This is the first microscopic model confirming such an effect, which was phenomenologically predicted long time ago and widely employed in several NLD models. In addition, the influence of collective vibrational enhancement on nuclear thermodynamic quantities such as excitation energy, specific heat capacity and entropy is also studied by using the proposed model [3].

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Presenter: Nguyễn Quang Hưng

O.14 – Oral, VCTP-45

Role of pairing correlation in the radiative strength function

L. Tan Phuc (1), N. Quang Hung (1), N. Dinh Dang (2), L. T. Quynh Huong (3), N. Ngoc Anh (4), N. Ngoc Duy (5), L. Ngoc Uyen (6), and N. Nhu Le (7)

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The enhancement of radiative strength function (RSF) in the region of low γ-rays energy (E$\gamma \leq$ 12 MeV), which is caused by the pygmy dipole resonance (PDR), is treated within the phonon damping model (PDM) plus exact pairing (EP) at finite temperature without adding any extra PDR fitting peak. The numerical calculations performed for 161-163 Dy show that, because of the effect of exact thermal pairing, the EP+PDM can describe reasonably well the total RSF data in both low- and high-energy regions of γ-rays. Consequently, as compared to the conventional description within the phenomenological generalized Lorentzian (GLO) and standard Lorentzian (SLO) models, the EP+PDM calculations are free from at least six free parameters. This indicates the important role of microscopic approaches towards the precise prediction of the RSF. In particular, temperature is found to have significant contributions to the RSF below the neutron separation energy, questioning again the validity of the Brink-Axel hypothesis

Presenter: Le Tan Phuc

O.15 – Oral, VCTP-45

Morpho-kinematics of the molecular gas in a quasar host galaxy at redshift z=0.654

T. T. Thai (1), P. Tuan-Anh (1), P. Darriulat (1), D. T. Hoai (1), P. T. Nhung (1), P. N. Diep (1), N. T. Phuong (1)

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We present a new study of archival ALMA observations of the CO(2-1) line emission of the host galaxy of quasar RX J1131. The quasar, at redshift $z_s \sim 0.654$, is lensed by a foreground galaxy at $z_L \sim 0.30$. Particular attention is paid to the mechanism of gravitational lensing. A simple lens model, shown to well reproduce the optical images obtained by the Hubble Space Telescope, is applied to the ALMA CO(2-1)images, providing a tool to understand the uncertainties attached to the evaluation of the source brightness and kinematics. Uncertainties attached to the process of data reduction are carefully evaluated. Evidence for the robustness of previously published results is obtained. A system of polar coordinates is introduced to better match the specificity

of the imaging process. It provides particularly clear evidence for rotation of the gas contained in the galaxy. A simple rotating disc model is shown to give an excellent overall description of the morpho-kinematics of the source. It gives evidence for a hot spot of emission located near the quasar, overlapping the caustic and corresponding to an enhancement of emission by a factor ∼2.5. The possible presence of a companion galaxy suggested by some previous authors is not confirmed. The rotation curve is studied with reference to the predictions of the disc model. Detailed comparison between model and observations gives evidence for a more complex dynamics than implied by the model. Doppler velocity dispersion within the beam size in the image plane is found to contribute ∼60 km/s to the line width. It accounts for the observed line width when a 2-sigma cut is applied to the data. However, when using a less severe cut, a significant amount of turbulence may be accommodated, preventing a reliable evaluation of the contribution of turbulence to the line width.

Presenter: Tran Thi Thai

O.16 – Oral, VCTP-45

Fano effect caused by the pairing on neutron-nucleus elastic scattering

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The Fano effect has been known as the quantum interference effect caused by the correlation between continuum and a sharp resonance or bound state [1]. In quantum physics, there are many examples of the Fano effect such as Raman scattering [2,3], photoelectric emission [4], photoionization [5] etc. Very recently, we have succeeded to derive the Fano resonance parameters for the neutron elastic scattering off the open-shell nucleus with the help of the HFB Jost function formalism [6,7]. This is the first derivation of the Fano parameters as the effect of the pairing correlation in quantum physics. We will introduce the derivation of the Fano parameters and the results of analysis at the conference.

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Presenter: Kazuhito Mizuyama

O.17 – Oral, VCTP-45

Vector boson scattering to diphoton at the LHC

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Diphoton production via vector boson scattering at the LHC is sensitive to electroweak quartic gauge boson couplings. In this talk we discuss the effects of next-to-leading order QCD

corrections to this process in the Standard Model. The QCD-induced background process will also be considered. Finally, we include the effects of anomalous gauge couplings coming from dimension-8 operators using an effective-field theory approach.

Presenter: Le Duc Ninh

O.18 – Oral, VCTP-45

Probing atmospheric electric fields under thunderstorm conditions by using radio emission from extensive air showers

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Energetic cosmic rays impinging on the atmosphere create a particle avalanche called an extensive air shower. In the leading plasma of this shower electric currents are induced that generate radio waves. During thunderstorms, radio emission from extensive air showers are influenced by atmospheric electric fields. These effects are observed at LOw Frequency ARray (LOFAR) radio telescope. We observe large differences in the intensity and polarization patterns of showers measured during thunderstorm conditions from the ones measured during fair-weather conditions. Thus, radio emission from air showers can be used as a tool to determine atmospheric electric fields. We show that the atmospheric electric fields are usually composed out of three layers. The height of the bottom layer near the ground depends on the seasons and large horizontal electric fields are observed.

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Presenter: Trinh Thi Ngoc Gia

O.19 – Oral, VCTP-45

Effects of velocity-dependent and spin-orbit term of Skyrme interaction on neutron elastic scattering observables

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Elastic scattering of a series of doubly closed-shell nuclei at low-energy has been described in the

framework of the optical potential model generated from the particle-vibration coupling (PVC) approach on top of the collective excited states obtained from the random phase approximation (RPA). We focus on the effects of the spin-orbit and velocity-dependent interaction on the angular distributions and analyzing powers by comparing these observables with experimental data. It has been found that the contribution of the two-body velocity-dependent and two-body spin-orbit terms are important to improve results for 16O, 40Ca, 48Ca, and 208Pb. The velocity-dependent interactions strongly reduce the absorption on the surface while the spin-orbit interactions sightly increase the absorption in the interior [1].

[1] N. Hoang Tung, D. Quang Tam, Vinh N. T. Pham, Chi Lam Truong, and T. V. Nhan Hao, Effects of velocity-dependent and spin-orbit term of Skyrme interaction on neutron elastic scattering observables, Physical Review C, accepted, (2020).

Presenter: Trần Viết Nhân Hào

O.20 – Oral, VCTP-45

Experimental study on the nuclear level scheme in Vietnam: examples of ^{153}Sm and ^{172}Yb

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Experimental study on the nuclear level scheme (NLS) at the Dalat Nuclear Research Institute (DNRI), Vietnam, is presented. Within the study, a NLS is constructed based on experimental two-step gamma cascades obtained from the (n,γ) reaction using a $\gamma - \gamma$ coincidence spectrometer, namely the (n,2γ) experiment. The neutron beam, whose flux is 1.7×10^5 n.cm^{-2} s^{-1}, is extracted from the Dalat Nuclear Research Reactor. Whereas, the coincidence spectrometer is self-installed [1]. The (n,2γ) experiment allows to achieve low Compton background spectra and to identify the correlated gamma transitions. The NLSs obtained for ^{153}Sm and ^{172}Yb reproduced a significant part of those extracted from the Evaluated Nuclear Structure Data File (ENSDF). Based on the comparison with the ENSDF library, we have deduced 18 excited levels and 126 gamma transitions of the NLS of ^{172}Yb, as well as 61 excited levels and 365 gamma transitions of the NLS of ^{153}Sm, as the new data [2,3]. In addition, in the case of ^{153}Sm, we have extended the maximum excitation energy, defined as the energy threshold below which most of the excited levels are observed, to about 1.2 and 1.8 MeV for the total and partial (for the spin range of [1/2, 3/2]$\hbar$) NLSs, respectively. This achievement permit to evaluate the predictive power of various phenomenological and microscopic nuclear level density models for ^{153}Sm. It turns out that the exact paring plus independent-particle model [4] is the best-fit one. Moreover, preliminarily result on the extraction of radiative strength function from the two-step gamma cascade intensity distribution is also shown.

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Presenter: Nguyen Ngoc Anh

O.21 – Oral, VCTP-45

Interaction-free measurement in IBM quantum computers

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(1) Nano and Energy Center, Hanoi University of Science, Vietnam National University, Hanoi; (2) Phenikaa Institute for Advanced Study, Phenikaa University

Interaction-free measurement is a type of quantum measurement that detects the state of an object without an interaction occurring between the object and the measuring device. A scheme for interaction-free measurement was proposed by Elitzur and Vaidman called Elitzur-Vaidman bomb tester where they used a Mach-Zehnder interferometer to detect whether a bomb is alive or dead. In 1992, Lucien Hardy proposed an experiment that a particle and its antiparticle may interact without annihilating each other which called Hardy's paradox. In this work, we demonstrate the above experiments using quantum computing, which are realized in IBM quantum computers.

Presenter: Tran Minh Duc

O.22 – Oral, VCTP-45

Wavelength dependence of high-order harmonic yields of Rydberg atom

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Currently, high-order harmonic generation (HHG), emitted by the atom/molecule-laser interaction, has been considered as the unique source for producing attosecond pulse, which is an effective tool for probing the ultrafast motion [1]. Thus, it is necessary to enhance HHG energy. One of the methods is using a laser with a long wavelength [2]. However, it leads to rapidly reduce the HHG efficiency with the universal scaling law λ^{-5}–λ^{-6} with the wavelength λ [2]. Therefore, many efforts focus on trying to slow down the wavelength scaling law [3]. Adopting Rydberg atom, i.e. an atom in the coherent superposition state, can lead to a slow scaling law $\sim \lambda^{-2.8}$ [3]. This result is interesting and should be further investigated in detail. In this report, we theoretically study the structure of the wavelength scaling law of HHG from an Rydberg atom. We found out that the scaling law of the Rydberg atom strongly oscillates with the wavelength. In addition, the oscillation depends on the frequency window to synthesis HHG yields, and also on the laser CEP. We attribute this property to the multi-node of the density population of the electron in the Rydberg state.

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Presenter: Phan Ngoc-Loan

O.23 – Oral, VCTP-45

Density of condensates of two-component Bose-Einstein condensates restricted between two planar walls

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The density of condensates of a binary mixture of Bose gases restricted by two parallel planar walls is investigated within the framework of Cornwal-Jackiw-Tomboulis effective action approach in improved Hartree-Fock approximation. It results that the density of condensates strongly depend not only on the distance between two walls but also on the interspecies interaction strength and they are equal their expectation values of the field operators after adding a term associated with the quantum fluctuations.

Presenter: Song Thế Phạm

O.24 – Oral, VCTP-45

Band Dispersion and Exciton Creation and Annihilation under Isotropic Strain in Monolayer WS2

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We present a density functionals study of the mechanism of creation and annihilation of excitons under strain in the monolayer WS2. With taking into account the influence of spin-orbit coupling (SOC) and van der Waals interaction by using optB86b-vdW functional, we investigate the vertical shift and displacement of the d and s partial orbitals of the W and S atoms, respectively, and the appearance of flattening valley, leading to the creation and decay of excitons under the isotropic strain in monolayer WS2. The crucial findings of this work are: (a) Based on the partial projected band structure, we explain the transition mechanism from the K-K direct to the K-Q and Γ-K indirect band gap under the isotropic compressive and tensile strained WS2 monolayer, respectively. Therewith, the notably decreased band gap is due to the occurrence of two phenomena, the vertical shifted valley and the flattened valley, in the partial projected band structure. Also due to these two phenomena, the carrier mobility at symmetrical points in the first Brillouin zone (BZ) is enhanced or reduced, and thus its applications as channel materials or high performance electronic devices can be exploited; (b) Thanks to the spin splitting with SOC effect, light and dark excitons are visually shown in the band structure, especially the exciton creation and annihilation with the isotropic strained WS2 monolayer, opening a possible path to manipulate excitons using strain scheme.

Presenter: Lương Thị Thêu

O.25 – Oral, VCTP-45

DFT study of water monomer adsorption on Nitrogen and Boron doped graphene

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Understanding the interaction between water and graphene is crucial for numerous practical applications of graphene such as water purification, desalination, and electrocatalysis. Herein, we provide the atomistic understanding of interfacial interactions of H2O/graphene by addressing the adsorption of a single water monomer on the pristine graphene, and Nitrogen-, and Boron-doped graphene using self-consistent van der Waals Density Functional (vdW-DF) method. The water monomer adsorption on the pristine graphene is revisited by using several vdW-DFs and vdW dispersion corrections, in which our results are consistent with quantum chemistry calculations. We find that by replacing C atoms of graphene with N or B atoms, interactions between water and the doped graphene surfaces are enhanced, but the water monomer is still physisorbed on the doped graphene. Unlike an independent orientation of water monomer on the pristine graphene, water is found to be preferable to adsorb on N-, and B- doped graphene with on-site O-down, and H-down geometries, respectively. The electronic structure is analyzed in detail. The increase in adsorption strength and the change in adsorbed geometries indicate that the wettability of graphene can be tailored by the chemical doping. Acknowledgement: This research was funded by Vietnam National University in Ho Chi Minh City under grant number C2020-20-39.

Presenter: Ngoc Son Do

P.1 – Poster, VCTP-45

Fast Estimation of the Blood-Brain Barrier Permeability by Pulling a Ligand through a Lipid Membrane

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The blood-brain barrier (BBB) is the physical barrier that regulates the homeostasis of the neural microenvironment. A relative estimate of the BBB permeability, which is important for drug design, may be experimentally provided by the logBB (the blood – brain concentration ratio) and the logPS (permeability – surface-area product), while many computational methods aim to identify key properties that correlate well with these quantities. Here, we use steered molecular dynamics simulation to estimate the BBB permeability of various compounds on the basis of simple lipid-membrane models by computing the nonequilibrium work, W_{neq}, produced by pulling the compounds through the membrane. We found that the values of W_{neq} correlate remarkably well with logBB and logPS for a range of compounds and pulling speeds. Moreover, our results provide insight into the role of hydrogen bonds, the energetic barriers on the ligands during their pulling. Our method is computationally easy to implement and fast. Therefore, we anticipate that it could provide a reliable pre-screening tool for estimating the relative permeability of the BBB to various substances.

Presenter: Nguyen Quoc Thai

P.2 – Poster, VCTP-45

Competition between heating and cooling effects on an optomechanical oscillator by a squeezed light

Vinh N.T. Pham (1), Chu Manh Hoang (2), Le Tri Dat (3,4), Tran Duong Anh Tai (1), and Nguyen Duy Vy (3,4,)*

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Squeezed light is a useful phenomenon that can be exploited to improve the sensitivity of specific classes of detectors based on optomechanical effects. In this work, we clarified the effect of the squeezed light by explicitly presenting the role of squeezing parameters on the final effective temperature and effective quantum number of the oscillator. The results show that the cooling and heating effects are strongly dependent on the squeezing parameter and phase. The lowest effective temperature and quantum number of three orders of magnitude smaller than that in the case of no squeezing can be obtained. The study gives important information for optimizing the cooling efficiency with squeezed light.

Presenter: Nguyen Duy Vy

P.3 – Poster, VCTP-45

Exact mode shapes of T-shaped and overhang-shaped microcantilevers

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Micro-mechanical systems have been widely used in vibration transducing, energy harvesting, and highly sensitive measurement. Observing a change of resonance frequencies or mode shapes of a microcantilever can reveal the physical or chemical properties of an object when it is adsorbed on the cantilever surface. The commonly used structure of the cantilever is a rectangular-shaped beam; however; the T-shaped and overhang-shaped structures have recently attracted many researchers due to their wide application. Nevertheless, obtaining the frequency of the cantilever is challenging from the analytical viewpoint. In this work, we figured out the exact modes for T-shaped and overhang-shaped cantilevers. The obtained mode shapes show significant deviations comparing to the approximate forms of a rectangular cantilever. Moreover, based on these exact solutions, the frequencies of microcantilevers with these complicated dimensions were revealed.

Presenter: Le Tri Dat

P.4 – Poster, VCTP-45

Interfacial characteristics, Schottky contact and optical performance of Graphene/Ga2SSe van der Waals heterostructure: Strain engineering and electric field tunable

Le M. Duc (1), Vo T. T. Vi (2), Nguyen V. Hieu (3), Nguyen N. Hieu (4), Chuong V. Nguyen (1)

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Vietnam (3) University of Education, The University of Da Nang, Da Nang, Vietnam (4) Duy Tan University, Danang, Vietnam

Two-dimensional graphene-based van der Waals heterostructures have received considerable interests because of their intriguing characteristics as compared with the constituent single-layered two-dimensional materials. Here, we investigate the interfacial characteristics, Schottky contact and optical performance of Graphene/Ga2SSe van der Waals heterostructure using first principles calculations. The effects of stacking patterns, electric gating and interlayer coupling on the interfacial properties of graphene/Ga2SSe heterostructures are also examined. Our results demonstrate that the Dirac cone of graphene is well preserved at the Γ point in all stacking patterns due to the weak vdW interactions, which keep the heterostructures feasible such that they can be obtained in further experiments. Moreover, depending on the stacking patterns, a small band gap of about (13 - 17) meV opens in graphene and has a high carrier mobility, indicating that the graphene/Ga2SSe heterostructures are potential candidates for future high-speed nanoelectronic applications. In the ground state, the graphene/Ga2SSe heterostructures form an n-type Schottky contact. The transformation from n-type to p-type Schottky contact or to Ohmic contact can be forced by eletric gating or by varying the interlayer coupling. Our findings could provide physical guidance for designing controllable Schottky nanodevices with high electronic and optical performances.

Presenter: Nguyen V. Chuong

P.5 – Poster, VCTP-45

Chaoticity and mixing in a dilute suspension of rods

Lance Christopher VI M. Plan (1), Stefano Musacchio (2), Dario Vincenzi (2), and Massimo Cencini (3)

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It has been previously shown (Groisman and Steinberg, Nature, 2000) that the a dilute amount of extensible polymers at low Reynolds number create the so-called elastic turbulence, a chaotic regime that has characteristics reminiscent of hydrodynamic turbulence, albeit smoother. Here we show that the rotational dynamics of microscopic rods in a viscous fluid at low Reynolds number causes a significant increase of the flow resistance and can likewise generate a turbulent-like behaviour. Numerical simulations of the dynamics of the solution reveal that this phenomenon is associated to a transition from laminar to chaotic flow. Polymer stresses give rise to flow instabilities which, in turn, perturb the alignment of the rods. This coupled dynamics results in the activation of a wide range of scales. The temporal decay of the variance of the scalar field and its gradients shows that this chaotic flow strongly enhances mixing.

Presenter: Emmanuel Lance Christopher VI M. Plan

P.6 – Poster, VCTP-45

Gas adsorption on Sc2CO2 monolayer from first-principles calculations

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By first principle calculations, we systematically studied the adsorption properties of different gases (H2, N2, CO2, O2, SO2, CO, NO, NO2) on monolayer Sc2CO2. The preferred adsorption site for each gas are identified. To determine the adsorption mechanism, properties such as the structural characteristics, adsorption distance, absorption energy, amount of charge transferred between gas molecules and Sc2CO2 monolayer were calculated. Our calculations show that CO2, CO, N2 and H2 molecules are physically adsorbed on the Sc2CO2 monolayer, while O2, NO, SO2 and NO2 molecules are chemically adsorbed. The assessment of the adsorption energy and the charge transfer between the monolayer and the gas molecule show that the selectivity in the adsorbed gas belongs to NO2 and O2 molecules. The chemical adsorption of O2 molecule on the Sc2CO2 monolayer changes the electronic properties of this monolayer and this makes the electronic properties of the Sc2CO2 monolayer difficult to control in the air. In our opinion, this will limit the prospect of monolayer application Sc2CO2 in gas sensors or toxic gas capture devices.

Presenter: Phạm Dinh Khang

P.7 – Poster, VCTP-45

Multicomponent dark matter in noncommutative B-L gauge theory

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A higher weak isospin symmetry, $SU(P)_L$ with $P \geq 3$, the baryon minus lepton charge $B - L$ neither commutes nor closes algebraically with $SU(P)_L$ similar to the electric charge Q, which all lead to a $SU(3)_C \otimes SU(P)_L \otimes U(1)_X \otimes U(1)_N$ gauge completion, where X and N determine Q and $B - L$, respectively. As a direct result, the neutrinos obtain appropriate masses via a canonical seesaw. While the version with $P = 3$ supplies the schemes of single-component dark matter well established in the literature, we prove in this work that the models with $P \geq 4$ provide the novel scenarios of multicomponent dark matter, which contain simultaneously at least $P - 2$ stable candidates, respectively. In this setup, the multicomponet dark matter is nontrivially unified with normal matter by gauge multiplets, and their stability is ensured by a residual gauge symmetry which is a remnant of the gauge symmetry after spontaneous symmetry breaking. The three versions with $P = 4$ according to the new lepton electric charges are detailedly investigated. The mass spectrum of the scalar sector is diagonalized when the scale of the $U(1)_N$ breaking is much higher than that of the usual 3-4-1 symmetry breaking. All the interactions of gauge bosons with fermions and scalars are obtained. We figure out viable parameter regimes given that the multicomponent dark matter satisfies the Planck and (in)direct detection experiments.

Presenter: Le Xuan Thuy

P.8 – Poster, VCTP-45

The influence of confined acoustic phonon on the quantum Peltier effect in

doped semiconductor superlattice in the presence of electromagnetic wave

Hung Le Thai (1), Quynh Nguyen Thi Lam (2), Anh Nguyen Thi Nguyet (2), Bau Nguyen Quang (2)

(1) VNU University of Education; (2) VNU University of Science

Based on the kinetic equation method, the quantum Peltier effect has been theoretically studied under the influence of confined acoustic phonon in doped semiconductor superlattice in the presence of the electromagnetic wave (laser radiation). There were complicated dependences of the analytical expression of the Peltier coefficient (PC) on quantities such as doped concentration of the superlattice, amplitude of the laser radiation, the cyclotron frequency of electrons and temperature of the system. In detailed consideration, the quantum number m was changed in order to characterize the influence of confined acoustic phonon. When setting the m to zero, we obtained the results that corresponded to the case of unconfined phonons. The theoretical results have been numerically evaluated and discussed for the GaAs:Si/GaAS:Be doped semiconductor superlattice (DSS). We found the oscillation of the PC according to enhancement of cyclotron frequency of electrons. Moreover, position of resonant peaks has shifted under the influence of phonons confinement. In the case of low doped concentration (nD), the PC decreased in non-linear way; then it reached a negative constant in high nD value. The non-linear change of the PC also has been detected when investigating its dependence on the laser amplitude. All numerical results have shown that the magnitude of the PC decreased due to the increase of phonon confinement effect. In short, the confinement of acoustic phonons caused the change of the quantum Peltier effect in DSS of GaAs:Si/GaAS:Be in quantitatively as well as qualitatively.

Presenter: Nguyễn Thị Lâm Quỳnh

P.9 – Poster, VCTP-45

The melting curve of gold up to 500 kbar

Pham Duy Tan (1), Pham Dinh Tam (2)

(1) Research Department, Tank Armour Command; (2) Le Quy Don Technical University

The melting temperature Tm of gold has been determined from ambient pressure to 500 kbar using the statistical moment method (SMM) and the Lindemann criterion. The equation of the melting curve obtained is a quadratic polynomial of the melting temperature Tm with coefficients that are explicitly dependent on pressure P. Number calculation is simple and easily verify. Numerical results for the melting temperature of gold up to 500 kbar are in good agreement with the experimental data.

Presenter: Phạm Duy Tân

P.10 – Poster, VCTP-45

Thermodynamic properties of Cu3Au alloy

Pham Duy Tan (1), Pham Dinh Tam (2)

(1) Research Department, Tank Armour Command; (2) Le Quy Don Technical University

Based on the general expression of the Helmholtz free energy of alloys with L12 structure obtained in previous works, we calculate the equations of the long-range order (LRO) parameter, and order-disorder transition(ODT) temperature in the Cu3Au alloy, and obtained thermodynamic quantities of Cu3Au alloy as simple functions of temperature and LRO-parameter, at pressures P = 0. Numerical results of the linear thermal expansion coefficient, isochoric and

isobaric heat capacities, isothermal and adiabatic bulk modulus are in good agreement with experiments.

Presenter: Phạm Duy Tân

P.11 – Poster, VCTP-45

Effects of hydrophobic and electrostatic interactions of the ribosomal exit tunnel on the escape and folding of nascent proteins

Phuong Thuy Bui (1) Trinh Xuan Hoang (2)

(1) Duy Tan University; (2) Institute of Physics, Vietnam Academy of Science and Technology

After the determination of ribosome structures, there has been increasing attention to understanding the role of the ribosomal exit tunnel in protein biosynthesis and folding inside cells. In recent works, we have shown that the exit tunnel, as a passive conduit with only excluded volume interaction, has a significant impact on the escape process and early post-translational folding of nascent proteins. In the present study, we continue to study the impact of the tunnel on the escape and folding processes by considering the effects of hydrophobic and electrostatic interactions between the tunnel and nascent chains. The study is carried out by using molecular dynamics simulation method with an atomistic model of the ribosome tunnel and a coarse-grained Go-like model for nascent proteins. We show that while the hydrophobic interaction slows down the protein escape process, the electrostatic interaction may speed it up depending on the net charge of a protein. Interestingly, like the escape time, the folding time at the tunnel also follows a proposed diffusion model of a drifting Brownian particle in a linear potential field, suggesting that the tunnel helps proteins to bypass a free energy barrier for folding which would exist without the tunnel.

Presenter: Bui Phuong Thuy

P.12 – Poster, VCTP-45

Structural and mechanical properties in densified (AlN)0.85(Si3N4)0.15 ceramics: A molecular dynamics simulation study

Nguyen Thi Thao (1), Dinh Thi Hinh (2), Nguyen Manh Hung (3), Nguyen Ba Phuong (4), Le Van Vinh (2)

(1) Hanoi National University of Education, (2) Phenikaa University, Hanoi, Vietnam, (3) Thuyloi University, (4) Institute of Materials Science

Molecular dynamics simulations have been carried out to investigate the microstructures and mechanical properties of densified (AlN)0.85(Si3N4)0.15 ceramics under uniaxial deformation. The samples with different densities were cooled down from 5000 K to 300 K. At the temperature of 300 K, these samples contain the poly-crystalline AlN embedded by the amorphous Si3N4. The poly-crystalline AlN contains major fcc-AlN and minor hcp-AlN. At the low density of sample, the amorphous Si3N4 contains major SiN3 units, but it contains major SiN4 units with the high density. The strengthening enhancement of the samples is observed with increasing density.

Presenter: Le Van Vinh

P.13 – Poster, VCTP-45

Investigation of S-shaped heat capacity in hot nuclei

Le Thi Quynh Huong (1), Nguyen Quang Hung (2)

(1) University of Khanh Hoa, (2) Institute of Fundamental and Applied Sciences, Duy Tan University

The clear S shape of the heat capacity is found around the critical temperature $T_c \sim 0.6-0.9$ MeV by using extrapolating the experimental level densities. Since the experimental data only covers the excitation energy up to 6.0–8.5 MeV, the back-shifted Fermi-gas model is used to extend the experimental level densities up to an excitation energy of ∼180 MeV. The characteristic feature of the heat capacities is known as a signature of the pairing transition and investigated in some hot nuclei.

Presenter: Le Thi Quynh Huong

P.14 – Poster, VCTP-45

The influence of confined acoustic phonon on the quantum Ettingshausen effect in cylindrical quantum wire with a infinite potential in presence of Strong electromagnetic Wave

Hoang Van Ngoc (1), Nguyen Thi Nguyet Anh (2), Tang Thi Dien (2), Nguyen Quang Bau (2), Nguyen Vu Nhan (3)

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Based on the kinetic equation method, the quantum Ettingshausen effect has been theoretically studied under the influence of confined acoustic phonon in cylindrical quantum wire with a infinite potential in presence of strong electromagnetic wave. We considered a quantum wire in the presence of constant electric field, magnetic field and electromagnetic wave (EMW) with assumption that electron – confined acoustic phonon (AP) scattering is essential. The EC obtained depends on many quantities in a complicated way such as temperature, magnetic field, frequency and amplitude of EMW, Cyclotron frequency, radius of cylindrical quantum wire and quantum numbers which specify confined AP. In detailed consideration,the quantum number m1, m2 were changed in order to characterize the influence of confined acoustic phonon.When setting the m1, m2 to zero, we obtained the results that corresponded to the case of unconfined phonons. The theoretical results have been numerically evaluated and discussed for the GaAs/GaAsAl quantum wire (CQW). The results show that phonon confinement has changed both the qualitative and quantitative Ettingshausen coefficients. The magnitude of the Ettingshausen coefficient increased many times, the position of the peak magnetic resonance changes and the peak number of magnetic resonances increases due to the size reduction effect. These results are new and different from bulk semiconductor and unconfined phonon.These findings have perfectly contributed to the theory of the Ettingshausen effect in low-dimensional semiconductor systems.

Presenter: Nguyễn Thị Nguyệt Ánh

P.15 – Poster, VCTP-45

Effect of ionic potential in a model of magnetic topological insulators

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Research on the effect of different factors such as energy level splitting, disorder, spin-orbit couplings (SOC), spin-exchange (SE) on topological and magnetic properties in topological insulators doped with magnetic impurities has gained much attention from physical scientists. In this report, we only focused attention on the effect of the sonic potential in the Kane-Mele model of magnetic topological insulators. The dynamical mean-field theory (DMFT) was employed to investigate the electron dynamics. Both magnetic long-range order and the topological invariants were calculated within the mean-field theory. From the investigated results, we analyzed the effects of the ionic potential on the topological and long-range ordering properties as well as on their phase transitions. The insulator states were observed at half-filling, quarter-filling, and three-quarter filling. At half-filling, an antiferromagnetic topological insulator, which exhibits the quantum spin Hall effect, exists in the phase region between the paramagnetic topological insulator and the trivially topological antiferromagnetic insulator, like in the without energy level splitting case. Especially, the emergence of new phases besides the observed states. In comparison with the without energy level splitting case, the phase diagram becomes very rich when the energy level splitting is present.

Presenter: Nguyễn Hồng Sơn

P.16 – Poster, VCTP-45

A DFT Study of Some VOCs Adsorption on the Pristine Graphene

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In this study, the adsorption properties of two volatile organic compounds (VOCs) - acetone (CH3)2CO and dicchlomethane CH2Cl2 - in human breath on the surface of pristine graphene are investigated using the density functional theory (DFT) method. The most favorable adsorption configurations of considered VOC molecules on the graphene surface are obtained first from scanning method [1], and then the adsorption energy profiles are calculated in framework of three van der Waals functionals: revPBE-vdW, optPBE-vdW, and vdW-DF2. All of these VOCs are found to orient parallel to the graphene surface at the distance of approximately 3.00 Å. We found that the highest occupied molecular orbitals (HOMO) of the considered VOCs shift backward the Fermi level during adsorption. The HOMO orbitals of VOCs interact with p orbitals of graphene's C and a tunneling band gap occurs at the Dirac cone. These results suggest the charge donation tendency of VOC molecules to graphene. Bader charge analysis shows that these VOCs act as donors on graphene and 0.03e and 0.075e of charge was transferred from dicchlomethane and acetone, respectively, to graphene surface. The larger charge transfer, the larger the change in electrical conductance, which indicates the stronger effect to the sensor response towards VOCs. Recommendations on the enhancement of the selectivity of graphene-based sensing materials have also been made by other methods such as introducing a vacancy or doping transition metal molecules on the graphene surface.

Reference: [1] Computational DFT-based Nanoscope developed by Van An Dinh, Vietnam Japan

University (2018).

Presenter: Phung T. V. Bac

P.17 – Poster, VCTP-45

Longitudinal excitations of the Heisenberg model: a functional integral approach

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We study the longitudinal excitations in the Heisenberg model by a functional integral approach. We represent the partition function of the quantum systems in terms of the functional integral over coherent Grassmann variables with Popov-Fedotov imaginary chemical for excluding non-physical states appeared due to transformations from spin operators to fermion ones. We go beyond the one-loop approximations taking into account coupling between transverse and longitudinal spin components. We compare our results with Xian's ones, obtained on analogue to Feynmann's theory on the low-lying excited states of the helium-4 superfluid (Y.Xian, Phys. Rev. B74 212401(2006)).

Presenter: Nguyen Van Hinh

P.18 – Poster, VCTP-45

Molecular dynamics simulation of the structure and mechanical properties of CuNi alloy

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The structure and mechanical properties of Cu80Ni20 alloy with the size of 8788 atoms have been investigated by means of molecular dynamic (MD) simulation. The interactions between atoms of the system were calculated by Quantum Sutton-Chen type of embedded atom method. Using cooling rate of 0.01 K/ps, we find that both Ni and Cu atoms are crystallized into face centered cubic (fcc) and the hexagonal close packed (hcp) phases when the sample was cooled down to 300K at the pressure of 45 GPa. The transformation to crystalline phase is analyzed through the dependence on temperature of potential energy; the radial distribution function, the Common Neighbor Analysis (CNA) methods and the visualization. Furthermore, we focus on the study of mechanical properties of Cu80Ni20 alloy.

Presenter: Nguyen Thi Thao

P.19 – Poster, VCTP-45

Study on anharmonic effects in the material with the cubic crystal structure by an analytic statistical moment method.

Cao Huy Phuong

Hung Vuong University

Vibrations of atoms or ions around the lattice points are inhamonic that cause the thermodynamic effects for the materials with the crystal structure. Using the moment statistical method in the statistical physics, within the fourth order moment approximation, we have found out that the change of the length, volume and shape of the material with the cubic crystal structure are determined by the anharmonic effect. Increasing temperature leads to the more strong anharmonic lattice vibrations that cause changing size of the material.

Presenter: Cao Huy Phương

P.20 – Poster, VCTP-45

Investigate the recollision dynamics in the nonsequential double ionization induced by an orthogonal two-color laser field

Thu D. H. Truong (1), Hanh H. Nguyen (1), Thang N. Tran (1), Giau N. Ngoc (1), Vinh N. T. Pham (1)

(1) Ho Chi Minh City University of Education

In this study, we comprehensively investigate the essential quantities associated with the returning electron as the relative phase of the laser field changes. The results indicate that these characteristics, such as the returning moment, returning energy, and energy sharing ratio, strongly depend on the relative phase of the orthogonal two-color laser field. Thus the mechanism governing the nonsequential double ionization process can be controlled by tuning the relative phase.

Presenter: Pham Nguyen Thanh Vinh

P.21 – Poster, VCTP-45

Derivation of the magnetic induction vector for a rectangular permanent magnet

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(1) Ho Chi Minh City University of Education

In this work, a rigorously analytical procedure is proposed to deduce the scalar potential of a rectangular permanent magnet oriented along the Oz axis, at any arbitrary position in space. The negative of divergence of the scalar potential provides the exact expression for the magnetic induction. The accuracy of the analytical formula is validated by numerical calculation.

Presenter: Pham Nguyen Thanh Vinh

P.22 – Poster, VCTP-45

Impact of magnetic dopants on magnetic and topological phases in magnetic topological insulators

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A topological insulator doped with random magnetic impurities is studied. The system is mod-

elled by the Kane-Mele model with a random spin exchange between conduction electrons and magnetic dopants. The dynamical mean field theory for disordered systems is used to investigate the electron dynamics. The magnetic long-range order and the topological invariant are calculated within the mean field theory. They reveal a rich phase diagram, where different magnetic long-range orders such as antiferromagnetic or ferromagnetic one can exist in the metallic or insulating phases, depending on electron and magnetic impurity fillings. It is found that insulator only occurs at electron half filling, quarter filling and when electron filling is equal to magnetic impurity filling. However, non-trivial topology is observed only in half-filling antiferromagnetic insulator and quarter-filling ferromagnetic insulator. At electron half filling, the spin Hall conductance is quantized and it is robust against magnetic doping, while at electron quarter filling, magnetic dopants drive the ferromagnetic topological insulator to ferromagnetic metal. The quantum anomalous Hall effect is observed only at electron quarter filling and dense magnetic doping.

Presenter: Trần Minh Tiến

P.23 – Poster, VCTP-45

Surface plasmon resonance of plasmonic polymers

Do Thi Nga (1), Do Chi Nghia (2), Vu Thi Thuy Duong (3)

(1) Institute of Physics, VAST; (2) Hanoi Pedagogical University 2; (3) Ministry of Science and Technology

We theoretically investigate optical properties of plasmonic polymers consisting of chains of TiN and Au nanoparticles. The plasmonic polymers are more flexible, and have hot spot excitation between two adjacent particles and anisotropic resonant modes. We find that the strong near-field coupling changes absorption and scattering spectrum compared to the random dispersion of nanoparticles at the same volume fraction. Thus, a gradient of laser-induced temperature rise is also varied. In biological medium, this temperature increase has a significant influence on the inactivation of proteins. In this work, we employ the Arrhenius model to determine the protein inactivation.

Presenter: Do Thi Nga

P.24 – Poster, VCTP-45

Morphologies and strengths of magnetic fields in LkHα-101

Nguyen Bich Ngoc, Pham Ngoc Diep and the BISTRO collaboration

Department of Astrophysics, Vietnam National Space Center, Vietnam Academy of Science and Technology

Magnetic fields play important roles in the formation and evolution of interstellar clouds and protostars. Polarized dust emission is a key tool for measurement of magnetic field morphology. I will present the first measurement of the magnetic field in the LkHα-101-S region from polarized dust thermal emission. The LkHα-101-S region is one of the densest regions with an early-B star in the Auriga cloud, a nearby giant molecular cloud of the Gould Belt. This study is a part of the "B-fields In STar-forming Region Observations" (BISTRO) survey which is a large program of the James Clerk Maxwell Telescope (JCMT). The polarized dust thermal emission was taken by the POL-2 polarimeter at 850-micron wavelength. The morphology and strength of the B-field have been obtained. We applied two methods to calculate the B-field strengths, un-sharp

masking and structure function, and they gave consistent results.

Presenter: Nguyen Thi Bich Ngoc

P.25 – Poster, VCTP-45

Spin excitations in the Kitaev-Heisenberg model on the square lattice

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We study a Kitaev-Heisenberg model of spin 1/2 on a square lattice. We derive the elementary magnetic excitation spectrum employing a functional integral method within one-loop approximation with exact on- site constraint. The result is discussed in relation to the data obtained by the equation of motion method and with the result of the linear spin wave theory in Holstein-Primakoff representation.

Presenter: Pham Thi Thanh Nga

P.26 – Poster, VCTP-45

Magnetic competition in magnetic topological kagome systems

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A minimal model is proposed to describe the magnetic competition between out-plane and in-plane magnetizations observed in topological kagome magnets. The model consists of the spin-orbit, an anisotropic Hund and an anisotropic spin exchange couplings. Using variational calculations based on the Bogoluibov inequality, we find the ground state is either the out-plane ferromagnetic or the in-plane 120 antiferromagnetic, depending on the model parameters. There is a crossover from the in-plane 120 antiferromagnetism to the out-plane ferromagnetism when temperature decreases. In the crossing region, the in-plane 120 antiferromagnetism and the out-plane ferromagnetism coexists. A universal relation between the in-plane and the out-plane components of the Hund and the spin-exchange couplings is obtained.

Presenter: Trần Minh Tiến

P.27 – Poster, VCTP-45

Effect of electric fields on the electronic structures of zigzag buckling silicene nanoribbons

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In this study, we used the tight-binding model to investigate the band structure as well as the density of state (DOS) of zigzag buckling silicene nanoribbons (ZBSiNRs). In addition, external electric fields are also added into the Hamiltonian to investigate the effect of transverse and vertical electric fields on the electronic properties of ZBSiNRs. First, we noticed that ZBSiNRs

have a small bandgap and it depends on the buckling distance. Second, by comparing the effects of the two electric fields, we showed that the vertical field opens the bandgap more significantly than the transverse one. The band gap opening is proportional to the strength of the vertical potential. Unlike the vertical electric field, the gap within the transverse field decreases if the strength of the field reaches a critical value. Within the vertical fields, ZBSiNRs are found to be are impacted more strongly than zigzag flat silicene nanoribbons (ZFSiNRs) and zigzag graphene nanoribbons (ZGNRs). In particular, when we investigated both fields simultaneously, we found that they have a mutual impact on the gap of ZBSiNRs. These results are important to understand more comprehensively the effects of electric fields on ZBSiNRs. Corresponding author: vttra@ctu.edu.vn

Presenter: Pham Nguyen Huu Hanh

P.28 – Poster, VCTP-45

Asymmetric matter from B-L symmetry breaking

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We show that the present matter content of the universe may be governed by a $U(1)_{B-L}$ symmetry. The B-L breaking scalar field inflates the early universe successfully and then decays to right-handed neutrinos, which reheats the universe and generates both normal matter and dark matter.

Presenter: Dương Văn Lợi

P.29 – Poster, VCTP-45

Electronic and magnetic properties of HfO2 and HfMnO2: First priniciples prediction

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In this work, the electronic structure and magnetic properties of HfO2 and HfMnO2 are comprehensively investigated using first principles calculations. The Mn incorporation into the HfO2 fluorite structure increases the lattice parameter and reduces slightly the mechanical resistance. HfO2 is insulator with an indirect band gap X - Γ of 5.96 eV, exhibiting no magnetism. While the half-metallicity can be obtained by adding Mn. Specifically, HfMnO2 exhibits the semiconductor spin-up state and metallic spin-dn state. The total spin magnetic moments of 3.00 μB is obtained in HfMnO2, respectively, being produced mainly from the transition metal. Results suggest that the HfMnO2 compound may be prospective material for spintronic applications provided that it possesses perfect spin-polarization at the Fermi level vinicities.

Presenter: Hoat Do Minh

P.30 – Poster, VCTP-45

Tomography of partially aligned molecules

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High-order harmonic generation (HHG), emitted from atoms and molecules exposed to an ultrashort intense laser pulse, is rich in structured information. One of the applications of HHG is to reconstruct the highest-occupied molecule orbital (HOMO) of molecules. In many theoretical studies on tomography, the authors have assumed that the molecules are perfectly aligned before interacting with the probe laser [1], [2]. However, with the recent alignment techniques [3], [4] the perfect alignment is impossible to archive [5]. Therefore, considering and clarifying the effect of the partial alignment of molecular samples into the tomography procedure is necessary. To our best of knowledge, this issue is rarely reported. In this report, we study the influence of molecular alignment on the quality of the reconstructed molecular HOMO using HHG form simple molecules N2 and O2. The HHGs are calculated by the semi-classical Lewenstein three-step model [6]. The alignment quality is varied in two ways: (i) using an approximated analytical formula, and (ii) adopting a numerical solution of solving the time-dependent Schrodinger equation for rotating molecules in the alignment laser field. Results show that the molecular HOMO of a molecular sample with a low degree of alignment is less structural due to the averaged effect.

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Presenter: Tran Cong Minh

P.31 – Poster, VCTP-45

Understanding the electronic band structures of single-layer and bilayer graphene nanoribbons: An intensive comparison

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Aiming to provide an insightful and general comparison about the electronic band structures of the single-layer and bilayer graphene nanoribbons, three distinct structures including single-layer, the AA and AB stacking-bilayers in both armchair and zigzag edge orientations in the presence of external electric fields were investigated. Using the Tight-Binding calculations, we observed noticeable effects, for instance, the opening of the bandgap Eg strongly depends on the edge states and the magnitude of external electric fields. Furthermore, each type of electric field (vertical or transverse) affects differently the electronic gap of each structure. When comparing the effect of applying the electric field, the AB stacking bilayer structures exhibit more remarkably in the change in the band structure as well as the opening of the bandgap. Besides, the intriguing consequence is that there are the similarities between the variation of the band structure and Eg of mono-layer and the AA stacking bilayers because of the origin of the charge-density distribution. All of the change of the electronic band structure is reflected by

the density of states (DOS) with the essential features. From the obtained results, we hope that these will provide a more comprehensive understanding of the electronic properties of single-layer and bilayer graphene, without and with electric fields, contributing to bringing these material structures into electronic applications in the future.

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Presenter: Nguyen Lam Thuy Duong

P.32 – Poster, VCTP-45

Size effect on melting of silicene nanoribbons by molecular dynamics simulation

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An analysis of a phase transition in silicene nanoribbons (SiNNRBs) carried by molecular dynamics simulation (MDs) under non-periodic boundary conditions. A crystal SiNNRBs models containing 3000, 6000 and 10000 atoms are arranged a honeycomb structure with the low-buckling of z=0,44A and a bond length of d=2,28A. All models are heated to temperature much higher melting point with melting rate 2.10^{11} K/s . Evolution of structure and thermodynamics properties upon melting are investigated and discussed, such as radial distribution functions (RDF), temperature dependence of total energy, potential energy, coordination number, bond and angle distribution, interatomic distance between Si-Si. 2D visualization of atomic configurations are also presented. Melting of SiNNRBs from the crystal state has been effected by size of model.

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Presenter: Huỳnh Anh Huy

P.33 – Poster, VCTP-45

Melting point of silicene nanoribbons affected by pressure

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We present molecular dynamics (MD) simulations of melting of silicene nanoribbons (SiNNRBs) from the crystal state under non-periodic boundary conditions. We prepared a model containing 10000 atoms Si, arranged a honeycomb structure with the low-buckling z=0,44A and interatomic distance d=2,28A. We heat a model to 3500K, much higher melting point of silicene sheet. Temperature increased from 50K to 3500K with melting rate 2.10^{11} K/s. The pressure is increased during the melting. Structure and thermodynamics properties upon melting are studied and presented, such as temperature dependence of total energy per atoms, radial distribution functions g(r), coordination number, bond and angle distribution, interatomic distance between

Si-Si. We also present 2D visualization of atomic configurations at certain temperature. Melting of SiNNRBs from the crystal state has been effected by pressure, we find superheating limit and melting point from the dependence temperature on pressure curve.

Acknowledgements: This research is funded by Vietnam National Foundation for Science and Technology Development (NAFOSTED) under Grant 103.02-2019.377.

Presenter: Huỳnh Anh Huy

P.34 – Poster, VCTP-45

The decay of the Standard model-like Higgs boson $h \to Z\gamma$ in the 3-4-1 model

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One loop contributions to the amplitude of the decay of the Standard model-like $h \to Z\gamma$, are presented in the framework of the 3-4-1 model constructed based on the gauge group $SU(3)_C \otimes SU(4)_L \otimes U(1)_X$. In this work, the Feynman diagrams, the Feynman rules and analytical formulas corresponding to the one loop contributions calculated in the unitary gauge are given in detailed.

Presenter: Nguyen Thi Tham

P.35 – Poster, VCTP-45

The optical absorption coefficients and the refractive index changes in MoTe2 monolayer

Tran N. Bich (1), Le Dinh (1), Luong V. Tung (2), Pham T. Vinh (3), Huynh V. Phuc (3)

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In this work, the optical absorption coefficients (OACs) and the refractive index changes (RICs) in monolayer MoTe2 are theoretically investigated in the presence of a magnetic field. Our results indicated that both OACs and RICs present blue-shift behavior when the magnetic field increases. Besides, the strong spin-orbit coupling in monolayer MoTe2 leads to a significant difference in the peak due to spin up and down. The OACs and RICs due to intra-band transition display only one peak in the THz range, while the inter-band spectra show a series of peaks in the near-infrared to the visible optical range, making monolayer MoTe2 to be a promising candidate for novel optoelectronic applications.

Presenter: Huynh V. Phuc

P.36 – Poster, VCTP-45

Correlated phases in three-component Falicov-Kimball model

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Mott insulator and charge ordered phases in a three-component Falicov-Kimball model is studied by the dynamical mean-field theory. The three-component Falicov-Kimball model consists of itinerant single-component and localized two-component fermions, and local Coulomb interac-

tions between the components. Self consistent equations for charge susceptibilities are derived. It is found that the metal-insulator transition occurs at high temperature, whereas charge ordering is stable at low temperature. Different Mott insulator and charge ordering patterns are presented.

Presenter: Nguyễn Hồng Sơn

P.37 – Poster, VCTP-45

Resolving the octant of leptonic mixing angle θ_{23} with Hyper-Kamiokande experiment.

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Super-Kamiokande discovered neutrino oscillation in 1998 and Hyper-Kamiokande, which is effectively eight time larger than its predecessor and approved for reconstruction from 2020, will be a discovery machine for proton decays, CP violation in neutrino oscillation and detection of astrophysical neutrinos. This study explores the physics potential of Hyper-Kamiokande in measuring the θ_{23} mixing parameter, which presents a factional contribution of ν_μ and ν_τ in the neutrino mass eigenstate ν_3. If its value is exactly equal to $\pi/4$, it indicates some unknown symmetry between muon and tau. We use two types of simulated samples produced from the accelerator-based muon neutrino source: (i) survived muon neutrinos, and (ii) appeared electron neutrinos. The former can determine precisely $\sin^2 2\theta_{23}$ but can not know if θ_{23} is in lower octant ($\theta_{23} < \pi/4$) or in higher octant ($\theta_{23} > \pi/4$). The later depends on $\sin^2\theta_{23}$, but also on $\sin^2_{13}$ and δ_{CP}, which makes measurement statistically limited and parameter-degeneracy dependent. It will be shown that the θ_{23} octant resolving can be improved significantly with constraints established by reactor experiments and systematic improvement of appearance samples. It will be also shown how the octant determination can help the measurement of CP violation in the lepton sector.

Presenter: Phan To Quyen

P.38 – Poster, VCTP-45

Canonical seesaw implication for two-component dark matter

Phung Van Dong, Cao H. Nam, Duong Van Loi

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The seesaw mechanism is well motivated for explaining neutrino mass and baryon asymmetry. This work adds that it unravels the mystery of structured dark matter. The seesaw scale has a nontrivial physical vacuum structure that defines the usual matter parity and a new Z_3 symmetry, yielding a novel scenario of two-component dark matter. The component stabilized by matter parity populates the cold dark matter today, whereas the other component stabilized by Z_3 is boosted in cold dark matter annihilation successfully scattering on electrons in the XENON1T experiment. Here this fast dark matter has a large B-L charge strongly interacting with the normal matter causing the observed effect.

Presenter: Phung Van Dong

P.39 – Poster, VCTP-45

Device Physics and Design of InAs Line-Tunneling Field-Effect Transistors with Laterally Doped Pocket

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Related to the extension of the tunneling region, the line-tunneling architecture is known as the most effective method to enlarge the tunneling area in tunnel field-effect transistors (TFETs). Based on two-dimensional simulations with experimentally calibrated model parameters, this work examined the mechanism of laterally doped pocket in enhancing the on-off characteristics of line-tunneling FETs and investigated the pocket design to optimize the device performance. InAs with a low and direct bandgap of 0.37 eV was utilized to boost the on-current for the practical significance of the study. Without a laterally doped pocket, the point-tunneling is triggered earlier than the line-tunneling to cause a high subthreshold swing and low on-current in line-tunneling FETs. The laterally doped pocket properly modulates the vertical energy-band diagrams near the gate-oxide interface to narrow the tunneling barrier. With a laterally doped pocket, therefore, the line-tunneling can be triggered early to produce a low subthreshold swing and high on-current while still maintaining unchanged ambipolar behavior. The detailed investigation showed that the optimal concentration and thickness of laterally doped pocket are around 1E19 cm-3 and 4 nm, respectively. Both the pocket concentration and thickness are optimized at the values at which the onset voltage of line-tunneling is the same as that of point-tunneling. Using the laterally doped pocket with optimized design parameters is helpful in exploiting the advantages of line-tunneling in low-bandgap TFETs.

Presenter: Nguyễn Đăng Chiến

P.40 – Poster, VCTP-45

Transport and localization of waves in complex random potential with power-law correlations: A numerical study

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In this paper, we investigate numerically wave propagation and localization in a complex random potential with power-law correlations. Using a discrete stationary Schrodinger equation with the simultaneous presence of the spatial correlation and the non-Hermiticity of the random potential in the diagonal on-site terms of the Hamiltonian, we calculate the disorder-averaged logarithmic transmittance and the localization length. From the numerical analysis, we find that the presence of power-law correlation in the imaginary part of the on-site disordered potential gives rise to the localization enhancement as compared with the case of absence of correlation. Depending on the disorder's strength, we show that there exist different behaviors of the dependence of the localization on the correlation strength.

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Lyra, Phys. Rev. Lett. 81, 3735 (1998). [3]. A. Basiri, Y. Bromberg, A. Yamilov, H. Cao, and T. Kottos, Phys. Rev. A 90, 043815 (2014). [4]. B. P. Nguyen, T. K. T. Lieu, and K. Kim, Waves Random Complex Media, DOI:10.1080/17455030.2020.1774680 (2020).

Presenter: Nguyen Ba Phi

P.41 – Poster, VCTP-45

The distribution of counterions in a hexagonal DNA lattice within mean field theory

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Understanding electrostatics of DNA system is essential for better understanding and design of DNA as a biomaterial and as a biological structure. In this work, we consider the concentration of counterions in a two-dimensional hexagonal lattice of DNAby solving numerically the Poisson-Boltzmann equation within mean-field theory using finite element method.Additionally, the dielectric discontinuity of the electric potential at the DNA surface is taken into account. The dependence of ion concentrations on the inter-DNA distance in the bundle and the condensation of counterions on the DNA surface are investigated. The effect of the entropic confinement of the ions is also demonstrated.

Presenter: Nguyen Thi Thu Hang

P.42 – Poster, VCTP-45

The effect of parameters on interaction of two two-level atoms with a single-mode field in a squeezing-enhanced superposition of coherent state

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In this paper, we study the dynamical entanglements in the interaction between two two-level atoms with a single-mode field in a squeezing-enhanced superposition of coherent state. By using the master equation method and the linear entropy criterion in the Jaynes-Cummings model, we find that the squeezing parameter and relative phase in the single-mode field can effect on the entanglement degrees between subsystems such as atom-field, atom-atom. Besides, the dynamical behaviors of this model are found to be different compared to that of the corresponding squeezing superposition of coherent state.

Presenter: Le Thi Hong Thanh

P.43 – Poster, VCTP-45

Nonclasical properties and quantum teleportation of the superposition of two-mode photon-added pair coherent state

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In this paper, we introduce a new state called superposition of two-mode photon-added pair coherent state. Some nonclassical properties of this state are studied such as two-mode sum squeezing and two-mode antibunching. It indicates that this state has two-mode sum squeezing as well as two-mode antibunching. This state is an entangled state and the entanglement degree can be enhanced by adding photons to both modes. When using this state as an entangled resource for quantum teleportation, the results show that the quantum teleportation process is successful and the average fidelity of the process can be higher than the case where the pair coherent state is used if parameters are selected appropriately.

Presenter: Ho Sy Chuong

P.44 – Poster, VCTP-45

Investigation of radiative process $\tau \to \mu\gamma$ in the simple 3-3-1 model

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We study phenomenological constraints on the simple 3-3-1 model with flavor-violating Yukawa couplings. Both triplets Higgs couple to leptons and quarks, which generates flavor-violating signals in both lepton and quark sectors. We have shown that this model can allow for large Higgs lepton flavor-violating rate decay $h \to \mu\tau$ and also can be reached to perfect agreements with other experimental constraints such as $\tau \to \mu\gamma$ and $(g-2)_\mu$.

Presenter: Nguyen Tuan Duy

P.45 – Poster, VCTP-45

Optimizing of InGaAsSb/GaSb Layer for Infrared Optoelectronics Devices

Nguyen Tien Dai (1,2,), Man Minh Tan (1,2), Dang Van Thai (1,2), Truong Thi Hien (1,2), Le Anh Thi (3), Kim Jun Oh (4), Lee Sang Jun (4), and Dang Tran Chien (5)*

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We report the synthesis of $In_xGa_{1-x}As_ySb_{1-y}$ epi-layer on the GaSb (100) substrate by calculated theoretical and molecular beam epitaxy (MBE) growth. The result showed that the InGaAsSb lattice matching layer is suitable for our calculation and experimental. The layers with a y = 0.91×x [1] lattice matching condition might vary In concentration from 0-1 to obtains high device performance in the infrared (IR) range from 1.7 to 3.2 μm at 300 K, respectively. As a result, we used a theoretical model ($y = \frac{As_{Flux}}{(As_{Flux}+Sb_{Flux})}$) [2], and the MBE growth to optimize $In_{0.23}Ga_{0.77}As_{0.22}Sb_{0.78}/GaSb$ epi-layer for photodetector. This layer can absorb IR wavelength at 2.6 μm, 300 K that will be applied for detecting CO_2 gas and moisture further.

Presenter: Nguyen Tien Dai

P.46 – Poster, VCTP-45

Comparison of the contribution of the photon's vector and scalar Kaluza-Klein partners in the neutron lifetime

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A discrete extra dimension of size 11.8 fm would imply the existence of a vector X and scalar H bosons as photon's Kaluza-Klein partners. The massive vector X can be identified with the particle X17 suggested by ATOMKI's experiment. The particle model of extended photon sector coupled to extended nucleon, electron and neutrino also implies the neutron decay to its Kaluza-Klein partner. There are several different channels triggered by X and H. In this paper we compare the contributions from them and imply some physical consequences on the parameters of the model.

Presenter: Pham Tien Du

P.47 – Poster, VCTP-45

Improvement of quantum teleportation and controlled quantum teleportation via photon-added trio coherent state

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In this paper, we use the photon-added trio coherent state as an entangled resource to perform two quantum tasks in quantum information. Accordingly, a two-mode entangled state can be teleported and a single mode state can be controlled via the photon-added trio coherent state. The results show that the quantum teleportation processes are successful. Moreover, the average fidelities of the quantum teleportation processes are enhanced by increasing the number of photons addition as well as the amplitude r of the photon-added trio coherent state.

Presenter: Tran Quang Dat

P.48 – Poster, VCTP-45

Metal-insulator transitions of fermionic mixtures with mass imbalance in disordered optical lattice

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We study the metal-insulator transitions in the half-filled Anderson - Hubbard model with mass imbalance by the typical-medium theory using the equation of motion method as an impurity solver. The nonmagnetic ground state phase diagram of the system with mass imbalance is

constructed numerically. In addition to the three phases showed up in the balanced case, the phase diagram of the mass imbalanced case contains a spin-selective localized phase, where one spin component is metallic while the other spin component is insulating. We find that if one increases the mass imbalance the metal region in the phase diagram is reduced, while both Anderson and Mott insulator regions are enlarged.

Presenter: Hoang Anh Tuan

P.49 – Poster, VCTP-45

Iron-tin-based nanocomposite anodes for sodium-ion batteries

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We report a simple method to synthesize iron-tin-based nanocomposites (FexSnyOz NCs) as new anode materials for sodium-ion batteries. FexSnyOz NCs are synthesized via the reactions between Fe3+ ions and Sn at high temperature in triethylene glycol solvent. The as-prepared NCs consist of Fe3O4 and SnO2 at the nanometer scale ($<$ 6 nm). The NCs show high capacity, good cyclic stability, and excellent rate performance; for instance, FexSnyOz-18h NCs delivers a reversible capacity of 215 mAh g-1 after 100 cycles. The outstanding electrochemical performance is attributed to the presence of nanostructures and inactive phases that act as buffer spaces for the volume change of active materials during alloying and conversion reactions.

Presenter: Nguyen Tuan Loi

P.50 – Poster, VCTP-45

Phase diagrams of Falikov-Kimball model with Gaussian distribution for impurities and box distribution for Coulomb disorder

Nguyen Thi Hai Yen, Hoang Anh Tuan

Institute of Physics

The metal - insulator phase diagrams of the Anderson - Falikov Kimball model with Coulomb disorder are obtained via typical - medium theory within an approximation to the equation of motion. The equations determining boundary between the correlated metal, Mott insulator and Anderson localization phases are derived. We show that the metal and the Mott insulator regions shrink as the strength of Coulomb disorder increases.

Presenter: Nguyen Thi Hai Yen

P.51 – Poster, VCTP-45

Effect of electron-impurity scattering on the magneto-optical absorption property in MoS_2 monolayer

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In this work, we investigate the absorption of an electromagnetic wave in a MoS_2 monolayer

subjected to a perpendicular static magnetic field. The absorption coefficient is calculated by the perturbation taking account of the electron-impurity scattering. The absorption spectrum shows the appearance of cyclotron-impurity resonant peaks for one and two photon absorption. The position of the resonant peaks (the resonant photon energy) is proportional to the square root of the magnetic field strength ($\sqrt{B}$), while it does not affect by the temperature. In addition, the full width at half maximum of the resonant peaks increases linearly with the magnetic field but almost does not change with temperature. The contribution of two-photon absorption processes is much smaller than that of one-photon absorption ones but is significant and should be considered when studying nonlinear optics.

Presenter: Le Thi Thu Phuong

P.52 – Poster, VCTP-45

Studying the spread of epidemics by matrix logistic map

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One–dimensional logistic maps are considered as a basic and effective model for epidemic research and prediction in a closed environment. The results obtained from logistic models are often agreed with actual data gathering in isolated or semi–isolated communities. However, in a flat world, countries and territories are no longer closed in every sense, transactions with human involvement such as trading, transporting, ... are inevitable. In this context, recent outbreaks of epidemics in the world have been out of the forecast and outside the framework provided by an one–dimensional logistic map. An extended version of the logistic map so–called the matrix logistic map where growth rate and variables instead of ordinary numbers are replaced by corresponding matrices of which diagonal elements and off–diagonal elements characterize the native processes in each subsystem and the effective interactions between component systems, respectively. In that manner, the proposed extended model allows investigating changes of each component system in the presence of neighboring systems. In this report, the simplest case consisting of two subsystems is studied.

Presenter: Chu Thuy Anh

P.53 – Poster, VCTP-45

Non-Equilibrium Molecular Dynamics Simulations of Self-Diffusion Coefficient at Infinite Dilution: Applications to Fractionation of Noble Gases

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Classical equilibrium molecular dynamics (MD) simulations using the Green-Kubo formula or Einstein's relation have shown to be an efficient tool to compute the self-diffusion coefficient of various fluids. However, when dealing with highly dilute solutions that are rather ubiquitous in many fields including geological and petroleum engineerings, these approaches may provide

simulation results for solute self-diffusion coefficient with a poor statistics and so to very large error bars. In such situations, non-equilibrium molecular dynamics (NEMD) simulations that yield high signal-noise ratio is an option to improve the uncertainties. Thus, this work aims at proposing an efficient scheme of NEMD simulations to compute the self-diffusion coefficient of solute in infinite dilution solution. To do so, we have used theory of the thermodynamics of irreversible process (TIP) to derive the approach. It has been obtained that this scheme provides very good results for bulk solutions. However, it becomes less efficient for highly confined solutions in nanoporous medium due to a non-linear response. In such cases, we have proposed an extrapolation to determine the self-diffusion coefficient of solution in the linear response regime. Finally, the proposed scheme has been employed to investigate the fractionation of noble gases by molecular diffusion in bulk water and in saturated clays.

Presenter: Lục Hán Tường

P.54 – Poster, VCTP-45

Elemental and Isotopic Fractionation of Noble Gases by Molecular Diffusion

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Noble gases have been widely used as natural tracers to characterize storage, migration and origin of fluids in geological environments. Interestingly, they are chemically and biologically inert under geological conditions, and are so only fractionated by physical processes. Among existing physical processes, particularly, the molecular diffusion process has shown to significantly induce a fractionation between noble gases. Accurate estimate of such fractionation in geological fluids such as water, oil and gas is greatly demanded in geology and petroleum engineering. Thus, this work is devoted to investigate how to accurately predict elemental and isotopic fractionation of noble gases by molecular diffusion in geological fluids. To do so, we have first performed molecular dynamics simulations to compute the elemental and isotopic fractionation of noble gases in some geological fluids such as water, oil and gases in reservoir conditions. Then, capability of simple and predictive models (square-root relation and kinetic relation) to predict these fractionations have been investigated. Interestingly, it has been found that the square-root relation is able to provide a good prediction for elemental fractionation between major noble gas isotopes in all solvents, except for the cases relevant to the major Helium isotope. However, this relation cannot provide good results for the isotopic fractionation. Regarding the capability of the kinetic relation, the isotopic fractionation can be well computed in the gas, but often deteriorates in the water liquid and the oil. Finally, we have proposed a simple and predictive scheme for the isotopic fractionation of noble gases in the dense fluids (water liquid and the oil).

Presenter: Nguyễn Phúc

P.55 – Poster, VCTP-45

Probing degrees of orientation of polar molecules

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Determining the degrees of orientation of molecular sample is an important issue since it affects the outcomes of the chemical reactions and physical interactions. In experiment, there are different ways to directly measure the degrees of orientation, such as using a terahertz pulse [1], or two-color fields [2]. However, these methods using strong electric field thus leading to the destroying molecules [1, 2]. Recently, some nondestructive methods adopting high-order harmonic generation (HHG), resulted in the interaction between molecules and ultrashort, intense laser, are proposed to probe the orientation of polar molecular [3–6]. However, these methods are only validated when appropriate laser pulses are used. Moreover, the method can probe only the absolute value, but not the sign of the degrees of orientation. In this report, we present a comprehensive method to probe the full-range degrees of orientation of a sample of CO molecule using HHG. The method can be applied regardless of the laser shape and laser parameters. The method is performed by adopting the time-frequency profile of HHG. We found that, with an arbitrary laser pulse, the time-profile of a harmonic order strongly depends on the degrees of orientation. The method is highly reliable with considerably small errors.

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Presenter: Nguyen Huynh Kim Ngan

P.56 – Poster, VCTP-45

The effect of vacancies on the electronic properties of bilayer graphene nanoribbons

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Bilayer graphene nanoribbons (BGNRs) are intriguing candidates for semiconducting materials system because of their ability in modulation of the band gap under external excitations. In this study, we applied the Tight Binding (TB) method in combination with Green's function formalism to investigate the energy band and the density of states (DOS) of the studied structures. The difference between perfect and defected bilayer armchair graphene nanoribbons (BAGNRs) in the presence of external electric fields is presented. The results reveal that the electronic structure of BAGNRs strongly depends on the position as well as the density of vacancies. The defects are found to strongly impact the energy levels compared to that in the perfect structure. Besides, the effects of the external electric fields and defects are demonstrated in controlling the band gap.

Presenter: Nguyen Thi Kim Quyen

P.57 – Poster, VCTP-45

Rectangular Quantum Wire with an Infinite potential GaAs/AlGaAs: Quantum theory of Acoustomagnetoelectric effect in the presence of Electromagnetic wave

Nguyễn Thu Hương, Nguyễn Văn Nghĩa, Nguyễn Quyết Thắng, Nguyễn Quang Báu

Hanoi University of Science

The effect of Acoustomagnetoelectric in an GaAs/Al:GaAs infinite potential rectangular quantum wire (RQW) is investigated under the influence of Electromagnetic Wave (EMW) in term of using quantum kinetic equation method. We obtain the electron distribution function in the reaction with internal and external phonon. By solving the electron distribution inhomogeneous differential equation, the current density J and the acoustomagnetoelectric field EAME are obtained in the dependence on the EMW amplitude, external acoustic wave frequency, the system temperature and the RQW parameter (the quantum wire length). The results are numerically evaluated for GaAs/Al:GaAs quantum wire. Comparison it to the results which is obtained in case of the bulk semiconductors and others low dimension system in order to show the difference and the novelty of the results. The EAME depends non-linearly on the Wire Length Lz and exhibits an oscillatory behavior as the function of wire length, although the stability period in long wire length condition. Moreover, we survey the impact of EMW on EAME with the dependence on the external acoustic wave frequency wq. The result also indicates that the current density J increases as the temperature goes up with a exponential curved.

Presenter: Nguyễn Quyết Thắng

P.58 – Poster, VCTP-45

A Toy Model for Prediction of Pandemics

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The logistic map is well–known as a simple but capable model that exhibits chaotic behaviors in nonlinear dynamics systems. First, this model was proposed as a discrete-time demographic model in the statistical study of population, then widely applied in biological, physical, and sociological research, in which system behavior is unpredicted due to its complexity. In this report, a modified version of the logistic map is proposed to study the relationship between the growth rate in the logistic map and the initial conditions of the model. The results obtained from the calculations indicate the dependence of the growth rate on the model's initial conditions, thereby providing a control parameter for the critical growth rate where bifurcation happens. Application of these results in the COVID-19 outbreak investigation may show an effective measure of the health system's competence and readiness to intervene and control the prevention of disease spread in the community.

Presenter: Nguyễn Văn Hoa

P.59 – Poster, VCTP-45

Aggregation of microorganisms on engineered topographic surfaces: a simulation study

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Institute of Physics, Vietnam Academy of Science and Technology

Surfaces with engineered microtopographies are potential candidates for applications as a non-toxic antifouling technology to be used in marine environment. It has been shown that the sharkskin-mimetic (Sharklet) surface reduces the attachment of zoospores of the green alga Ulva as much as 77% compared to a smooth surface. In this work, we study the aggregation of Ulva linza zoospores on the Sharklet surfaces by using Monte Carlo simulations with an extended Surface Energetic Attachment (SEA) model that includes inter-organism interactions proposed in a recent work [1]. The energy parameters in the model are optimized based on experimental attachment probabilities. In agreement with reported experiments, it is shown that engineered topographies promote smaller aggregates compared to those on the smooth surface.

[1] Trinh X. Hoang, Ha T. H. Mai, Anthony B. Brennan and Ly Le, Biofouling 35, 684-695 (2019)

Presenter: Trinh Xuan Hoang

P.60 – Poster, VCTP-45

Counterion distribution near macroions, a field-theoretical treatments up to two-loop order

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Field-theoretical treatment of a counterion distribution near a charged surface is constructed in a systematic perturbative manner. The standard Hubbard–Stratonovich transformation is used to transform the system of interacting counterions in aquaeous solution into a scalar field theory. By using perturbative expansion in the interaction strength, Gaussian functional average and Wick's theorem, an analytical expression for the counterion distribution is obtained up to the two-loop Feyman diagrams. Numerical calculation and plotting show that the contribution of these higher order loops are already quite significant when the so-called plasma interaction strength parameter is about 0.5. Our results qualitatively agrees with previous Monte-Carlo simulation results. Some discrepancies are observed at stronger interaction parameter values, which indicates the need for higher order corrections for such systems.

Presenter: Tran Thanh Tuyen

P.61 – Poster, VCTP-45

On the Quatron State in Parabolic Quantum Dots

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In this work we consider a quatron state – a state of four particles – two electrons and two holes in quantum dots with parabolic potentials of confinement. By using the Hatree-Fock method, we obtain the binding energy of the quatron in the dependence of the system parameters, such as the mass ratios between the electron and the hole, the ratio between the electron and

hole confinement strengths in the quantum dots. The effect of the magnetic field has been also investigated on the binding energy of the quatron. We have established the relationship between the binding energy of the quatron and the biexciton. It is interesting to note that in the ground state for the certain ranges of the electron-to-hole mass and confinement ratios, while the biexciton as a state of two excitons is unbound, the quatron state as a state of two electrons and two holes as a whole is bound.

Presenter: Nguyen Hong Quang

P.62 – Poster, VCTP-45

Total decay rate of $\mu \to e\gamma$ in a model with electroweak scale right-handed neutrino

Dinh Nguyen Dinh

Institute of Physics, VAST

In this research, we briefly introduce an extended model of the SM with EW right-handed neutrino. Then the formula expression of the total branching ratio of $\mu \to e\gamma$ at one-loop level in the scenario of the model will be derived. Using the obtained branching ratio formula and current experimental upper bound on the channel, we expect to set constraints on some relevant parameters, and also constraint on the correlation of the expectation values of the model.

Presenter: Dinh Nguyen Dinh

P.63 – Poster, VCTP-45

A discrete differential evolution for fuel loading optimization of the DNRR reactor and comparison with genetic algorithm

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Fuel loading pattern optimization is one of the complicated tasks of nuclear reactor core design in order to maximize fuel utilization while satisfying operation and safety constraints. In the present work, a discrete differential evolution (DE) method has been developed and applied to the problem of fuel loading pattern optimization of the Dalat Nuclear Research Reactor (DNRR). A classic strategy DE/rand/1/bin was chosen for the mutation operator of the DE method. Numerical applications were performed based on the core configuration of the DNRR consisting of 100 highly enriched uranium (HEU) fuel bundles with various burnup levels. Comparison of the performance between the DE method and a genetic algorithm (GA) was also carried out. The results show that DE is more advantageous in exploring search space and approaching a global optimum than GA. Further investigation on the application of advanced DE variants to the fuel loading optimization problem is being conducted in the future work.

Presenter: Phan Thi Thuy Giang

P.64 – Poster, VCTP-45

Thermodynamics and control systems theory: Application to non-equilibrium single-phase or multi-phase processes

Hoang Ngoc Ha

Duy Tan University

In this work, we show how thermodynamic properties of irreversible systems, through the so-called exergy or availability open research perspectives on the mathematical modelling, analysis and control of non-equilibrium single-phase or multi-phase processes. As a consequence, we connect thermodynamics and the control systems theory.

Presenter: Hoang Ngoc Ha

P.65 – Poster, VCTP-45

Transmembrane Amyloid β-Peptide Structures: In Silico Study

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Amyloid beta (Aβ) peptides are considered the major causative agents of Alzheimer's disease (AD). In a widely accepted mechanism for AD pathogenesis, Aβ peptides are proposed to play multiple roles in damaging brain cells and their synaptic communications. Due to the heterogeneous nature Aβ oligomers, their in vivo structures have not been understood. Most experimental and computational studies favored β-rich structures of Aβ as observed in Aβ fibrils. To determine the putative structures of the transmembrane Aβ oligomers, the temperature replica exchange molecular dynamics (REMD) simulations with an explicit solvent has been employed to monitor its structural change when the membrane DPPC lipid bilayers is induced. The initial structure of the oligomers was modelled based on the current low-resolution data of these conformations. The physical insights into the forming transmembrane Aβ oligomers probably enhance the AD therapy.

Presenter: Ngo Son Tung

P.66 – Poster, VCTP-45

Diverse Structural and Electronic Properties of Si-Doped Graphene

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A complete theoretical framework has been developed under the first principles calculations to explore the diverse structural and electronic properties of Si-doped graphene systems, including the adatom-diversified geometric structures, atom-dominated electronic band structures, spatial charge density, variations in spatial charge density and atom- and orbital-projected density of states (DOSs). Such physical quantities draw together a distinct physical and chemical picture in the studying systems. The planar geometric structure still remains regardless of various Si doping concentrations, clearly evidencing for presence of the very strong Si-C chemical bonds on the nanosheet. An indirect energy gap of 2.5 eV is induced in the fully Si-substituted graphene nanosheet and it is much shrunk under the various atom arrangements in 50% Si-substituted

ones or even vanished in the single adatom-substituted one. The typical orbital hybridization mechanisms in the Si-doped graphene systems are fully identified by the developed first-principles quantities.

Presenter: On Van Vo

P.67 – Poster, VCTP-45

Thermoelectric and magnetic properties of gadolinium doped bismuth telluride: first-principles investigation

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Rare earth doped Bi2Te3 reveals many exotic magnetic properties in host materials which is promising for the functional-material applications such as thermoelectricity and spintronics. In this work, within the density functional theory, we carried out first-principles electronic structure calculation to examine ground states and thermoelectric properties of Gd doped bismuth telluride. The strong correlation and spin-orbital coupling effects were found to be important to describe the electronic structure of the alloy. Results show that Gd substituted alloy is ferromagnetic with the magnetic moment of 7μB which purely comes from f-states of Gd atoms. Interaction between the valence electrons produces Gd1/3Bi5/3Te3 to be semimetallic, which drastically reduces the Seebeck coefficient. To substantiate this point, we calculated the transport coefficients, i.e. the Seebeck coefficient, the electrical conductivity and the thermoelectric power factor by utilizing the solution of Boltzmann transport equation in a constant relaxation-time approximation. The bipolar conduction effect is responsible for a drastic reduction of the Seebeck coefficient thereby the power factor. We pointed out that optimizing the carrier concentration was a method to feasibly improve the power factor thereby the thermoelectric performance of Gd1/3Bi5/3Te3.

Presenter: Tran Van Quang

P.68 – Poster, VCTP-45

Simulation for CO2 capture and permanent underground geological storage

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The 2019 global fossil-fuel carbon emission was estimated to amount to approximately 36.8 billion tonnes of CO2 with a 0.6% increase from 2018 [1]. The global need to reduce the amount of CO2 emissions, as highlighted by international agreements and expert evaluations, such as the Kyoto protocol and the IPCC [2]. This increase is proportional to the global increase in the demand for fossil fuel, solutions for CO2 capture and storage must be found. The IPCC report [3] presents a review of the international status of three CO2 storage technologies: Underground geological storage, ocean storage, and mineral carbonation. The options for underground geological storage include storage in saline aquifers and oil reservoirs, where CO2 injection as a part of WAG (water-alternating-gas) technique can be used for enhanced oil recovery (EOR). There are many CO2 capture and storage projects in USA, Canada, Norway, Algeria. With thousand kilometer deep from the earth surface, the processes occurring during injection, post-injection, and

storage of CO2 occur in either porous rock or inside rust-covered pipes, making interactions and reactions between CO2, water, and minerals to be utmost importance. Calcite is one of the most abundant minerals in the Earth's crust. In this report, molecular dynamics (MD) simulation was chosen as the main scientific method for theoretical studies of aqueous interfacial systems involving CO2, H2O, and calcite. We disregarded all possible reactions between water, carbon dioxide, and calcite. Our main focus was to investigate the impact of calcite and temperature variations on transport, adsorption, and stability of CO2 and water as affected by the presence of hydrate and calcite surface. For the molecular dynamics set up, the starting composite system was constructed from the calcite slab, water slabs, hydrate crystal, and a carbon dioxide phase. The resulting primary simulation cell ranged 48 x 48 x 108 Å in size with 19245 total numbers of atoms. The molecular dynamics MDynaMix package [4] was used to keep the constant temperature of MD system at three different temperatures (277, 388, and 500 K) by the Nose-Hoover thermostat [5, 6, 7]. The Linux-based Message-Passing Interface (MPI) was used to run the MD simulations in parallel on 88 processors of Cray XT4 supercomputing facility at the University of Bergen, Norway. Our MD simulation results showed that CO2 transport, adsorption, and interface stability were heavily affected by temperatures, presence of calcite and clathrate hydrate. The results indicated that CO2 can cross the water layers to approach both calcite surface and hydrate. At all simulation temperatures, a number of CO2 molecules were adsorbed on calcite surface. At lower temperatures (277 K and 388 K), CO2 molecules were found to become trapped inside the open hydrate cages.

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Presenter: Phan Van Cuong

P.69 – Poster, VCTP-45

Adsorption of Gas Molecules on Sawtooth Penta-Graphene Nanoribbon

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We have studied the adsorption of gas molecules (CO, CO2, and NH3) on the surface and the edge of Sawtooth Penta-Graphene Nanoribbon (SSPGNR) using first principles methods. The adsorption geometries, adsorption energies, charge transfer, density of states, and electron difference density are obtained. We find that the adsorption of CO and CO2 on SSPGNR show chemical adsorption properties, meanwhile the adsorption of NH3 shows physical adsorption properties. The current voltage (I–V) characteristics have also been investigated using non-equilibrium green's function (NEGF) approach. The results indicate towards gas molecules have

little effect on modifying the conductance of SSPGNR. We also studied to compare the absorption capacity NH3 on SSPGNR at possible absorption sites. Quantum transport calculations further indicate that NH3 molecules can be detected by the SSPGNR-based sensor.

Presenter: Nguyen Thanh Tien

P.70 – Poster, VCTP-45

Study on structural and elastic properties of interstitial alloy FeSi with B2 structure under pressure

Nguyen Quang Hoc (1), Nguyen Duc Hien (2), Nguyen Minh Hoa (3), Dinh Cong Thanh (1) and Vu Trang Linh (1)

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The analytic expressions of the Helmholtz free energy, the cohesive energy, alloy parameters, mean nearest neighbor distance and elastic quantities such as the isothermal elastic modulus BT, the elastic moduli E, G, K and the elastic constants C11, C12, C44 for interstitial alloy AB with the B2 structure under pressure are derived from the statistical moment method. In limit case when the concentration of interstitial atoms is equal to zero, we obtain the elastic theory for the main metal A with the SC structure. The numerical calculations for the B2-FeSi are compared with available other calculations and experimental data. Keywords: B2 structure, interstitial alloys, statistical moment method

Presenter: Nguyen Minh Hoa

P.71 – Poster, VCTP-45

Feature-Rich Magnetic and Electronic Properties of Halogen-Doped Silicene

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Feature-rich magnetic and electronic properties of halogen-doped silicene are studied by the first-principles calculations. The developed ab initio quantities include the atom-dominated band structures, spatial spin density distributions, spatial charge density distributions, and atom- and orbital-projected density of states that sufficiently identify similar and different features in the double-side and single-side adsorptions. The double-side adsorptions belong to the concentration-depended finite gap semiconductors or p-type metals, while the single-side adsorptions only present the p-type metals. Both adsorption types show the halogen-related weakly dispersed bands at deep energies, the adatom-modified middle-energy σ bands, and the recovery of low-energy π bands during the decrease of the halogen concentrations. Such developed ab initio quantities can be fully generalized to other layered materials.

Presenter: On Van Vo

P.72 – Poster, VCTP-45

Effects of pH of the precipitation environment on SiO2 synthesis from rice husk ash

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The situation of SiO2 nanoparticle synthesis research is being concerned with many interesting applications by their adsorption properties. Sources of synthetic SiO2 nanoparticles may come from inorganic or organic matter but recently people often take advantage of agricultural waste such as straw, rice husk, bagasse with high SiO2 content. We synthesized SiO2 from rice husk ash by the method of precipitation in the laboratory to study the effect of pH of the precipitation medium on the structure formation and purity of nano SiO2. The samples S5, S6, S7 are synthesized with the pH respectively pH = 5, pH = 6 and pH = 7. From the analysis methods of UVis, FT IR, XRD, SEM spectroscopy, S5 results showed that SiO2 particles are clustered, amorphous structure, and organic substances have not been expelled from the sample. As the pH increases, the particle size gradually increased, the structure become porous and pure with an average size of about 20.6 nm for the S7 sample. Based on two isothermal adsorption models Langmuir and Freundlich, results show that nano SiO2 gives the adsorbent absorption capacity of MB solution about 81.69% in 90 minutes. From this research, opening the way for the application of SiO2 nanoparticles in wastewater treatment. Key words: nano SiO2, pH effect, methylene blue adsorption

Presenter: Nga Huynh Nguyen Thi

P.73 – Poster, VCTP-45

Exact electron-muon elastic scattering in QED at next-to-leading order: Soft-photon contribution

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Recently, the new experiment MUonE has been proposed to measure precisely the running of the fine-structure constant at space-like momenta via the electron-muon elastic scattering. The motivation is to resolve the current 3-sigma anomaly on the muon (g-2) measurement. For the MUonE measurement we have to calculate the cross section of electron-muon elastic scattering very precisely, at the level of 10 ppm relative accuracy. This requires that the electron and muon masses have to be kept and next-to-next-to-leading order QED corrections must be included. Already at next-to-leading order, the precise calculation keeping the electron mass is numerically challenging due to different scales involved. Here we report on our attempt to calculate the cross section of electron-muon elastic scattering in QED at next-to-leading order in the soft-photon approximation keeping the electron mass. We will present some numerical results for MUonE experiment setup.

Presenter: Le Duc Truyen

P.74 – Poster, VCTP-45

Isotropic Strain Effect on 2D Charge Density Wave Materials NbX2 (X = S,

Se)

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Based on density functional theory, we investigate the influence of strain on the electronic structure of charge density wave (CDW) materials NbX2 (X = S, Se) with taking the van der Waals interaction and spin-orbit coupling (SOC) into account. By using the optB88-vdW functional, we found that spin splitting induced by SOC effect is significantly large in the band that crosses the Fermi level, especially at the high symmetrical points in the Brillouin zone (BZ). Furthermore, the mobility of electrons and correspondingly the conductivity of the materials might be enhanced as an overlap between the bottom and the top of the two conducting bands occurs under the biaxial strain. Our results suggest an application of NbX2 as channel materials or high-sensitive materials for gas sensors.

Presenter: Lương Thị Thêu

P.75 – Poster, VCTP-45

Effect of dynamic core-electron polarization on odd-even high-order harmonic generation from CO molecule

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Many theoretically and experimentally reports have demonstrated that the high-order harmonic generation (HHG) emitted from asymmetric molecules contains both even and odd orders [1,2]. The emission of even harmonics is attributed to the symmetry breaking of the laser-molecule system [3]. Therefore, the even-to-odd ratio strongly depends on the symmetry-breaking degrees, such as, molecular orientation [4]. In work [5], the authors also indicated that the dynamic core-electron polarization (DCeP) affects the even-to-odd ratio when the molecule interacts with the laser with a specific intensity. However, how does this influence of DCeP for interacting laser with different intensity is still questionable. In this work, we investigate the DCeP effect on the even-to-odd ratio of HHG emitted from CO molecule, when interacting with laser with various parameters. The HHG is calculated by using a numerical method solving the time-dependent Schrödinger equation within the single-active-electron approximation. We show that, when considering the DCeP, with changing the laser intensity, the intensities of the odd and even harmonics are almost comparable. Meanwhile, when the DCeP is neglected, the even-to-odd ratio changes with varying the laser intensity. We then explain these phenomena by considering the separated ungerade and gerade components of the temporal transition dipole.

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Presenter: Nguyen Thi Hien

P.76 – Poster, VCTP-45

Transition-Metal Dichalcogenides MoX2 (X=Te, Se) under Biaxial Strain

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In recent years, monolayer transition-metal dichalcogenides (2D TMDs) have been interested by their direct band gap, no inversion center, strong spin-orbit coupling. In this work, we performed a systematic first-principles study of the electronic structure of 2D TMDs MoX2 (X= Te, Se) in 2H hexagonal phase. The influences of Van der Waals (vdW) interaction was investigated by employing the five van der Waals functionals: revPBE, optPBE, optB86b, optB88, and vdW-DF2 with and without taking spin-orbit coupling into account. Under spin-orbit coupling effect, the spin splitting at K and G point in the first Brillouin zone appears, and the bandgap is narrower. Under biaxial strain, the change of band gap from the direct to indirect was revealed. The creation and annihilation of quasi-particles under strain were also explored.

Presenter: Nguyễn Hoàng Hưng

P.77 – Poster, VCTP-45

DFT Study on Crystal and Electronic Structures of Potential Cathode Material $Na_2Ni_3(SO_4)_4$

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Aiming to find a promissing candidate of cathode materials for sodium rechargeable batteries, we proposed a new material $Na_2Ni_3(SO_4)_4$ and investigated its crystal and electronic structures, and reveals the diffusion mechanism of Na-ions inside this material by using the GGA + U and HSE06 methods. Bandgap of 4.2 eV was found and an open circuit voltage of 5.2 V was predicted. Based on the diffusion mechanism of small polaron-vacancy complexes [1], we calculate the activation energies of the diffusion processes. It is found that Na-ions can diffuse along the tunnels of the crystal structure but with higher activation energy than in $Na_2Mn_3(SO_4)_4$. However, with a considerably high voltage $Na_2Ni_3(SO_4)_4$ can be expected as a promising cathode material for Na rechargeable batteries.

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Presenter: Trần Thiện Lân

P.78 – Poster, VCTP-45

A connection between domain structure and dynamical properties of liquid

silica under pressure

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Molecular dynamics simulation is used to study liquid silica consisting of 4998 atoms at 3200K under pressure from 0 to 30 GPa. The compression was considered through domain analysis and voronoi polyhedral. The results show that the structure of liquid silica is heterogeneous at pressure below 10 and above 20 GPa. It comprises separate regions which are Dx (x = 4, 5, 6) and DB domains. The Dx domains occupy high-density regions while DB domains occupy low-density regions. Upon compression the structural change is accompanied with splitting and merging processes of domains. The dynamical properties are investigated firstly corresponding to domain structure. We found that there is a connection between domain structure and dynamical properties of liquid silica.

Presenter: Giap Thi Thuy Trang

P.79 – Poster, VCTP-45

Enhancement of the electric current in high-Tc superconductor interacting with an artificial pinning arrayan

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The dynamics of the flux lattice in the mixed state of high-Tc superconductor interacting with a periodic array of nano-solid (pinning center) is considered. We calculate analytically the current density for the case of the matching field (when the number of vortices is equal to that of the nano-solid) using Ginzburg-Landau equations in a magnetic field in the presence of strong thermal fluctuations. It is found that the current density increase considerably with increasing pinning strength. Physically in the presence of thermal fluctuations when the energy scale of the vortex lattice shear fluctuations becomes comparable to the pinning energy scale, it results in increase of the current density.

Presenter: Nguyen Minh Hoa

P.80 – Poster, VCTP-45

Exciton Creation and Annihilation Mechanism in Monolayer WSe2 under Tensile and Compressive Strains

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We present a density functional study on the effect of tensile and compresive strains on the electronic structure and the creation/annihilation mechanism of excitons in monolayer WSe2 using the van der Waals functional optB88-vdW with talking the spin-orbit coupling effect into account. Based on the partial projected band structure, the spin splitting of the band edges is carefully interpreted. Moreover, excitons arisen from the five valleys around the Fermi level are specifically indicated. The calculation gives a good agreement between the electronic structure

and emission spectra related to A and B excitons. Since the deformation of orbital state dz2 is sensitive to strain, the dispersion of the bands predominately occupied by dz2 at the band edges strongly changes and the band gap notably reduces when strain is applied. Furthermore, the excitons at K valleys are remarkably stabilized while the excitonic annihilation at the four remaining valleys occurs as applying tensile strain. Inversely, excitons at K and Q valleys might disappeared and the momentum excitons are strongly stabilized under compression. Our research suggests a guide to manipulate several kinds of excitons in TDM materials.

Presenter: Tran Thi Nhan

P.81 – Poster, VCTP-45

The possibility of supersolid phase in the hard-core boson model on the triangular lattice

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Supersolid is an unusual phase in which crystalline and superfluidity properties coexist simultaneously. The search for a supersolid phase in a natural crystal has just brought frustration and disappointment over the past decades. In recent years, the signal of a stripe supersolid phase observed booming on the optical lattice experiments with BEC have rekindled excitement for this hot topic. Intriguing by these positive expressions, we have explored the extended Bose-Hubbard model for hard-core boson on the triangular lattice in the cases of the nearest-neighbor and long-range interactions are taken account. By using the mean-field method, the phase diagrams were sketched. Notably, the supersolid exists in the middle of solid phases corresponding to densities $\rho = 1/3$ and $2/3$. Simultaneously, as the nearest neighbor interaction V1 increases, the region of the supersolid phase gradually broadens.

Presenter: Nguyen Oanh

P.82 – Poster, VCTP-45

First-principles insight into the structural, electronic and optical properties of cadmium selenium nanocrystals

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In this work, the structural, electronic, and optical properties of CdSe were studied using an ab initio calculation based on the generalized gradient approximation (GGA) method within the density functional theory. Geometrical optimization of the unit cell is in good agreement with our experimental data. The band-structure, density of states of the nanocrystals were presented. The results show that CdSe is a direct band gap with an estimated 0.63 eV. We also report

our results dielectric functions and the refractive index (n) characterized. It is indicated that CdSe materials have excellent photoelectric properties potential applications in optoelectronic devices.

Presenter: Đỗ Quang Tâm

P.83 – Poster, VCTP-45

Reconstruction of the highest-occupied molecular orbital

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Knowing the molecular structure, such as the highest-occupied molecular orbital (HOMO), is the desire of scientists since it reveals many physical and chemical properties. One method to reconstruct the HOMO is using high-order harmonic generation (HHG) reported in Ref. [1], called tomography. This tomography procedure bases on the semi-classical three-step model, including (i) tunnel ionization, (ii) propagation, and (iii) recombination [2]. Therein, the needed plane-wave amplitudes characterized the propagation step, is more difficult to measure or calculate. Therefore, the solution is using a reference atom whose ionization energy approximately equals that of the main molecule [1]. However, in the three-step model, the plane-wave approximation which assumes that the wave packet of the returning electron just depends on the laser parameter, and importantly, independent on the target [3]. Therefore, the question is whether the requirement of using a reference atom with the same ionization energy for tomography procedure is necessary. In this report, we study the role of the reference atom in the tomography procedure for HOMO of N2 molecule from HHG. We use various reference atoms with different ionization energy. This investigation is meaningful in the selection of reference atoms in experiments.

Presenter: Truong Quan Hao

P.84 – Poster, VCTP-45

The optical Stark effect of excitons in InGaAs/InAlAs prolate ellipsoidal quantum dots

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Abstract. In this paper, we study the optical Stark effect of excitons in InGaAs/InAlAs prolate ellipsoidal quantum dots using the renormalization wavefunction formulation. Our results show that the absorption spectrum appears two absorption peaks of excitons when there is a strong laser coupling of two-electron quantized levels. This provides clear evidence of the existence of the three-level optical Stark effect in this quantum structure. Besides, the dependence of the exciton absorption spectrum on the pump laser detuning, photon energy, size, and geometry of quantum dots were also investigated and explained in detail.

Presenter: Le Thi Ngoc Bao

P.85 – Poster, VCTP-45

Phenomenology study of the lepton sector in an S_3 flavor symmetry with

inverse seesaw mechanism

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A new S_3 flavor symmetry with inverse seesaw mechanism is added to the gauge group of the Standard Model. The Higss sector of the model with new flavons beside the Standard Model's Higgs is studied in detail. theThe phenomenology of the lepton sector, including charged lepton masses, neutrino masses and lepton mixing matrix are derived. Our numerical analysis shows that the current experimental data of the lepton sector, in both normal ordering and inverted ordering of active neutrino masses, are successfully explained by our model.

Presenter: Nguyễn Thanh Phong

P.86 – Poster, VCTP-45

Casimir effect in a single weakly interacting Bose gas at zero-temperature with Neumann boundary condition

Pham The Song

Tay Bac University

Developing Bogoliubov theory of weakly interacting Bose gas in uncompacted three-dimension space, quantum fluctuation energy of one component dilute gas of Bose-Einstein condensate (BEC) confined to two parallel plates is investigated at zero-temperature in grand canonical ensemble (GCE) with Neumann boundary condition (BC). The Casimir force is considered in comparison to the one with Robin BC, Dirichlet BC and periodic BC.

Presenter: Song Thế Phạm

P.87 – Poster, VCTP-45

Gelation of Anisotropic Colloids with Short-Range Attraction

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Colloidal gels are space-spanning networks that form solids at dilute particle volume fractions. The kinetic process of gelation is central to understand the flow of complex fluids. Here, we report a simulation study of colloidal gelation of anisotropic colloids with attractive Lennard-Jones potential. These forces quasi-model the critical Casimir effect far from the critical solvent fluctuations acting on colloidal patches. By tuning the depths of the patch-to-patch particle interactions and the selected colloidal patches, we dynamically arrest the colloids to form gels. We find that thermal density fluctuation is the key factor to activate colloidal cluster space spanning: the balance between clustering and break-up mechanism is important for the gelation process of anisotropic systems. These results open new opportunities for studying the structural modifications of colloidal gels formed by anisotropic particles, and shed light on non-equilibrium behavior of anisotropic colloidal building blocks. Acknowledgement: This research is funded by Vietnam National Foundation for Science and Technology Development (NAFOSTED) under grant number 103.01-2018.308

Presenter: Tran Van Thien

P.88 – Poster, VCTP-45

Numerical determination of the soft Coulomb in considering the nonsequential double ionization process

Truong Dang Hoai Thu (1,2,3), Luong Hoang Sang (3), Nguyen Thuy Uyen (3), Pham Nguyen Thanh Vinh (3)

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In this study, we propose a simple procedure to determine the soft parameter of Coulomb potential based on the classical ensemble model to avoid autoionization and to eliminate singularity in the potentials. The approach is illustrated for several nobel gas atoms and indicates good agreement between the calculated two-electron correlated momentum distribution with experimental data.

Presenter: Truong Dang Hoai Thu

P.89 – Poster, VCTP-45

Controlled teleportation between a continuous-variable state and a discrete-variable state using hybrid entanglement under decoherence effects

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We propose a linear optics scheme for teleporting two different types of qubits by using hybrid entanglement under the decoherence effects. Namely, the sender can teleport a single-rail qubit to the receiver in spite of the fact that she/he holds a coherent state and vice versa under the supervisor of two controllers who work in two different Hilbert spaces, e.g. finite-dimensional and infinite- dimensional spaces. The quantum channel to be used is a four-particle state which two particles live in finite-dimensional space and the others live in infinite-dimensional space. We calculate and compare the success probability and fidelity between two teleportation processes. In addition, the role of the two controllers is assessed via the analysis of the average fidelity of the teleportation protocol without their participations. It is found out that the power of the controller who holds discrete-variable state is always equal to or larger than that of the other controller who holds continuous-variable state.

Presenter: Cao Thi Bich

P.90 – Poster, VCTP-45

Parity violation by gravity in QCD as Discretize Kaluza-Klein theory

Nguyen Van Dat, Nguyen Ai Viet, Pham Tien Du

Trường Đại học Khoa học Tự nhiên, Đại học Quốc gia Hà Nội Viện Công nghệ Thông tin, Đại học Quốc gia Hà Nội Đại học Thủy lợi

Discretized Kaluza-Klein Theory (DKKT) can include non-abelian gauge fields as components of generalized gravity in space-time extended by a discrete extra dimension if the gauge group

is the same for left- and right-handed chiral quark-leptons or one group must be abelian. In this paper we construct the QCD coupled to gravity in the framework of DKKT while keeping the chiral symmetry of QCD. We show that for consistency, this theory must have different gravity coupling to left- and right-handed quarks. The consequences of this parity violation mechanism by gravity are discussed.

Presenter: Nguyễn Văn Đạt

P.91 – Poster, VCTP-45

The correlation function dependence on temperature in EXAFS spectra. Application for Cu-Ag alloys

Nguyen Ba Duc (1), Trinh Phi Hiep (2), Vu Quang Tho (3)

University of Tan Trao

Correlation ratios between the mean square displacement (MSD), mean square relative displacement (MSRD), and correlated displacement function were studied in extended X-ray absorption fine structure spectra (EXAFS). The expressions of MSD, MSRD, and correlation function were determined using Debye models. Hardy problems due to many-particles effects were considered and replaced by a calculation based on the effective anharmonic potential, including the interaction of absorbing and scattering atoms with their nearest neighbours atoms. Based on the Debye-Waller factor, the difference between MSRD and MRD was analyzed, and their ratios have calculated. The methods were applied to fcc crystals and their alloys. Numerical results for Cu crystal and CuAg50 alloys agreed with experimental values and other studies.

Presenter: Nguyen Ba Duc

P.92 – Poster, VCTP-45

Electronic properties of the pentagonal silicon dicarbide nanoribbons

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Structural stability and electronic properties of the pentagonal silicon dicarbide nanoribbons are theoretically studied by density functional theory (DFT). We evaluate the stability of the four nanoribbon structures cutting from pentagonal silicon dicarbide (p-SiC2) sheet. By comparing their energy formations, we figure out that p-SiC2 SSribbon (p-SiC2 SSNR) is the most stable and having indirect band gap. Electronic properties versus the ribbon width was studied by computing the band structure and density of state. With various width, LUMO and HOMO charge densities are restricted in edges. In particular, while HOMO charge densities are evenly distributed, LUMO ones mainly focus on the middle of SSribbon. We also investigated the electronic structures and the current–voltage (I–V) characteristics of the SSPGNRs under a sequence of uniaxial strains in range from 10% compression to 10% stretch. The value of the band gap of p-SiC2-SSNRs can be depicted as a parabola under uniaxial strain. Our calculations show that the current is monotonous increase with compressive strain at the same applied bias voltage. The results obtained from our calculations are beneficial to practical applications of

these strained structures in p-SiC2-SSNRs-based electromechanical devices.

Presenter: Nguyen Thanh Tien

P.93 – Poster, VCTP-45

Two-dimensional clusters of colloidal tetramers via droplet emulsion templating

Pham Van Hai

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In this report, using a kinetic Monte Carlo simulation method we consider a hierarchical assembly of square-shape tetramers , constrained in a plane, via droplet evaporation. We found that colloidal tetramers undergo a structural transition from initial square-shape tetramers to diamond-like tetramers. A variety range of resulting clusters of square-shape tetramers belongs to a particular class of geometrical shape, namely polyiamonds, that are previously reported to the clusters of single colloids. However, due to geometrical constrained of tetramers, many novel structures can be observed. Considering potential applications of colloidal clusters in electronics, photonic materials, our result could provide an effective way to control the formation of complex colloidal cluster structures.

Presenter: Pham Van Hai

P.94 – Poster, VCTP-45

Neutron bubble in ^{54}Ca nucleus

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The neutron-rich nucleus ^{54}Ca which far-stable-line isotope are recently considered since experimental evidence of this isotope related to the new nuclear 'magic number'. Especially, with $N = 34$, the orbital $3s_{1/2}$ in the neutron shell of ^{54}Ca is not occupied and can cause the bubble structure in the neutron density. Therefore, we calculate microscopically the nucleon (proton/neutron) density to examine the existence of the "bubble" structure at the zero and finite temperature. Particularly, establishing Skyrme-Hartree-Fock mean field plus thermal exact pairing solution (FTEP) described mainly nucleon density of ^{54}Ca. The obtained results show the existence of the neutron bubble in ^{54}Ca and the disappearance of this structure with increasing temperature.

Presenter: Le Ngoc Uyen

P.95 – Poster, VCTP-45

Discrete SHADE method for in-core fuel management of VVER-1000 reactor

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In-core fuel management (ICFM) is known as one of the most complicated tasks of reactor core design for determining an optimal core loading pattern of available fuel assemblies. This work

presents the development of a Success-History based Adaptive Differential Evolution (SHADE) method for the ICFM problem of a VVER-1000 reactor. SHADE is an advanced version of differential evolution (DE) method, which is originally developed for continuous-variable multi-objective optimization problems. However, the ICFM problem of a nuclear reactor works with integer variables corresponding the positions of fuel assemblies in the core. Several discretization approaches have been proposed and investigated for a discrete SHADE method. Comparison among the discretization approaches has been conducted based on numerical calculations for optimizing fuel loading pattern of a reference VVER-1000 core. Based on the numerical calculation and the comparison, a suitable discretization approach has been selected for the discrete SHADE method for further development.

Presenter: Tran Viet Phu

P.96 – Poster, VCTP-45

Otpical properties of slidding bilayer graphene

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Slidding bilayer graphene is a chiral system which has been recently shown to present circular dichroism. In this work, the optical properties of sliding bilayer graphene are theoretically. The Hall conductivity of the slidding bilayer graphene is calculated by the Kubo formula. The Kerr (Faraday) angle which is optical rotation of the polarization of light on slidding bilayer graphene are calculated by using a method based on transfer matrices.

Presenter: Tran Ky Vi

P.97 – Poster, VCTP-45

Opto-electronic property of Nitrogen doped graphene quantum dots

Nguyen Vo Anh Duy, Thanh Tien Nguyen, Van An Dinh, Minh Triet Dang

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Graphene quantum dots (QDs) have been widely studied in recent years due to its unique optical, electrical and optoelectrical properties in applications in solar devices. In this talk, we present the opto-electronic properties of graphene quantum dots (GQDs) and nitrogen doped graphene quantum dots (N-GQDs) using first principles methods. Based on density functional theory (DFT), we investigated the changes of geometry structure, density of states, projected density of states and optical absorption of quantum dots. We have shown that by doping nitrogen to graphene quantum dots, the optical absorption of quantum dots experience a red shift compared to that of the pristine graphene quantum dots. These results opens a new opportunity to develop nanoscale devices using graphene quantum dots in applications in solar devices.

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Presenter: Nguyen Vo Anh Duy

P.98 – Poster, VCTP-45

Structural, Electronic and Mechanical Properties of Few-layer Porous Nanosheet from spheroidal cage-like ZnO polymorph

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The low-dimensional II-VI group semiconductors have recently emerged as interesting candidate materials for the tailoring of two dimensional (2D) layered structures. Herein, a series of the cage-like nanoporous composed of spheroidal hollow cages (ZnO)12 , cutting from the high symmetrical cubic SOD cage-like polymorph as building block, is proposed. We have performed the density-functional tight binding (DFTB+) calculations on the structural, electronic and mechanical properties of this few- layer (ZnO)9 - , (ZnO)12 - and (ZnO)16 -cage-block nanosheet series, to investigate the effects of structural modification and sheet thickness on their structural, electronic, and mechanical properties. Optimized geometries, formation energy, phonon spectra, electronic band structure, and elastic tensor calculation has ensured the energetically, dynamical and mechanical stability for the sheets. Furthermore, the theoretically found nanosheet series possess an intrinsic wide direct band gap preserving from wurtzite tetragonal-based bonding. This high symmetry wide bandgap semiconductor nanosheet series and their derivatives are expected to have broad applications in photocatalysis, and biomedicine.

Presenter: Vu Ngoc Tuoc

P.99 – Poster, VCTP-45

Investigate the dependence of multiple recollision on laser wavelength in the nonsequential double ionization process

Nang V. Do (1) Truong Dang Hoai Thu (2), (3), (4) Quach Ai Mi (4) Nguyen Hong Hanh (4) Pham Nguyen Thanh Vinh (4)

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We investigate the recollision dynamics of the nonsequential double ionization process induced by linearly polarized laser pulses with the three dimensional classical ensemble model. The results show that the two electron correlated momentum distribution is significantly contaminated by the multiple recollision events for sufficiently short laser wavelength. The effect of multiple recollision decreases as the laser wavelength grows. The mechanisms governing the nonsequential double ionization process are also thoroughly studied.

Presenter: Truong Dang Hoai Thu

P.100 – Poster, VCTP-45

Molecules on β_{12} borophene: chemical bonding analysis and van der Waals density functional assessment

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Recently, β_{12} borophene has been received great attention due to its potential properties to

be applied in electronic devices such as possessing spin gapless Dirac cone, rich band structure, and high Young's modulus, etc. However, the interaction between common gases and β_{12} borophene has been still remaining ambiguous. To provide an insight into adsorption behavior of borophene, we study the interactions of β_{12} borophene towards five hazardous gases namely CO, NO, NH_3, NO_2, and CO_2 using van der Waals density functionals (vdW-DFs) method. Among considered gases, CO_2 is physisorbed meanwhile other gases have chemically bonding with β_{12} borophene. Notably, NO_2 exhibits its superior interaction with borophene, suggesting the potential of borophene in sensing or capturing this gas. Besides, we take into account the effects of vdW correlation models and constraint of geometry. We found that the adsorption energies given by vdW-DFs increase as the order of vdW-DF1 vdW-DF2 $<$ optPBE-vdW $<$ rev-vdW-DF2. Besides, CO and NH_3 are likely to be susceptible with the constraint on geometry of borophene. By COOP, PDOS and vibrational analysis, we also provide the details of orbital hybridization between atomic orbitals of boron and molecular orbitals of molecules; thereby, elucidating the adsorption mechanism, the origin of preferable adsorption site and redshift of molecules' stretching modes. The results are expected to benefit experiments related to this topic in very near future.

Presenter: Dinh Van An

P.101 – Poster, VCTP-45

Novel orthorhombic Tavorite-like material for lithium ion batteries: DFT investigation

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Recently, lithium-ion batteries have been emerged as the most successful commercial energy storage for portable devices such as laptop, smartphone, camera. Since the cathode material determines the overall voltage of rechargeable batteries, more and more endeavors have been made to investigate cathode material with excellent voltage and high capacity. Using density functional theory (DFT), we proposed a novel orthorhombic cathode material Li_xVPO_4F which its structure have Tavorite-like framework with the typical F-V-F-V-F finite chain along the [100] direction. In fully charging and discharging states, Li_xVPO_4F is predicted to be thermally stable because no imaginary frequency is found in the phonon spectra at x = 0 and 1. Our DFT results show that the intermediate ($0<x<1$) states experience two bi-phase reactions in the concentration ranges [0.125; 0.5] and [0.5; 1.0]. The proposed material exhibits an excellent average voltage of 4.12 V and a high theoretical capacity of 156 mAh/g. Therefore, the Tavorite-like material could be a promising cathode material in the future.

Presenter: Dinh Van An

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