



Program & Abstracts

44th Vietnam Conference on Theoretical Physics

**HỘI NGHỊ VẬT LÝ LÝ THUYẾT VIỆT NAM
LẦN THỨ 44**



Đồng Hới

29 July - 1 August, 2019

Program & Abstracts

44th Vietnam Conference on Theoretical Physics

Muong Thanh Nhat Le Hotel
121 Trương Pháp, Đồng Hới
Quảng Bình, Việt Nam

29 July - 1 August, 2019

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Welcome Message

It is a great pleasure to welcome you in the *44th Vietnam Conference on Theoretical Physics* (VCTP-44) in Dong Hoi.

The VCTP-44 is organized by the Institute of Physics – 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 for over 40 years, and has become the most well-known annual scientific forum dedicated to the dissemination of the latest development in the field of theoretical physics within the country.

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.

Coming to this year conference are 148 participants from about 30 research and educational institutions in Vietnam and 11 invited speakers from abroad. 13 invited talks, 22 oral and 104 poster contributions will be presented at the conference.

We wish you enjoy the scientific atmosphere at the conference and have a memorable stay in Dong Hoi.

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, Ha Noi)

Chair

- Bach Thanh Cong (VNU University of Science, Ha Noi)

Organizing Committee

- Trinh Xuan Hoang (Institute of Physics, VAST, Ha Noi), Chair
- Dinh Nguyen Dinh (Institute of Physics, VAST, Ha Noi), Chair
- Le Van Hoang (Ho Chi Minh City Pedagogical University)
- Dang Van Soa (Hanoi Metropolitan University)

Program Committee

- Hoang Anh Tuan (Institute of Physics, VAST, Ha Noi), Chair
- Phung Van Dong (Phenikaa University, Ha Noi)
- Nguyen The Toan (VNU University of Science, Ha Noi)
- Vu Ngoc Tuoc (Hanoi University of Science and Technology)

Secretariat

- Duong Thi Man (Institute of Physics, VAST, Ha Noi)

Sponsors

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

General Information

Conference Venue

The VCTP-44 conference takes place in:

Muong Thanh Nhat Le Hotel

121 Truong Phap street

Dong Hoi city

Quang Binh province, Viet Nam



Direction

Travelers may come to Dong Hoi by road transport, train or airplane. Dong Hoi has a domestic airport, the Dong Hoi Airport (VDH). International travelers may have flight connections in Ha Noi or Ho Chi Minh city.

The conference venue is about 6 km from Dong Hoi Airport. To get to the conference venue from the airport, participants can use taxis.

Instructions for Speakers

Speakers are requested to be present in their respective session room at least 10 minutes prior to the commencement of the session.

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.

Speakers should bring their own laptop ready for presentation. Laptop needs to be checked with the projector to be sure it is working before the session starts.

Instructions for Posters

Two poster sessions will be held during 08:30 AM - 10:00 AM in the mornings of 30 July and 1 August. However, it is recommended that posters are hung the whole day (morning and afternoon) of the respective dates of the sessions to facilitate interested viewers and discussions.

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.

Instructions for Session Chairs

Please be aware of the time frame designated to each presenter, and warn the presenters as follows:

- Invited talk: first warning at 20 minutes, second warning at 25 minutes.
- Regular talk: first warning at 15 minutes, second warning at 17 minutes.

Meeting Room

All sessions take place in one conference room of the Muong Thanh Nhat Le Hotel. Please follow the direction in the lobby for getting to the conference room.

Lunches

Lunches are provided for conference participants in the Muong Thanh Nhat Le Hotel. 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: 31 July 2019, from 18:30 PM

Place: Muong Thanh Nhat Le Hotel.

For your accompanied family members to attend Gala Dinner, please buy tickets from the conference secretary on 30 July.

Excursion

A full-day tour to visit Thiên Đường Cave (Paradise Cave) will be organized on Wednesday, 31 July. The cave is about 60 km northwest of Dong Hoi city, and is within the Phong Nha - Kẻ Bàng National Park, UNESCO's World Heritage Site. The cost of the tour is only partially sponsored by the organizers. Please register and pay a registration fee for the tour with the conference secretary on 29 July.

VTPS Young Research Award

On 29 July, at the opening session of the conference will be an announcement and the delivery of the 2019 VTPS Young Research Awards to Mr. Le Tan Phuc (Institute of Fundamental and Applied Sciences, Duy Tan University).

VTPS Meeting

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

Time: 17:30 PM - 18:00 PM, Monday, 29 July 2019.

Place: Conference Hall, Muong Thanh Nhat Le Hotel.

Program Timetable

Time	Monday 29 July	Tuesday 30 July	Wednesday 31 July	Thursday 1 August
08:30 – 10:00	Opening (8:40) Mahn-Soo Choi (I.1) Do Quoc Tuan (O.1) (Chair: Nguyen Ba An)	Poster Session 1 (Chair: Hoang Anh Tuan)	Excursion Gala Dinner (18:30 - 20:30)	Poster Session 2 (Chair: Nguyen Quang Hung)
10:00 – 10:30	Coffee break	Coffee break		Coffee break
10:30 – 12:00	Diep The Hung (I.2) Ngo Van Thanh (O.2) Huynh Thanh Duc (O.3) Nguyen Nhu Dat (O.4) (Chair: Bach Thanh Cong)	Nguyen Ba An (I.6) Kieu Quang Tuan (O.9) Hirobumi Mineo (O.10) Phan Thi Ngoc Loan (O.11) (Chair: Truong Minh Duc)		Takeo Inami (I.10) Cao Van Son (I.11) Phan Anh Vu (O.16) Le Xuan Thuy (O.17) (Chair: Nguyen Anh Ky)
12:00 – 14:00	Lunch	Lunch		Lunch
14:00 – 15:30	Yoji Shibutani (I.3) Jer-Lai Kuo (I.4) Vu Ngoc Tuoc (O.5) (Chair: Nguyen Manh Duc)	Philippe Derreumaux (I.7) Nguyen Hoang Phuong (I.8) Trinh Xuan Hoang (O.12) (Chair: Mai Suan Li)		Toshifumi Noumi (I.12) Tran Minh Hieu (O.18) Tran Quang Loc (O.19) Le Duc Ninh (O.20) (Chair: Takeo Inami)
15:30 – 16:00	Coffee break	Coffee break		Coffee break
16:00 – 17:30	Le Tan Phuc (I.5) Tran Viet Nhan Hao (O.6) Kazuhito Mizuyami (O.7) Nguyen Quang Hung (O.8) (Chair: Le Van Hoang)	Mai Suan Li (I.9) Diep The Hung (O.13) Dinh Van An (O.14) Dang Minh Triet (O.15) (Chair: Trinh Xuan Hoang)		Nguyen Manh Duc (I.13) Nguyen Thi Kim Quyen (O.21) Nguyen Thi Loan (O.22) (Chair: Nguyen Hong Quang) Closing
from 17:30	VTPS Meeting			

Conference Program

Monday, 29 July 2019

Opening Session

Chair: Bach Thanh Cong

08:40 - 08:50 Opening

08:50 - 09:00 Delivery of VTPS Young Research Award

Oral Session:

Chair: Nguyen Ba An

09:00 - 09:30 I.1 – Invited

Weak-Strong Coupling Duality in the Cavity QED
Mahn-Soo Choi (Korea University)

09:30 - 09:50 O.1 – Oral

On a five dimensional counterexample to the cosmic no-hair conjecture
Do Quoc Tuan (VNU Faculty of Physics)

09:50 - 10:00 Photo session

10:00 - 10:30 Coffee break

Oral Session: *Condensed Matter Physics*

Chair: Bach Thanh Cong

10:30 - 11:00 I.2 – Invited

Spin Waves and Skyrmions in Magneto-Ferroelectric Superlattices
Diep The Hung (University of Cergy-Pontoise)

11:00 - 11:20 O.2 – Oral

Wang-Landau simulation of smectic phases
Ngo Van Thanh (Institute of Physics)

11:20 - 11:40 O.3 – Oral

Photovoltaic effect due to asymmetric electron-hole interaction in semiconductor quantum wells
Huynh Thanh Duc (Ho Chi Minh City Institute of Physics, VAST)

11:40 - 12:00 O.4 – Oral

LO-Phonon-limited Electron Mobility in a Core-Shell Polar Semiconductor Quantum Wire

Nguyen Nhu Dat (ITAR, Duy Tan University)

12:00 - 14:00 Lunch

Oral Session: *Condensed Matter Physics*

Chair: **Nguyen Manh Duc**

14:00 - 14:30 I.3 – Invited

Physics of Plasticity from Atomistic Views; Defect Mechanics

Yoji Shibutani (Osaka University)

14:30 - 15:00 I.4 – Invited

Ab Initio Anharmonic Algorithms to Understand Structures and Vibrational Spectra of Molecular Systems

Jer-Lai Kuo (Institute of Atomic and Molecular Sciences, Academia Sinica)

15:00 - 15:20 O.5 – Oral

Computational predictions of two-dimensional covalent organic frameworks (COF) based on 2D square lattice topology

Vu Ngoc Tuoc (Hanoi university of Science and Technology)

15:30 - 16:00 Coffee break

Oral Session: *Particle, Nuclear, and Astro- Physics*

Chair: **Le Van Hoang**

16:00 - 16:30 I.5 – Invited

Renormalizing random-phase approximation by using exact pairing

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

16:30 - 16:50 O.6 – Oral

Deuteron elastic scattering based on Faddeev-Alt-Grassberger-Sandhas equations within the realistic potentials

Tran Viet Nhan Hao (Faculty of Physics, University of Education, Hue University)

16:50 - 17:10 O.7 – Oral

Introduction of the extended Jost function formalism for S-matrix analysis of nucleon-nucleus scattering

Kazuhito Mizuyama (Duy Tan University)

17:10 - 17:30 O.8 – Oral

Second-order phase transition in an odd-odd deformed and hot-rotating nucleus

Nguyen Quang Hung (Institute of Fundamental and Applied Sciences, Duy Tan University)

17:30 - 18:00 VTPS Meeting

Tuesday, 30 July 2019

Poster Session 1

Chair: Hoang Anh Tuan

- 08:30 - 10:00 P.1 – Poster
Computational study of the effect of protonation states of PSA protein zinc fingers on its DNA binding
Nguyen Hai Ly (Hanoi university of science)
- 08:30 - 10:00 P.2 – Poster
New one-loop formulas for Higgs $\rightarrow VV^*$
Tran Tri Dung (University of Science, 227 Nguyen Van Cu, Dist. 5, Ho Chi Minh City, Vietnam)
- 08:30 - 10:00 P.3 – Poster
Study of Dark Matter in the 3-3-1 with CKS mechanism
Hoang Ngoc Long (IOP)
- 08:30 - 10:00 P.4 – Poster
Self-Diffusion Coefficient of Solute Molecule in Diluted Mixtures: A Non-Equilibrium Molecular Dynamics Approach
Thieu Quang Quoc Viet (Can Tho University)
- 08:30 - 10:00 P.5 – Poster
Fractionation of Noble Gases in Normal Alkanes at Equilibrium: Monte-Carlo molecular simulation
Luc Han Tuong (Ho Chi Minh University of science,)
- 08:30 - 10:00 P.6 – Poster
Spontaneous decay rate and Casimir–Polder interaction of a two-level atom in a Bragg-reflector cylindrical structure
Nguyen Dung Chinh (IFAS, Duy Tan University)
- 08:30 - 10:00 P.7 – Poster
On anisotropic power-law Gauss-Bonnet inflation
Do Quoc Tuan (VNU Faculty of Physics)
- 08:30 - 10:00 P.8 – Poster
On the derivation of the entropy of ideal quantum gases confined in a three-dimensional harmonic potential
Pham Nguyen Thanh Vinh (Department of Physics, Ho Chi Minh City University of Education)
- 08:30 - 10:00 P.9 – Poster
Strain and electric field tunable electronic properties and Schottky barrier of Graphene/GaX (X = S, Se) heterostructures
Nguyen Van Chuong (Le Quy Don Technical University)
- 08:30 - 10:00 P.10 – Poster

Cyclotron-phonon resonance via one and two-photon absorption in asymmetrical Gaussian potential quantum wells

Le Dinh (University of Education, Hue University)

- 08:30 - 10:00 P.11 – Poster
Specific Ion Effects on Static and Dynamic Properties of Aqueous Solution Confined between Uniformly Charged Hydrophobic Plates
Nguyễn Minh Hiền (Department of Education and Training, University of Khanh Hoa, Nha Trang City, Khanh Hoa Province, Vietnam)
- 08:30 - 10:00 P.12 – Poster
Effect of Rigidity on Thermophysical Properties of Lennard-Jones Chains: A Molecular Simulation Study
Nguyễn Phúc (Ho Chi Minh University of science)
- 08:30 - 10:00 P.13 – Poster
Minimal flipped 3-3-1 model
Nguyen Tuan Duy (Center for Theoretical Physics, Institute of Physics, VAST)
- 08:30 - 10:00 P.14 – Poster
Resonance energy transfer rate in the presence of a cylindrical photonic band-gap structure
Nguyen Van Phuoc (Trường ĐH Tôn Đức Thắng)
- 08:30 - 10:00 P.15 – Poster
The study of neutron star: Nuclear matter Equation of state and Symmetry energy
Ngô Hải Tân (Phenikaa Institute for Advanced Study (PIAS))
- 08:30 - 10:00 P.16 – Poster
Debye model for heat capacity of liquid water at normal condition
Tran Thi Nhan (Hanoi University of Industry)
- 08:30 - 10:00 P.17 – Poster
DFT calculation of electronic and optical properties of quaternary sulfide $\text{Cu}_2\text{HgSnS}_4$: a prospective photovoltaic semiconductor
Vu Van Tuan (Institute for Computational Science, Ton Duc Thang University)
- 08:30 - 10:00 P.18 – Poster
Is the Nonlocal Band-to-Band Tunneling Model Proper for Calculating the Tunneling Current in Tunnel Devices?
Nguyen Dang Chien (Dalat University)
- 08:30 - 10:00 P.19 – Poster
Optical absorption coefficients and relative refractive index changes in monolayer silicene
Huynh V. Phuc (Dong Thap University)

- 08:30 - 10:00 P.20 – Poster
Mechanisms of nonsequential double ionization process of argon by near-single cycle laser pulse
Truong Dang Hoai Thu (Ho Chi Minh city University of Education)
- 08:30 - 10:00 P.21 – Poster
Controlling the recolliding properties in nonsequential double ionization by orthogonal two-color laser field
Truong Dang Hoai Thu (Ho Chi Minh city University of Education)
- 08:30 - 10:00 P.22 – Poster
Band-gap Modulation of Sawtooth Penta-graphene Nanoribbons under Uniaxial Elastic Strain
Thanh Nhật Lê (Đại học Cần Thơ)
- 08:30 - 10:00 P.23 – Poster
Classical interpretation of dynamics of ultracold atoms in the tilted optical lattice
Pham Nguyen Thanh Vinh (Department of Physics, Ho Chi Minh City University of Education)
- 08:30 - 10:00 P.24 – Poster
Effect of spatially modulated magnetic field and spin-orbit coupling in Lieb lattice
Nguyễn Hồng Sơn (Trường Đại học Công đoàn)
- 08:30 - 10:00 P.25 – Poster
The formation of magnetization plateaus in the Sastry-Sutherland lattice with disorder.
Bach Huong Giang (VNU University of Science)
- 08:30 - 10:00 P.26 – Poster
Molecular dynamics simulation of microstructure and atom-level mechanism of crystallization pathway in iron nanoparticle
Giap Thi Thuy Trang (Department of Computational Physics, Hanoi University of Science and Technology)
- 08:30 - 10:00 P.27 – Poster
A review of using re-quantized classical molecular dynamics simulation method for spectral shape study
Ngo Hoa Ngoc (Hanoi National University of Education)
- 08:30 - 10:00 P.28 – Poster
Non-equilibrium condensation of Polaritons I: kinetics of the Excitations
Đoàn Trí Dũng (Viện Vật TP. Hồ Chí Minh)
- 08:30 - 10:00 P.29 – Poster
Sampling the folding transition state ensemble in a tube-like model of protein
Nguyen Ba Hung (Faculty of physics and biophysics, Vietnam military medical university)

- 08:30 - 10:00 P.30 – Poster
The geometry of ribosomal exit tunnel affects post-translational escape of nascent proteins
Bui Phuong Thuy (Duy Tan University)
- 08:30 - 10:00 P.31 – Poster
Study on elastic and nonlinear deformations of BCC interstitial alloy FeC
Nguyễn Đức Hiền (Sở Giáo dục và Đào tạo Gia Lai)
- 08:30 - 10:00 P.32 – Poster
Structural and electronic properties of silicene/gallium selenide van der Waals heterostructure: A first principles study
Nguyen Ngoc Hieu (Duy Tan University)
- 08:30 - 10:00 P.33 – Poster
Transient super-slow power-law decay of the time-dependent reflection induced by correlations in semi-infinite disordered media
Ngô Thị Hồng Vy (Department of Physics, Quy Nhon University)
- 08:30 - 10:00 P.34 – Poster
Investigation of thermodynamic properties and self-diffusion of AuCu superlattice by an analytic statistical moment method
Cao Huy Phuong (Hung Vuong University)
- 08:30 - 10:00 P.35 – Poster
Vibration effect on the elastic differential cross section in the gas-phase electron diffraction within the multiple scattering model
Nguyen Thi Hien (Department of Physics, Faculty of Natural Sciences and Technology, Tay Nguyen University)
- 08:30 - 10:00 P.36 – Poster
Molecular dynamics simulations of structural transformation and mechanical properties in densified MgSiO₃
Le Van Vinh (Phenikaa University)
- 08:30 - 10:00 P.37 – Poster
A comparative study of the localization properties of eigenstates in conservative and non-conservative systems: Effects of long-range correlation disorder
Lieu Thi Kim Thoa (Department of Physics, Quy Nhon University)
- 08:30 - 10:00 P.38 – Poster
Elementary excitation in the layered ferroics
Nguyễn Từ Niệm (VNU University of Science)
- 08:30 - 10:00 P.39 – Poster
Decay of neutron with participation of the light vector boson X₁₇
Pham Tien Du (Energy Department, Thuy Loi University)
- 08:30 - 10:00 P.40 – Poster
Electric-field-enriched electronic and optical properties of Bernal stacked bi-

- layer graphene nanoribbons
Vu Thanh Tra (Can Tho University)
- 08:30 - 10:00 P.41 – Poster
 A model to predict the thermal diffusion factors in binary mixtures
Nguyen Tu Khai Nam (Ho Chi Minh University of Science)
- 08:30 - 10:00 P.42 – Poster
 Dark matter and flavor changing in the flipped 3-3-1 model
Thiện Đức Lê (leducthienhvt1@gmail.com)
- 08:30 - 10:00 P.43 – Poster
 Algebraic relation between bases of the nine-dimensional MICZ-Kepler problem
Le Dai Nam (Atomic Molecular and Optical Physics Research Group, Advanced Institute of Materials Science, Ton Duc Thang University)
- 08:30 - 10:00 P.44 – Poster
 Equation of state and thermal expansion of metals Cu, Au, Ag
Pham Duy Tan (Research Department, Tank Armour Command)
- 08:30 - 10:00 P.45 – Poster
 Mott transition in the mass imbalanced ionic Hubbard model at half filling
Nguyen Thi Hai Yen (Institute of Physics)
- 08:30 - 10:00 P.46 – Poster
 Adsorption of Gas Molecules on Sawtooth Penta-Graphene Nanoribbons
Vo Van On (University of Thu Dau Mot)
- 08:30 - 10:00 P.47 – Poster
 Molecular dynamics simulation of amorphous silica under pressure
Giap Thi Thuy Trang (Department of Computational Physics, Hanoi University of Science and Technology)
- 08:30 - 10:00 P.48 – Poster
 Neutrino mass and mixing in an A4 model with inverse seesaw mechanism
Ngo Minh Ket (Can Tho University)
- 08:30 - 10:00 P.49 – Poster
 Decay of SM-like Higgs $h \rightarrow \mu\tau$ in an A4 model with inverse seesaw mechanism
Ho Viet Thang (Can Tho University)
- 08:30 - 10:00 P.50 – Poster
 Retrieval of structural parameters of monolayer transition-metal dichalcogenides from the exciton energy spectrum
Ly Duy-Nhat (HCMC University of Education)
- 08:30 - 10:00 P.51 – Poster
 Magnetic orders of Heisenberg models with arbitrary spin in semi-fermionic representation

Pham Thị Thanh Nga (Thuy loi University)

08:30 - 10:00 P.52 – Poster
 Nonlocal properties and quantum teleportation in the photon-pair-subtracted and photon-pair-added two-mode squeezed vacuum state
Tran Quang Dat (University of Transport and Communications - Campus in Ho Chi Minh City)

10:00 - 10:30 Coffee break

Oral Session: *Molecular Physics, Quantum Optics and Quantum Information*

Chair: **Truong Minh Duc**

10:30 - 11:00 I.6 – Invited
 Joint Remote Preparation of General Quantum States of Arbitrary Dimensions
Nguyen Ba An (Thang Long University)

11:00 - 11:20 O.9 – Oral
 Probe-controlled-system approach to direct state measurement
Kieu Quang Tuan (Department of Theoretical Physics, University of Science, Ho Chi Minh City)

11:20 - 11:40 O.10 – Oral
 Quantum method for probing molecular chirality of enantiomer specific coherent pi-electron angular momentum
Hirobumi Mineo (Ton Duc Thang University)

11:40 - 12:00 O.11 – Oral
 Extracting molecular structure from the laser-induced electron diffraction spectra
Phan Thi Ngoc-Loan (Ho Chi Minh City University of Education)

12:00 - 14:00 Lunch

Oral Session: *Soft Matter, Biological and Interdisciplinary Physics*

Chair: **Mai Suan Li**

14:00 - 14:30 I.7 – Invited
 Computer simulations of amyloid proteins in various environments and folded proteins in a cell-like environment
Philippe Derreumaux (Laboratory of Theoretical Biochemistry, UPR9080 CNRS, Université de Paris)

14:30 - 15:00 I.8 – Invited
 Ultrasound interacts with biological systems
Nguyen Hoang Phuong (Laboratory of theoretical biochemistry, CNRS)

15:00 - 15:20 O.12 – Oral
 Local symmetry determines the phases of linear chains: a simple model for the self-assembly of peptides

Trinh Xuan Hoang (Institute of Physics, VAST)

15:30 - 16:00 Coffee break

Oral Session: *Soft Matter, Biological and Interdisciplinary Physics*

Chair: **Trinh Xuan Hoang**

16:00 - 16:30 I.9 – Invited

Protein aggregation and neurodegenerative diseases

Mai Suan Li (Institute of Physics, Polish Academy of Sciences)

16:30 - 16:50 O.13 – Oral

Social Conflicts Studied by Means of Statistical Physics and Monte Carlo Simulations

Diep The Hung (University of Cergy-Pontoise)

16:50 - 17:10 O.14 – Oral

Adsorption Trend of Volatile Organic Compounds on monolayer MoS₂

Dinh Van An (Vietnam Japan University)

17:10 - 17:30 O.15 – Oral

Micro-mechanical properties of colloidal aggregates with critical Casimir forces

Dang Minh Triet (Can Tho University)

Wednesday, 31 July 2019

Excursion

18:30 - 20:30 Gala Dinner

Thursday, 1 August 2019

Poster Session 2

Chair: **Nguyen Quang Hung**

08:30 - 10:00 P.53 – Poster

Role of pairing in maintaining the constant value of nuclear temperature at low excitation energy

Le Thi Quynh Huong (University of Khanh Hoa)

08:30 - 10:00 P.54 – Poster

The effect of external electric fields on the electronic band structure of AA-stacking bilayer graphene ribbons

Dao Thuy Tuong Vi (School of graduate, College of Natural Sciences, Can-Tho University)

08:30 - 10:00 P.55 – Poster

Electronic structures in armchair silicene nanoribbons

Danh Tan Xuan ((1) School of graduate, CanTho University; (2) Thot Not

Highschool, Can Tho, Vietnam.)

- 08:30 - 10:00 P.56 – Poster
Investigation of the magneto-dynamical dielectric function of monolayer phosphorene
Bui Dinh Hoi (University of Education, Hue University)
- 08:30 - 10:00 P.57 – Poster
Metal-insulator phase diagram of the half-filled Anderson-Hubbard model
Hoang Anh Tuan (Viện Vật lý)
- 08:30 - 10:00 P.58 – Poster
Theoretical investigation of quantum beat of excitons in GaAs/AlGaAs quantum dots
Le Thi Ngoc Bao (Hue University of Sciences)
- 08:30 - 10:00 P.59 – Poster
Improved Simulated Annealing Methods for core loading pattern optimization of VVER-1000 reactor
Tran Viet Phu (Institute for Nuclear Science and Technology - VINATOM)
- 08:30 - 10:00 P.60 – Poster
A theoretical study of the exciton quantum beats in GaAs/AlGaAs cylindrical quantum wires
Dương Đình Phước (Hue University of Education)
- 08:30 - 10:00 P.61 – Poster
Dynamical properties of the photon-added two-mode $SU(1,1)$ coherent state in the Jaynes-Cummings-model
Le Thi Hong Thanh (Quang Nam University)
- 08:30 - 10:00 P.62 – Poster
Particle-type Burnable Poison for Improving Neutronics Characteristics and Thermal Conductivity of VVER-1000 Assembly
Tran Hoai Nam (Duy Tan University)
- 08:30 - 10:00 P.63 – Poster
Method of solving the time-dependent Schrödinger equation and its implementation in strong field physics
Le Thi Cam Tu (Ton Duc Thang University)
- 08:30 - 10:00 P.64 – Poster
The classical effects of Einstein's GRT for some $f(R)$ modified gravity models in the Sun system
Vo Van On (University of Thu Dau Mot)
- 08:30 - 10:00 P.65 – Poster
Temperature-dependent transport properties of two-dimensional hole gas in Ge channel modulation-doped square quantum wells
Tran Thi Hai (Hong Duc University)

- 08:30 - 10:00 P.66 – Poster
Investigation of the frequency shift of microcantilever depends on positions and the correlation between two absorbed mass on the surface.
Le Tri Dat (Laboratory of Applied Physics, Advanced Institute of Materials Science, Ton Duc Thang University)
- 08:30 - 10:00 P.67 – Poster
Distributions transition under orthogonal random fluctuations
Chu Thuy Anh (Institute of Physics, VAST)
- 08:30 - 10:00 P.68 – Poster
Anisotropic magnetoresistance of nickel nanowires with various diameters
Ngo Van Thanh (Institute of Physics)
- 08:30 - 10:00 P.69 – Poster
Performance of quantum algorithms on the IBM quantum computers
Nguyen Quoc Hung (Nano and Energy Center, Hanoi University of Science, VNU)
- 08:30 - 10:00 P.70 – Poster
Theoretical study for mid-infrared graphene plasmons
Do Thi Nga (Institute of Physics, VAST)
- 08:30 - 10:00 P.71 – Poster
Self-assembly of anisotropic colloids with critical Casimir forces: A simulation study
Dang Minh Triet (Can Tho University)
- 08:30 - 10:00 P.72 – Poster
Mechanical-thermodynamic responses of 2D penta-graphene materials under applied forces
Nhân Hoàng Lê (Can Tho University)
- 08:30 - 10:00 P.73 – Poster
Ab initio Study on Adsorption of Volatile Organic Compounds on Germanene
Duong Thi Diem My (University of Education, Hue University)
- 08:30 - 10:00 P.74 – Poster
First-principles study of $\text{Na}_2\text{Fe}_3(\text{SO}_4)_4$: A new material of potential cathodes for the sodium-ion rechargeable batteries
Tran Thien Lan (Nguyen Hue Highschool)
- 08:30 - 10:00 P.75 – Poster
Performance of quantum algorithms on the IBM quantum computers
Tran Minh Duc (Hanoi University of Science and Technology)
- 08:30 - 10:00 P.76 – Poster
Generation of entangled states in Kerr-like nonlinear coupler pumped by external fields
Doan Quoc Khoa (Quang Tri Teacher Training College)

- 08:30 - 10:00 P.77 – Poster
Dynamics heterogeneity and diffusion mechanism in sodium-silicate melts.
Molecular dynamics simulation
Nguyen Thi Thanh Ha (Department of Computational Physics, Hanoi University of Science and Technology)
- 08:30 - 10:00 P.78 – Poster
Determination of the mass diffusion coefficient of H₂O diluted in N₂ using classical molecular dynamic simulation
Ngô Hoa Ngọc (Hanoi National University of Education)
- 08:30 - 10:00 P.79 – Poster
Quantitative measures of entanglement and quantum teleportation in the photon-added and photon-subtracted two-mode pair coherent state
Hồ Sỹ Chương (Dong Nai University)
- 08:30 - 10:00 P.80 – Poster
Effects of the gold nanoparticle size on resonance energy transfers in optics system
Nguyễn Minh Hoa (Trường Đại học Y Dược Huế)
- 08:30 - 10:00 P.81 – Poster
The quantum Etingshausen effect in parabolic quantum well with in-plane magnetic field in the presence of laser radiation under the influence of confined optical phonon
Nguyễn Thị Lâm Quỳnh (Hanoi University of Science)
- 08:30 - 10:00 P.82 – Poster
Effects of pairing correlations on the reactions observables of nucleon-nucleus elastic scattering
Nguyen Hoang Tung (Department of Nuclear Physics and Nuclear Engineering, Faculty of Physics and Engineering Physics, VNUHCM-University of Science)
- 08:30 - 10:00 P.83 – Poster
Proton-nucleus elastic scattering based on microscopic approaches at low-energy
Trần Diệu Thùy (Faculty of Physics, University of Education, Hue University)
- 08:30 - 10:00 P.84 – Poster
High-pressure melting curves of and phases of iron
Nguyễn Thị Hồng (Hong Duc university)
- 08:30 - 10:00 P.85 – Poster
Numerical mean-field solution for the distribution of counterions in a hexagonal DNA lattice
Tuyền Thanh Trần (Trường THPT Quế Võ số 3)
- 08:30 - 10:00 P.86 – Poster

- Dependence of lattice spacing on the temperature and pressure for ordered Cu₃Au alloy.
Pham Duy Tan (Research Department, Tank Armour Command)
- 08:30 - 10:00 P.87 – Poster
 Diverse Electronic Transport of Sawtooth Penta-Graphene Nanoribbons by Substitutional Doping
Pham Thi Bich Thao (Can Tho University)
- 08:30 - 10:00 P.88 – Poster
 New analysis characterizing the dynamics heterogeneity and microstructure in liquid silicates
Nguyen Thu Nhan (Hanoi University of Science and Technology)
- 08:30 - 10:00 P.89 – Poster
 Biexciton in two dimensional parabolic quantum dots
Nguyen Hong Quang (Institute of Physics, Vietnam Academy of Science and Technology)
- 08:30 - 10:00 P.90 – Poster
 Interaction between two soft-particles with different sizes
Nguyen Thi Lam Hoai (Institute of physics)
- 08:30 - 10:00 P.91 – Poster
 Non-equilibrium condensation of Polaritons II: luminescence of the Excitations
Đoàn Trí Dũng (Viện Vật TP. Hồ Chí Minh)
- 08:30 - 10:00 P.92 – Poster
 Conceptual design of a small modular reactor with AP1000 fuel assembly
Hoang Van Khanh (Institute for Nuclear Science and Technology)
- 08:30 - 10:00 P.93 – Poster
 Electron-nucleon scatterings in light of ATOMKI'S IPC anomalies
Nguyen Van Dat (Information Technology Institute, VNU)
- 08:30 - 10:00 P.94 – Poster
 Wave functions: from phenomenological to microscopic approaches
Nguyen Nhu Le (Physics Department, Hue University of Education)
- 08:30 - 10:00 P.95 – Poster
 Quantum computation with cloud services: a new paradigm for physicists
Nguyen Quoc Hung (Nano and Energy Center, Hanoi University of Science, VNU)
- 08:30 - 10:00 P.96 – Poster
 Lepton mass and mixing in an extension of the standard model based on $\Delta(54)$ discrete symmetry
Vo Van Vien (Tay Nguyen University)

- 08:30 - 10:00 P.97 – Poster
Electrically controlled magnetism in iron thin film
Tran Van Quang (University of Transport and Communications)
- 08:30 - 10:00 P.98 – Poster
Calculations of beta energies spectra in beta-decay of Rb unstable isotopes
Pham Ngoc Son (Nuclear Research Institute)
- 08:30 - 10:00 P.99 – Poster
Molecular study of interactions of mu-opioid receptor in binding with biased and unbiased ligands by molecular dynamic simulation
Tran Ky Thanh (VNU Vietnam Japan University)
- 08:30 - 10:00 P.100 – Poster
Multi-scale simulation of low-cost metal-organic framework for hydrogen storage
Cao Cong Phuong (VNU Key Laboratory)
- 08:30 - 10:00 P.101 – Poster
Formation of Two-Dimensional Penta-Germanene by Molecular dynamics (MD) simulation
Nguyen Hoang Giang (HCM City Univ. of Technology, Vietnam National Univ.-HCM City, Vietnam)
- 08:30 - 10:00 P.102 – Poster
Composition-dependent microstructural properties of liquid lead silicate
Mai Van Dung (Thu Dau Mot University)
- 08:30 - 10:00 P.103 – Poster
Gravitational waves for a central gravitational field in an $f(R)$ -theory of gravitation
Nguyen Anh Ky (Institute of Physics, VAST)
- 08:30 - 10:00 P.104 – Poster
Scatterings of proton proton to leptons in the Standard Model
Nguyen Tran Quang Thong (HCMUS + IFIRSE)
- 10:00 - 10:30 Coffee break
- Oral Session: Particle, Nuclear, and Astro- Physics**
Chair: Nguyen Anh Ky
- 10:30 - 11:00 I.10 – Invited
Higgs potential at Planck scales and quantum gravity effects
Takeo Inami (RIKEN)
- 11:00 - 11:30 I.11 – Invited
Neutrino Oscillations: Present Landscape and Future Prospects
Cao Van Son (KEK/J-PARC)
- 11:30 - 11:50 O.16 – Oral

Higgs boson mass in Next-to-Minimal Supersymmetric Standard Model with Inverse Seesaw Mechanism

Phan Anh Vũ (VNU HCM - University of Science)

11:50 - 12:10 O.17 – Oral

Kinetic mixing effect in noncommutative B-L theory

Le Xuan Thuy (Vinh Long University Of Technology Education)

12:10 - 14:00 Lunch

Oral Session: *Particle, Nuclear, and Astro- Physics*

Chair: Takeo Inami

14:00 - 14:30 I.12 – Invited

Cosmic inflation as a very high energy particle detector

Toshifumi Noumi (Kobe University)

14:30 - 14:50 O.18 – Oral

Prospect of dark matter searches in split SUSY models

Tran Minh Hieu (Hanoi University of Science and Technology)

14:50 - 15:10 O.19 – Oral

Constraining new physics from Higgs measurements with Lilith: update to LHC Run 2 results

Tran Quang Loc (IFIRSE, ICISE)

15:10 - 15:30 O.20 – Oral

Single top-quark production in association with two jets at the LHC

Le Duc Ninh (Institute For Interdisciplinary Research in Science and Education)

15:30 - 16:00 Coffee break

Oral Session: *Condensed Matter Physics*

Chair: Nguyen Hong Quang

16:00 - 16:30 I.13 – Invited

Predictive modelling of steady-state configuration in non-equilibrium physics

Nguyen Manh Duc (Culham Centre for Fusion Energy)

16:30 - 16:50 O.21 – Oral

Tight binding description for the electronic band structure of penta-graphene

Nguyen Thi Kim Quyen (KienGiang University)

16:50 - 17:10 O.22 – Oral

Spin-dependent tunneling and spin current in semiconductor heterostructures

Nguyen Thi Loan (Graduate University of Science and Technology, VAST and Hong Duc University)

17:10 - 17:20 Closing

Conference Abstracts

I.1 – Invited, VCTP-44

Weak-Strong Coupling Duality in the Cavity QED

*Mahn-Soo Choi**

*Department of Physics, Korea University, Seoul 02841, Korea, *E-mail: choims@korea.ac.kr*

We reveal the duality in the Rabi Hamiltonian, which describes the various physical systems and phenomena. In particular, the superconducting circuit QED systems provide a wide range of scientific platforms from quantum computer to accurate quantum sensing of elementary charge or spin [5]. Further, due to its ultra-strong coupling constant, it has drawn a renewed interested in the Rabi Hamiltonian. In this talk, we reveal the duality in the Rabi Hamiltonian, where the weak and strong coupling regime are mathematically equivalent and related to each other by a unitary transformation. Several examples of the implications of the duality will be discussed including the ground-state squeezing [1,2], the Majorana bound states [3], and the photon localization-delocalization double transitions [4].

[1] M.-J. Hwang , Mahn-Soo Choi, and Rosa Lopez, Phys. Rev. B 76, 165312 (2007).

[2] M.-J. Hwang and Mahn-Soo Choi, Phys. Rev. A 82, 025802 (2010).

[3] M.-J. M.-J. Hwang and Mahn-Soo Choi, Phys. Rev. B 87, 125404 (2013).

[4] M.-J. Hwang, M. Kim, and Mahn-Soo Choi, Phys. Rev. Lett. 116, 153601 (2016).

[5] M. M. Desjardins et al., Nature 545, 71 (2017).

Presenter: Mahn-Soo Choi

I.2 – Invited, VCTP-44

Spin Waves and Skyrmions in Magneto-Ferroelectric Superlattices

H. T. Diep (1) and I. Sharafullin (2)

(1) Laboratoire de Physique Théorique et Modélisation Université de Cergy-Pontoise, CNRS, UMR 8089, 2 Avenue Adolphe Chauvin, 95302 Cergy-Pontoise, Cedex, France; (2) Bashkir State University, 32, Validy str, 450076, Ufa, Russia.

We present in this talk the effects of Dzyaloshinskii-Moriya (DM) magnetoelectric coupling between ferroelectric and magnetic layers in a superlattice formed by alternate magnetic and ferroelectric films. Magnetic films are modeled with the Heisenberg spins interacting with each other via an exchange J and a DM interaction with the ferroelectric interface. Electrical polarizations are assumed to be spins of Ising type occupying the lattice sites in the ferroelectric films. We determine the ground-state (GS) spin configuration in the magnetic film. In zero

applied magnetic field, the GS is periodically non collinear. In an applied field H perpendicular to the superlattice layers, we show the existence of skyrmions at the interface. Using the Green's function method we study the spin waves (SW) excited in the magnetic layer sandwiched between two ferroelectric films, in zero field. We show that the DM interaction strongly affects the long-wave length SW mode, changing from ferromagnetic behavior to antiferromagnetic one with increasing DM interaction. We also calculate the zero-point spin contraction at temperature $T=0$ and the magnetization at low T . In an applied magnetic field H where skyrmions appear, we use Monte Carlo simulations to calculate various physical quantities at finite temperatures such as the critical temperature, the layer magnetization and the layer polarization, as functions of the magnetoelectric DM coupling and H . Phase transition to the disordered phase is studied in detail.

Presenter: Diep The Hung

I.3 – Invited, VCTP-44

Physics of Plasticity from Atomistic Views; Defect Mechanics

Yoji Shibutani

Department of Mechanical Engineering, Osaka University

Plasticity stems from the Greek “*plaitikos*” of forming. Thus, the metals can be plastically deformed by introducing the line defect, called “dislocation”, to obtain the permanent shape of object which has a physical function for the practical application. The dislocation dynamics is the fundamental process of the macroscopic plasticity. Phenomenological plasticity has been academically systematized by the continuum theory, that is, “The Mathematical theory of Plasticity” (R. Hill, 1950). On the other hand, physical plasticity based on the crystallography and elastic theory can be summarized by “Theory of Dislocations” (J. P. Hirth and J. Lothe, 1982). When we link together with the two views over time and length scales, the defect interactions among the point defect such as vacancy and interstitial, the line defect of dislocation, and the planar defect such as grain boundary and surface should be resolved. The talk will be focused on the physical interactions between the defects using the large scale molecular dynamics and the linear elasticity, putting much emphasis on the followings.

- (i) Strength and ductility; interaction between dislocation and grain boundary
- (ii) Strength, ductility and fracture toughness; interaction among crack, dislocation, and grain boundary.

Presenter: Yoji Shibutani

I.4 – Invited, VCTP-44

Ab Initio Anharmonic Algorithms to Understand Structures and Vibrational Spectra of Molecular Systems

Jer-Lai Kuo

Institute of Atomic and Molecular Sciences, Academia Sinica, Taiwan

Modeling the structures and properties of molecular systems has been a challenging task for Physics, Chemistry and Material Science. The relatively weak interaction and intrinsic structural flexibility has given rise to a rich phases and properties. In our group, we have been working on developing a framework of computational algorithms to engage different models (ranging from empirical model, semi-empirical methods, DFT to high-level quantum chemistry

methods) for molecular modeling. To search for structures, we have build an array for structural searching schemes to utilize the efficiency of empirical and semi-empirical methods to explore the configurational space. Structural info. obtained will further been refined using high-level methods. Furthermore, different molecular properties require different level of quantum mechanical theories. As a example, we will present our recent effort to understand the vibrational motion of proton in various molecules using the computational algorithms we developed including both types of proton (Zundel [1] and Eigen [2,3]) under different solvation environments. If time permits, we will also access the performance of a few approximate treatments on vibrational coupling/anharmonicity to treat larger hydrogen-bonded molecular (water, alcohols and amines) clusters [4,5].

[1] J.A. Tan and J.-L. Kuo. *J. Phys. Chem. A.*, 119, 11320 (2015).

[2] J-W Li, M. Morita, T. Takahashi, and J-L Kuo, *J. Phys. Chem. A*, 119, 10887 (2015).

[3] Q. Huang, T. Nishigori, M. Katada, A. Fujii J. Kuo, *Phys. Chem. Chem. Phys* 20, 13836 (2018)

[4] K-L Ho, L-Y Lee, M. Katada, A. Fujii, J-L Kuo, *Phys. Chem. Chem. Phys.*, 18, 30498 (2016)

[5] Q-R Huang, Y-C Li, K-L Ho, and J-L Kuo, *Phys. Chem. Chem. Phys*, 20, 7653 (2018)

Presenter: Jer-Lai Kuo

I.5 – Invited, VCTP-44

Renormalizing random-phase approximation by using exact pairing

L. Tan Phuc (1,2), N. Quang Hung (1), N. Dinh Dang (3)

(1) Institute of Fundamental and Applied Sciences, Duy Tan University, Vietnam. (2) Faculty of Physics and Engineering Physics, Vietnam National University Ho Chi Minh City-University of Science, Vietnam. (3) Quantum Hadron Physics Laboratory, RIKEN Nishina Center for Accelerator-Based Science, Japan.

We proposed a fully self-consistent renormalized random-phase approximation by using the self-consistent Hartree-Fock mean field plus exact pairing solutions (EP). Within this approach, the particle number is exactly conserved. The Pauli principle, which is violated in the conventional particle-hole random-phase approximation (RPA), is preserved, and the energies-weighted sum rule, which is violated in the conventional renormalized RPA, is restored.

This approach is applied to calculate several light, medium, and heavy-mass nuclei, such as 22, 24, 28O, 60Ni, and 90Zr nuclei by using the MSk3 interaction. We found that taking into account ground-state correlations beyond the RPA by means of the occupation numbers obtained in EP affects the RPA solutions within the whole mass range, and this effect decreases with increasing the mass number. Moreover, the anti-pairing effect is also observed via a significant reduction of pairing in neutron-rich nuclei. The enhancement of Pygmy Dipole Resonance (PDR) is found in most of neutron-rich nuclei under consideration within our method.

Presenter: Le Tan Phuc

I.6 – Invited, VCTP-44

Joint Remote Preparation of General Quantum States of Arbitrary Dimensions

Nguyen Ba An (1,2)

(1) *Thang Long Institute of Mathematics and Applied Sciences, Thang Long University;* (2) *Institute of Physics, Vietnam Academy of Science and Technology*

Information can be encoded in quantum states. Secure and intact transfer of quantum information between distant nodes of a global quantum network is a demanding task for quantum communication and distributed quantum computation. Thanks to weird quantum entanglement, such task can be done only by means of local operations and classical messages, i.e., quantum information is transferable even though the state itself is not actually transported. Most famous is the protocol called quantum teleportation [1] which requires (a) physical supply of the state and (b) ability of performing Bell-state measurement. Later, a different protocol called remote state preparation (RSP) [2] was proposed that is free from the two requirements (a) and (b). However, RSP suffers from two drawbacks: (i) failure with a probability of 50% and (ii) leakage of full information to the preparer. Recently, a new protocol called joint remote state preparation (JRSP) [3] was put forward to get rid of all the above-mentioned weak points (a), (b), (i) and (ii). JRSP of arbitrary quDit states of dimensions $D = 2, 4$ and 8 was studied intensively using standard procedures. JRSP of equatorial single-quDit states as well as equatorial hybrid quDit-quNit entanglements of any dimensions have also been investigated. Nevertheless, JRSP of the most general quDit and quDit-quNit states turns out impossible by standard techniques. In this talk we propose nonstandard protocols using positive operator-valued measurements (POVMs), which are suitably designed so that our protocols work deterministically for arbitrary dimensions D and N . Furthermore, we also construct quantum circuits to realize the concerned POVMs [4]. The obtained results might be of interest from both theoretical and experimental point of view.

[1] C.H. Bennett et al., Phys. Rev. Lett. 70, 1895 (1993)

[2] See, e.g., A.K. Pati, Phys. Rev. A 63, 014302 (2000)

[3] N.B. An, J. Kim, J. Phys. B: At. Mol. Opt. Phys. 41, 095501 (2008)

[4] N.B. An, L.T. Dat, J. Kim, Phys. Rev. A 98, 042329 (2018)

Presenter: Nguyen Ba An

I.7 – Invited, VCTP-44

Computer simulations of amyloid proteins in various environments and folded proteins in a cell-like environment

Philippe Derreumaux

Laboratory of Theoretical Biochemistry, UPR9080 CNRS, Université de Paris, Paris Sciences Lettres, IBPC, 13 rue Pierre et Marie Curie, 75005, Paris, France

I shall present where OPEP coarse-grained force field and atomistic force fields coupled to advanced sampling techniques stand in the context of amyloid proteins associated with Alzheimer's disease. The understanding of protein behavior in cell-like environments is a challenge because of the size and the spread of length- and time-scales characterizing the systems, and I shall show where we are in this context using OPEP simulations.

[1] Nasica-Labouze J, Nguyen PH, Sterpone F, Berthoumieu O, Buchete NV, Coté S, De Simone A, Doig AJ, Faller P, Garcia A, Laio A, Li MS, Melchionna S, Mousseau N, Mu Y, Paravastu A, Pasquali S, Rosenman DJ, Strodel B, Tarus B, Viles JH, Zhang T, Wang C, Derreumaux P. Chem Rev. 2015 May 13;115(9):3518-63.

[2] Sterpone F, Melchionna S, Tuffery P, Pasquali S, Mousseau N, Cragolini T, Chebaro Y, St-Pierre JF, Kalimeri M, Barducci A, Laurin Y, Tek A, Baaden M, Nguyen PH, Derreumaux P. Chem Soc Rev. 2014 Jul 7;43(13):4871-93.

Presenter: Philippe Derreumaux

I.8 – Invited, VCTP-44

Ultrasound interacts with biological systems

Nguyen Hoang Phuong (1,2)

(1) CNRS, Université de Paris, UPR 9080, Laboratoire de Biochimie Théorique, 13 rue Pierre et Marie Curie, F-75005, Paris, France; (2) Institut de Biologie Physico-Chimique, Fondation Edmond de Rothschild, PSL Research University, Paris, France

Ultrasound has a wide range of medical applications. Nowadays, the diagnostic and therapeutic ultrasound procedures are routinely used, but effects of ultrasound on biological systems at the molecular level are, however, not fully understood even for the simplest biological components such as cell membranes and proteins. This limits the development and application of ultrasound in the emerging important fields such drug delivery to the brain or cancer cells. In principle, the molecular dynamics simulation method can provide molecular insights into the interaction between ultrasound and biological systems. However, its applications in this field are still at infancy. In this talk, we will present our recent development of the methods for performing molecular dynamics simulations under focused ultrasound and ultrasound induced bubble cavitation. The applications of the methods are illustrated with the studies of the bubble cavitation induced amyloid fibril dissociation, lipid cell membrane pore formation, damage and molecular nanometers propelled by bubble.

Presenter: Nguyen Hoang Phuong

I.9 – Invited, VCTP-44

Protein aggregation and neurodegenerative diseases

Mai Suan Li (1,2)

(1) Institute of Physics, Polish Academy of Science, Al. Lotnikow 32/46, 02-668 Warsaw, Poland; (2) Institute for Computational Science and Technology, Ho Chi Minh city, Vietnam

Protein aggregation is associated with a large group of major human diseases, including Alzheimer's disease, prion disorders, type 2 diabetes etc [1]. Therefore, understanding the key factors that govern this process is of paramount importance. It was well-known that the fibril formation time strongly correlated with the hydrophobicity, charge and population of the fibril-prone state of proteins [2]. In this talk, we show that the aggregation rate depends on the mechanical stability of fibril [3] and the beta-content of the monomer [4]. The higher the beta-content, the faster the fibril elongation, and this dependence can be described by a single exponential function. Our results open up a new way of understanding the self-assembly of bio-molecules at the monomer level, and this has been confirmed by all-atom molecular dynamics simulations of amyloid beta ($A\beta$) peptides and in vitro experiments. Recent research revealed that soluble complexes of $A\beta$ peptides and copper are efficient catalysts in dioxygen activation and, therefore, are potentially dangerous species triggering an irreversible oxidative pathway in Alzheimer's disease. We have shown [5] that in the presence of Cu(II) the beta-content of monomer is reduced substantially compared with the wildtype $A\beta_{42}$ suggesting that, in accord with experiment, metal ions facilitate formation of amorphous aggregates rather than amyloid fibrils with cross- β structures. For the Cu: $A\beta$ stoichiometric ratios of 1:1 Cu delays the $A\beta$ dimerization process as observed in a number of experiments. The mechanism underlying this phenomenon is associated with decreased hydrophobicity of monomer upon Cu-binding.

- [1] J. Nasica-Labouze, et al., Amyloid beta-protein and Alzheimer's disease: when computer simulations complement experimental studies, *Chemical Reviews* 115, 3518-3563 (2015).
- [2] M.S. Li, N.T. Co, G. Reddy, C-K Hu and D. Thirumalai, Factors governing fibrillogenesis of polypeptide chains revealed by lattice models, *Phys. Rev. Lett.* 105, 218101 (2010).
- [3] M. Kouza et al, Kinetics and mechanical stability of the fibril state control fibril formation time of polypeptide chains: A computational study, *J. Chem. Phys.* 148, 215106 (2018).
- [4] TTM Thu, NT Co, LA Tu, and MS Li, Aggregation rate of amyloid beta peptide is controlled by beta-content in monomeric state, *J Chem Phys.* 150, 225101 (2019).
- [5] P.D.Q. Huy et al., Impact of Cu(II) binding on structures and dynamics of A β 42 monomer and dimer: Molecular dynamics study, *ACS Chem. Neurosci.* 10, 1348 (2016).

Presenter: Mai Suan Li

I.10 – Invited, VCTP-44

Higgs potential at Planck scales and quantum gravity effects

Takeo Inami

RIKEN, Wako, Japan

Presenter: Takeo Inami

I.11 – Invited, VCTP-44

Neutrino Oscillations: Present Landscape and Future Prospects

Cao Van Son

KEK/J-PARC, Japan

Massiveness of neutrinos, confirmed by the so-called neutrino oscillation phenomenon, up-to-date is the only palpable evidence of physics beyond the description of the Standard Model of the elementary particles. Measurements of neutrino oscillations have been become a very useful and important tool for answering the fundamental questions: What is neutrino mass hierarchy? Is CP violated in the leptonic sector? Does the sterile neutrinos exist? Recently T2K experiment has provided a hint that CP is violated in the leptonic sector with more than 95.5% C.L. Besides most of neutrino experiments are favoring the normal mass hierarchy of neutrinos and there is no conclusive evidence of the sterile neutrinos. The talk will review the present landscape and discuss the future prospects of neutrino oscillation measurements.

Presenter: Cao Van Son

I.12 – Invited, VCTP-44

Cosmic inflation as a very high energy particle detector

Toshifumi Noumi

Kobe University, Japan

The energy scale of cosmic inflation could be as high as 10^{14} GeV, hence it is the highest energy scale we may explore. It is therefore interesting to explore a possibility to use inflation as a probe of new particles predicted by high energy theories (ex. supergravity, GUT, extra dimension). Such an idea is dubbed “cosmological collider physics.” In this presentation, I will

discuss how to use primordial non-Gaussianities to detect new particles by analogy with particle colliders.

Presenter: Toshifumi Noumi

I.13 – Invited, VCTP-44

Predictive modelling of steady-state configuration in non-equilibrium physics

Duc Nguyen-Manh

Department of Materials Science and Scientific Computing, CCFE, United Kingdom Atomic Energy Authority, Abingdon OX14 3DB, UK

Nuclear fusion offers the potential of predictable, safe power with no carbon emissions and fuel sources lasting for millions of years. However, it is notoriously difficult to achieve in a controlled, steady-state fashion. A magnetic confinement nuclear fusion power plant requires many different science (including theoretical physics), technology and engineering challenges to be met simultaneously. An integrated approach from the outset is needed to bring fusion electricity closer if the other challenges are resolved in harmony.

In this talk, a recent breakthrough in predicting steady-state solution of the phase stability under strong irradiation in multiple-component systems as plasma-facing materials for fusion devices is presented. The work has been carried out within an international collaboration between the UKAEA leading modelling team and different experimental groups at Los Alamos National Laboratory, Argonne National Laboratory and Pacific Northwestern National Laboratory (USA) in finding outstanding radiation resistance materials based on W-based so-called high-entropy alloys (HEAs) [1]. Our theoretical work is developed by using the constrained thermodynamic formalism combining ab-initio construction of many-body Hamiltonian to model for to model K-component alloy system under irradiation for which irradiated defects are being considered as the additional elements in the system. It is found that the formalism can be mathematically represented within matrix formulation for the K-component alloys via many-body cluster correlation functions which in turn can be computed efficiently from Monte-Carlo simulations in a combination with first-principles cluster-expansion Hamiltonian [2]. Applying the theory for bcc W-Ta-Cr-V based HEAs, it is predicted that there is a strong phase decomposition between W, Ta and Cr, V as a function of composition and temperature. The formation of Cr and V rich phase found from the MC simulations is in an excellent agreement with the precipitates observed with Atom Probe Tomography analysis for W 38 Ta 36 Cr 15 V 11 alloy irradiated at high temperatures. The competition between phase segregation and radiation effects is discussed to understand the origin of observed outstanding radiation resistance.

[1] O. El-Atwani, N. Li, M. Li, A. Devaraj, J. K. S. Baldwin, M. M. Schneider, D. Sobieraj, J. S. Wróbel, D. Nguyen-Manh, S. A. Maloy, E. Martinez, *Science Advances*, 5 (2019) eaav2002

[2] A. Fernandez-Caballero, M. Fedorov, J.S. Wrobel, P.M. Mummery, D. Nguyen-Manh, *Entropy*, 21 (2019) 00068

Presenter: Nguyen Manh Duc

O.1 – Oral, VCTP-44

On a five dimensional counterexample to the cosmic no-hair conjecture

Tuan Q. Do

Faculty of Physics, VNU University of Science, Vietnam National University, Hanoi

We will present main results of our recent study on a five dimensional counterexample to the cosmic no-hair conjecture [T. Q. Do and W. F. Kao, Eur. Phys. J. C 78, 531 (2018)].

Presenter: Do Quoc Tuan

O.2 – Oral, VCTP-44

Wang-Landau simulation of smectic phases

Phuong-Thuy Nguyen (1), T.-L. Hoai Nguyen (1), V. Thanh Ngo (1), H. T. Diep (2)

(1) Institute of Physics, Vietnam Academy of Science and Technology, 10 Dao Tan, Ngoc Khanh, Ba Dinh, Hanoi; (2) Laboratoire de Physique Théorique et Modélisation, Université de Cergy-Pontoise, CNRS, UMR 8089, 2 Avenue Adolphe Chauvin, 95302 Cergy-Pontoise Cedex, France

Liquid crystals have been extensively studied for more than 30 years due to their applications in electronic display devices. In spite of this, macroscopic models for the formation of ordering in liquid crystals are still missing. Much works have been based on the phenomenological Frank's free energy. In this work, using a microscopic Hamiltonian we study the transition of smectic phases by the Wang-Landau Monte-Carlo simulation. We use the mobile q-states Potts model for the molecules which can move from one site to another on a lattice. The Potts spin has 6 states corresponding to 6 different spatial molecular orientations. The simulation results clearly showed the existence of two melting points which is observed in the experiments

Presenter: Ngo Van Thanh

O.3 – Oral, VCTP-44

Photovoltaic effect due to asymmetric electron-hole interaction in semiconductor quantum wells

Huynh Thanh Duc (1), Ngo Thanh Cong (1), and Torsten Meier (2)

(1) Ho Chi Minh City Institute of Physics, Vietnam Academy of Science and Technology; (2) Department of Physics, University of Paderborn

We demonstrate the existence of a ballistic photocurrent which results from the excitation of excitons in non-centrosymmetric semiconductor quantum wells. Unlike several other cases, where excitonic effects quantitatively modify photocurrents which originate from single-particle properties, the photocurrent we discuss is a true many-body effect that caused by asymmetric electron-hole attraction. We also show that the coherent dynamics of excitons gives rise to oscillations in the photocurrent transients.

Presenter: Huynh Thanh Duc

O.4 – Oral, VCTP-44

LO-Phonon-limited Electron Mobility in a Core-Shell Polar Semiconductor Quantum Wire

Nguyen Nhu Dat (1) and Le Thanh Hai (2)

(1) Institute of Theoretical and Applied Research (ITAR), Duy Tan University (2) Hanoi University of Civil Engineering

Electron scattering rate and electron mobility limited by LO-phonons are calculated for a cylindrical polar semiconductor quantum wire with core-shell structure. Longitudinal optical phonons

modes are developed within a dielectric continuum model. The influence of the thickness of the shell on the electron scattering rate by phonons is studied. Numerical calculations performed for a GaAs/AlGaAs quantum wire show that the electron–LO-phonon scattering rate changes with the thickness of the shell layer and is reduced considerably in the quantum wires having thicker shell, leading to higher electron mobility. The mobility can be improved up to several orders of magnitude.

Presenter: Nguyen Nhu Dat

O.5 – Oral, VCTP-44

Computational predictions of two-dimensional covalent organic frameworks (COF) based on 2D square lattice topology

Vu Ngoc Tuoc (1), Nguyen Thi Thao (2) Le Thi Hong Lien (1)

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We have studied several structure's family to explore the applicability of the formation of Covalent Organic Frameworks (COFs) - the lightweight, organic crystalline porous materials constructed via strong covalent bonds between elements, e.g. C, B, O, N. from their defined individual building blocks. The square lattice's symmetry node and linear linker building blocks have been selected for designing high symmetry square shape's COF layers. Using Density Functional Theory (DFT) and the derived from its Density Functional based tight-binding (DFTB) method, we have designed, optimized and investigated these set of hypothetical 2D COFs. The various high-symmetry stacking sequence. e.g. AA and AB, are also considered in details. The designed COF series, revealing a variety of promising mechanical and electronic properties, which can potentially find future realistic in bio-medical and/or energetic applications.

Presenter: Vu Ngoc Tuoc

O.6 – Oral, VCTP-44

Deuteron elastic scattering based on Faddeev-Alt-Grassberger-Sandhas equations within the realistic potentials

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In few-body physics, the Faddeev-Alt-Grassberger-Sandhas (FAGS) equations [1] are well known the only existing formalism which can describe simultaneously and exactly the elastic, inelastic, and rearrangement process. In this contribution, we discuss the possibility of using the realistic

nucleon-nucleon and nucleon-nucleus potentials in FAGS equations to study the (d,p) reactions. Some preliminary results for d(12C, 12C)d reactions are shown and discussed.

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Presenter: Tran Viet Nhan Hao

O.7 – Oral, VCTP-44

Introduction of the extended Jost function formalism for S-matrix analysis of nucleon-nucleus scattering

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The structure of sharp resonances which are observed at several MeV region of the nucleon-nucleus (NA) scattering is one of the most useful and important characteristic of nucleus. The candidates of the origin of the sharp resonances are the channel-coupling and pairing effect (configuration mixing of the particle and hole states).

The application of the particle-vibration-coupling (PVC) method to the NA scattering [1,2,3] has shown the results which is consistent with the qualitative consequences from the Feshbach projection theory[4]. The cPVC calculation [1] has succeeded also the partial reproduction of the sharp resonances. These recent progresses may indicate that the PVC model is the candidate of a new optical model which covers both resonance and continuum energy region for NA scattering. The pairing correlation is one of the most important fundamental properties of nuclear structure, however, the role of the pairing correlation for the NA scattering is still not so clear yet.

The S-matrix analysis is one of the most powerful way for the investigation of resonances. The Jost function [5] has been known as very useful framework for the description of the S-matrix and the bound states structure of the system. Very recently, we extended the Jost function framework based on the Hartree-Fock-Bogoliubov formalism [6] in order to investigate the role of the pairing correlation for the NA scattering and the nuclear structure at the same time.

In our presentation, we are planning to introduce the Jost function, our recent results and progress, and also explain about our future plan.

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Presenter: Kazuhito Mizuyama

O.8 – Oral, VCTP-44

Second-order phase transition in an odd-odd deformed and hot-rotating nucleus

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The thermodynamic properties of ^{200}Tl , ^{211}Po , and ^{212}At nuclei are studied by using the angular-momentum gated nuclear level densities (NLDs) extracted from the experimental particle evaporation spectra in the excitation energy range of 2-15 MeV. The experimental NLDs are found in very good agreement with the results of the exact pairing plus the independent-particle model at finite temperature (EP+IPM) [1]. Consequently, the heat capacities of the above nuclei at finite angular momentum have been extracted using the EP+IPM NLDs. The results obtained show that while the heat capacities of ^{200}Tl , ^{211}Po , and ^{212}At (near spherical nuclei) follow the trend as expected in odd-odd and even-odd masses, surprisingly an *S*-shaped heat capacity, which is the signature of the superfluid-to-normal (second-order) phase transition, is found in an odd-odd deformed nucleus ^{184}Re . This *S*-shaped heat capacity observed in ^{184}Re is microscopically explained by not only the breaking of nucleon Cooper pairs but also the change of pairing induced by deformation within the EP+IPM [2].

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Presenter: Nguyen Quang Hung

O.9 – Oral, VCTP-44

Probe-controlled-system approach to direct state measurement

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A complex wave function in quantum mechanics is the fundamental representation of the quantum state of a system. In its statistical interpretation, the wave function predicts the results of measurements made on the system. Therefore, a complete determination of the wave function, or in general, the density matrix, of quantum states is crucially important and is one of the main tasks in quantum mechanics. In practice, quantum state tomography (QST) is widely employed for quantum state measurements. This method measures multiple copies of the system in a complete set of non-commuting observables, which is used to reconstruct the quantum state. It is, however, difficult to apply in large systems where exponentially complicated calculations and precise measurements are required. Alternatively, one can use direct state measurement [1, 2]. Here, the system of interested interacts with a pointer to obtain weak value, which are proportional to the amplitude of the wave functions. So far, the DSM approach has been verified based on weak interaction [2], arbitrary strong interaction [3], coupling-deformed pointer observables [4], and enlarged Hilbert spaces [5].

In this work, we focus on the DSM using the probe-controlled-system method [6]. This approach uses a probe-controlled-system transformation instead of a system-probe interaction to obtain the desired quantum state. We first analyze the precision of our approach in comparison to

the weak- and strong-measurement approaches. Then, we present our simulation and analytic calculation results. We believe that this approach provides a simpler and more effective tool to measure the quantum wave function directly.

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Presenter: Kieu Quang Tuan

O.10 – Oral, VCTP-44

Quantum method for probing molecular chirality of enantiomer specific coherent pi-electron angular momentum

Hirobumi Mineo (1)

(1) Ton Duc Thang University

Detection of molecular chirality is one of the important topics and chirality is an essential concept for a discussion of the stereochemistry. In biochemistry many biologically active molecules are chiral molecules including the amino acids and sugars. In natural biological system most of these naturally produced chiral molecules have the specific chirality, e.x., amino acids have L-enantiomers, and sugars have the D-enantiomers, while the chemically synthetic chiral molecules have both L-, D-enantiomers equally. Therefore the concept of molecular chirality and its detection are practically very important. The circular dichroism (CD) or optical rotatory dispersion (ORD) spectroscopy techniques are typically used to investigate the electronic and geometric structures of chiral molecules in UV/Vis frequency region, however the observed strengths of CD and ORD are very weak due to its indirect spectroscopic methods. Recently some ultrafast new methods are proposed, imaging photoelectron CD (PECD) or multiphoton (PECD) to discriminate the chiral molecules. In this paper we propose an efficient laser control scheme for a ultrafast probing the enantiomers of chiral aromatic ring molecules using the linearly polarized (LP) laser pulses. Here phenylalanine, which is an essential amino acids, is used as an example of chiral aromatic ring molecules to demonstrate a numerical simulation of this laser control scenario. In our previous work we utilized the dynamic Stark effect (DSE) to generate the unidirectional pi-electron angular momentum. Here the two electronic excited states are subject to dynamical Stark shift, and the degeneracy is induced by the two LP stationary lasers.

Presenter: Hirobumi Mineo

O.11 – Oral, VCTP-44

Extracting molecular structure from the laser-induced electron diffraction spectra

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Laser-induced electron diffraction (LIED) has been found as a promising tool for molecular imaging with high spatiotemporal resolution [1, 2]. First, based on the quantitative rescattering theory [3] the laser-free elastic differential cross section (DCS) can be extracted from the LIED spectra. Then, by comparing with the theoretical DCS calculated by the independent-atoms model (IAM) of molecules, the molecular structures can be retrieved. This approach was applicable only for the mid-infrared laser, which induces electron-molecular collision with high energy [1, 2]. Therefore, we have recently upgraded the multiple-scattering model (MS) to expand the range of electron-ion collision to low energy induced by the near-infrared laser [4]. These IAM and MS models were useful in the reconstruction of the molecular information for not only diatomic but also polyatomic molecules but not including the vibration effect [1, 2, 4].

Many studies have shown the necessity of including the molecular vibration and anharmonicity in the DCS calculation of the conventional gas-phase electron diffraction [5, 6]. This inclusion leads to the right corrections of structural retrieval parameters of the molecules [5], or the shrinkage effect [6]. Therefore, the vibration and anharmonicity may affect the quality of extracting molecular structure from the electron-ion collision obtained from LIED spectra. In this report, we discuss the influence of molecular vibration on the electron-ion DCS and, consequently, on the extracted molecular structure from LIED spectra.

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Presenter: Phan Thi Ngoc-Loan

O.12 – Oral, VCTP-44

Local symmetry determines the phases of linear chains: a simple model for the self-assembly of peptides

Tatjana Škrbić (1), *Trinh Xuan Hoang* (2), *Amos Maritan* (3), *Jayanth R. Banavar* (1), and *Achille Giacometti* (4)

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We discuss the relation between the emergence of new phases with broken symmetry within the framework of simple models of biopolymers. We start with a classic model for a chain molecule of spherical beads tethered together, with the steric constraint that non-consecutive beads cannot overlap, and with a pairwise attractive square well potential accounting for the hydrophobic ef-

fect and promoting compaction. We then discuss the consequences of the successive breaking of spurious symmetries. First, we allow the partial interpenetration of consecutive beads. In addition to the standard high temperature coil phase and the low temperature collapsed phase, this results in a new class of marginally compact ground states comprising conformations reminiscent of α -helices and β -sheets, the building blocks of the native states of globular proteins. We then discuss the effect of a further symmetry breaking of the cylindrical symmetry on attaching a side-sphere to the backbone beads along the negative normal of the chain, to mimic the presence of side chains in real proteins. This leads to the emergence of a novel phase within the previously obtained marginally compact phase, with the appearance of more complex secondary structure assemblies. The potential importance of this new phase in the de novo design of self-assembled peptides is highlighted.

Presenter: Trinh Xuan Hoang

O.13 – Oral, VCTP-44

Social Conflicts Studied by Means of Statistical Physics and Monte Carlo Simulations

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(2) Department of Physics, Cleveland State University, USA. (3) Levin College of Urban Affairs, Cleveland State University, USA.

Statistical physics models of social systems with a large number of members, each interacting with a subset of others, have been used in very diverse domains such as culture dynamics, crowd behavior, information dissemination and social conflicts. We observe that such models rely on the fact that large societal groups display surprising regularities despite individual agency. Unlike physics phenomena that obey Newton's third law, in the world of humans the magnitudes of action and reaction are not necessarily equal. The effect of the actions of group n on group m can differ from the effect of group m on group n . We thus use the spin language to describe humans with this observation in mind. Note that particular individual behaviors do not survive in statistical averages. Only common characteristics remain.

We have studied two-group conflicts as well as three-group conflicts. We have used time-dependent Mean-Field Theory and Monte Carlo simulations. Each group is defined by two parameters which express the intra-group strength of interaction among members and its attitude toward negotiations. The interaction with the other group is parameterized by a constant which expresses an attraction or a repulsion to other group average attitude. The model includes a social temperature T which acts on each group and quantifies the social noise. One of the most striking features is the periodic oscillation of the attitudes toward negotiation or conflict for certain ranges of parameter values. Other striking results include chaotic behavior, namely intractable, unpredictable conflict outcomes.

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Presenter: Diep The Hung

O.14 – Oral, VCTP-44

Adsorption Trend of Volatile Organic Compounds on monolayer MoS₂

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Nanotechnology Program, Vietnam Japan University

Screening tests to detect lung cancer at an early stage is very important for localizing the cancer cells and significantly improving the possibility of the curability of the disease. Human breath contains volatile organic compounds (VOCs) as clinically useful markers which can be detected by electronic sensors. The monolayer material MoS₂ is strongly expected to be a promising material for the gas sensors in detecting the VOCs because of its very high sensitivity in adsorption of gases.

In this work, the adsorption mechanism of various VOCs on MoS₂ by using the Density Functional Theory (DFT) is investigate. Scanning images of the adsorption possibility are shown for the several types of VOCs in breath of lung cancer patients on these materials by using Computational DFT-base Nanoscope to determine the potential energy surfaces, potential adsorption areas and the diffusion path of VOCs. The adsorption energy is calculated with employing five functionals of van der Waals interaction: vdw-revPBE, vdw-optPBE, vdw-optB88, vdw-optB86b and DFT-DF2. The trend of adsorption is evaluated in respect of the chemical functional groups of VOCs.

Presenter: Dinh Van An

O.15 – Oral, VCTP-44

Micro-mechanical properties of colloidal aggregates with critical Casimir forces

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Microscopically, gel networks, formed by the aggregation of attractive colloidal particles, are widely used to control the rheological properties of complex materials. Network elasticity characterized via the storage and loss moduli, bending stiffness is highly sensitive to the connectivity, rearrangement of particle aggregates and shows a strong time evolution due to their complex energy landscape. This network elasticity is central in foods and in the cell cytoskeleton, where networks of biopolymers give the cell the mechanical properties. In this talk, we investigate the role of both spherical and anisotropic colloids with novel critical Casimir forces on the bonding morphology and micro-mechanical properties of these chain-like colloidal aggregates. Computer simulations using an effective critical Casimir pair potential with modern experimental confocal observations show the morphology changes and the increase of storage and loss moduli with aging time. These results highlight the impact of engineering building blocks on the way to design colloidal superstructures with tunable mechanical behavior.

Acknowledgement: This research is funded by Vietnam National Foundation for Science and Technology Development (NAFOSTED) under grant number 103.01-2018.308.

Presenter: Dang Minh Triet

O.16 – Oral, VCTP-44

Higgs boson mass in Next-to-Minimal Supersymmetric Standard Model with Inverse Seesaw Mechanism

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The Higgs in Next-to-Minimal Supersymmetric Standard Model (NMSSM), while can be a candidate for the experimentally detected Higgs boson, has some differences from the one proposed in the Standard Model. At the same time, the unnatural smallness of neutrino mass is obtained through Inverse Seesaw mechanism so that newly appearing particles can be on TeV scale. This mechanism has effects on the mass of Higgs boson, but to investigate such changes, one-loop calculation is essential. With the help of the package NMSSMCALC, numerical analysis of one-loop Higgs mass, its dependence on the neutrino sector and experimental constrains is conducted.

Presenter: Phan Anh Vũ

O.17 – Oral, VCTP-44

Kinetic mixing effect in noncommutative B-L theory

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The $SU(P)_L$ gauge symmetry for $P \geq 3$ can address the question of generation number due to anomaly cancellation, but it neither commutes nor closes algebraically with electric and baryon-minus-lepton charges. Hence, two $U(1)$ factors are required, yielding a complete gauge symmetry $SU(P)_L \otimes U(1)_X \otimes U(1)_N$ apart from the color group, which provides neutrino mass, dark matter and inflation. However, this gauge structure may present kinetic mixing effects associated to the $U(1)$ gauge fields and affect the electroweak precision test such as the ρ parameter and Z couplings. Additionally, it presents interesting mixing phenomena in the new neutral gauge sector. We will construct the model and examine the new physics effects in detail.

Presenter: Le Xuan Thuy

O.18 – Oral, VCTP-44

Prospect of dark matter searches in split SUSY models

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The recent results from the XENON1T/Panda-X and IceCube experiments have set the most severe upper limits on spin-independent (SI) and spin-dependent (SD) scattering cross section of weakly interacting massive particles on nuclei. In the framework of split supersymmetry scenario supported by the LHC constraints, we investigate the prospect of dark matter (DM) direct and indirect detection experiments. Assuming a relation among gaugino masses at the grand unification scale, we have specified the parameter regions that predict the right DM relic abundance as well as satisfy the constraints on SI and SD scattering cross sections of DM. In the

case of universal gaugino masses, the XENON1T/Panda-X results have ruled out completely the well-tempered neutralino region. We have found that 200 times smaller than the current IceCube bound is the sensitivity limit that a future DM indirect detection experiment should have at least in order to have a certain impact beyond the current XENON1T/PandaX results. The future results from XENON1T will be able to test a significant portion of the Higgsino-like region. Although there are points in the Higgsino-like region that cannot be reached by future DM detection experiments, direct production channels of neutralino/chargino can be used to test the model at the LHC/HL-LHC. In the case of non-universal gaugino masses, beside showing the allowed parameter space, we have specified the regions that can be tested at both future DM direct and indirect detection experiments. One of them are Higgsino-like region, while the others two predict a well mixed bino-wino DM. The DM properties in each region have been examined and demonstrated with a benchmark of -ino spectrum. Interestingly, points in the mixed bino-wino region with rather light chargino can be tested the LHC 14 TeV.

Presenter: Tran Minh Hieu

O.19 – Oral, VCTP-44

Constraining new physics from Higgs measurements with Lilith: update to LHC Run 2 results

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Lilith is public python library for constraining new physics from Higgs signal strength measurements. We here present version 2.0 of Lilith together with an updated database which includes the full set of ATLAS and CMS Run 2 Higgs results for 36 fb^{-1} . Both the code and the XML database were extended from the ordinary Gaussian approximation employed in Lilith-1.1 to using variable Gaussian and Poisson distributions. Moreover, Lilith can now make use of correlation matrices of arbitrary dimension. We provide detailed validations of the implemented experimental results as well as a status of global fits for i) reduced Higgs couplings and ii) Two-Higgs-doublet models of Type-I and Type-II. Lilith-2.0 is available on GitHub and ready to be used to constrain a wide class of new physics scenarios.

Presenter: Tran Quang Loc

O.20 – Oral, VCTP-44

Single top-quark production in association with two jets at the LHC

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We present a next-to-leading order study of QCD corrections to the process of single on-shell top-quark production in association with two jets at the LHC. The tW channel is assumed to be measured independently. This study is important for the measurement of the electroweak tbW coupling and of the V_{tb} element of the CKM matrix.

Presenter: Le Duc Ninh

O.21 – Oral, VCTP-44

Tight binding description for the electronic band structure of penta-graphene

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Penta-graphene, a new carbon allotrope discovered recently has attracted great attention from researchers due to its high potentials as a large bandgap semiconductor, which is an intriguing feature for many applications in nanoelectronics. Understanding of the electronic properties of this materials is therefore necessary to modulate its properties. In this work, we present an effective tight-binding (TB) model which can induce the energy bands that being consistent with results from ab initio calculations. Besides the comparison of our simple TB model to previous ones, we also supplemented further neighbor interactions into the TB Hamiltonian to analyze the band structure and considered the impact of each type of TB parameters such as onsite and hopping energies, overlap terms of wave functions on the shape of the energy bands. Then a set of appropriate parameters was selected to reproduce reasonably important characters in the band structure captured by ab initio calculations. Further analysis was also carried out to examine the density of states by using Green's function. Moreover, we also investigated the impact of a vertical electric field on the electronic properties of penta-graphene and showing a strong modulation of the bandgap in the presence of such external field.

Presenter: Nguyen Thi Kim Quyen

O.22 – Oral, VCTP-44

Spin-dependent tunneling and spin current in semiconductor heterostructures

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We present our recent research concerning anomalous spin-dependent tunneling of electron and holes through semiconductor heterostructures involving both spin-orbit and exchange interactions. We carefully introduce the concept of spin current and derive its analytical expression in the simplest cases where only conduction or valence bands are involved. Numerical calculations have been performed, base on multi-band k.p approaches and scattering matrix descriptions, step by step incorporating the higher-order bands of the material band-structure. As an illustration, we show the spin-current profiles through a GaMnAs/GaAs/GaMnAs heterostructure in three specific magnetization configurations.

Presenter: Nguyen Thi Loan

P.1 – Poster, VCTP-44

Computational study of the effect of protonation states of PSA protein zinc

fingers on its DNA binding

Nguyen Hai Ly, Nguyen The Toan

VNU, Hanoi University of Science

In this study, we investigate the binding of the Zinc finger (ZF) structure on a short DNA molecule. Zinc finger of a protein where a Zn^{2+} ion binds to 4 cysteine or histidine amino acids in a tetrahedral structure is a very common motif of nucleic acid binding proteins. This structure is ubiquitous and the corresponding interaction model is present in 3% of the genes of the human genome. ZF has been shown to be extremely useful in various therapeutic and research capacities, as well as in biotechnology. A recent computational study has shown that Zn finger structure is stable if the cysteine amino acids are in deprotonated. Here, we investigate how these deprotonated states influence protein structure, dynamics, and function by studying the binding of ZF to short DNA molecules in normal and in deprotonated states using molecular dynamics simulations in sub-microsecond range. Our results show that the Zn $2+$ ion and the deprotonated state of cysteine are essential for mechanical stabilization of the functional, folded conformation. Not only this state stabilizes the ZF structure, but it also stabilizes the DNA binding structure. Our result has a potential impact on the better design of zinc fingers for various biotechnological application.

Presenter: Nguyen Hai Ly

P.2 – Poster, VCTP-44

New one-loop formulas for Higgs $\rightarrow VV^*$

Khiem Hong Phan (1) and Dzung Tri Tran (1)

(1) VNUHCM-University of Science, 227 Nguyen Van Cu, Dist. 5, Ho Chi Minh City, Vietnam

In this talk, we derive new one-loop formulas for Higgs $\rightarrow VV^*$ with $V, V^* = \gamma(\text{photon}), Z$. Analytic results are expressed in terms of generalized hypergeometric functions which are valid in general space-time dimension. We also confirmed previous results in $d = 4$.

[1] One-loop three-point Feynman integrals with Appell F1 hypergeometric functions, Khiem Hong Phan and Dzung Tri Tran, accepted by PTEP.

[2] New one-loop formulas for Higgs $\rightarrow VV^*$ in terms of hypergeometric functions, Khiem Hong Phan and Dzung Tri Tran, to be submitted.

[3] Hypergeometric representation of one-loop Higgs decay to two photons, Khiem Hong Phan, Canadian Journal of Physics: cjp-2018-0944.

[4] Scalar 1-loop Feynman integrals as meromorphic functions in space-time dimension d , Khiem Hong Phan and Tord Riemann, Physics Letter B 791(2019) 257-264.

Presenter: Tran Tri Dung

P.3 – Poster, VCTP-44

Study of Dark Matter in the 3-3-1 with CKS mechanism

N.V.Hop, L.T.Hue, H.N.Long

IOP

The full Higgs potential of the 3-3-1 with CKS mechanism is considered. We find the SM-like

Higgs boson and one pseudoscalar boson as a candidate for Dark Matter.

Presenter: Hoang Ngoc Long

P.4 – Poster, VCTP-44

Self-Diffusion Coefficient of Solute Molecule in Diluted Mixtures: A Non-Equilibrium Molecular Dynamics Approach

*Quang Quoc Viet Thieu (1), Hai Hoang (2), Julien Collell (3), Magali Pujol (3), Guillaume Galliero (4),**

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Accurate estimates of self-diffusion coefficient of solute molecule at infinite dilution in mixtures plays a key role in many fields, in particular in geological and petroleum engineering. Molecular dynamics simulations have become a powerful tool to predict thermophysical properties of fluids including the self-diffusion coefficient. This quantity is often computed by performing equilibrium MD (EMD) simulations using classical algorithms such as Green-Kubo or Einstein relations. However, when dealing with an infinitely diluted mixture these relations are difficult to apply because of the poor statistics, and so may lead to very large error bars. Thus, an efficient algorithm to calculate this property in MD simulations is highly desired. In this work, we have employed the Thermodynamic of Irreversible Process (TIP) formalism combined with the Einstein's relation to propose an efficient algorithm used in MD simulations for the estimation of self-diffusion coefficient of solute molecule at infinite dilution. The algorithm consists in applying an external force on the solute molecule, and computing its steady velocity, i.e. carrying out Non-equilibrium MD (NEMD) simulations. As an application of the method we have studied the self-diffusion coefficients of noble gases in bulk water and saturated clay to check the accuracy of mass square-root relation.

Presenter: Thieu Quang Quoc Viet

P.5 – Poster, VCTP-44

Fractionation of Noble Gases in Normal Alkanes at Equilibrium: Monte-Carlo molecular simulation

Han Tuong Luc (1), Hai Hoang (2), Magali Pujol (3), Guillaume Galliero (4)

(1) Ho Chi Minh University of science, 227 Nguyen Van Cu, District 5, Ho Chi Minh City 7000, Vietnam; (2) Institute of Fundamental and Applied Sciences, Duy Tan University, 10C Tran Nhat Duat Street, District 1, Ho Chi Minh City 700000, Viet Nam; (3) TOTAL S.A., CSTJF, Avenue Larribau, Pau, 64018, France; (4) Laboratoire des Fluides Complexes et leurs Réservoirs (UMR-5150 with CNRS, and TOTAL), Université de Pau et des Pays de l'Adour, BP 1155, F-64013 Pau Cedex, France

Noble gases are natural tracers allowing characterizing the origin, migration, trapping of hydrocarbon reserves. This is because that they are chemically inert under geological conditions and are so fractionated only by physical processes. Accurate estimate in the fractionation of noble

gases enable to better describe complex natural processes involved for identifying and extracting oil and gas discoveries. Partition equilibrium between the gas and oil is an important physical process which leads to a fractionation of noble gases. Such fractionation is usually quantified by Henry's coefficient. Thus, this work is devoted to investigate Henry's coefficients of noble gases in n-alkanes and their mixtures, i.e. simple gases and oils. To do so, we have performed extensive Monte-Carlo molecular simulations using Trappe-ua force field to model the n-alkanes. Simulation results have shown that the mean field theory is able to well describe the equilibrium fractionation of noble gases in the n-alkanes. Hence, we have employed this theory combined with the simulation results to develop an accurate correlation which yields Henry's coefficients of noble gases in pure n-alkanes. In addition, a simple extension of this correlation to mixtures of n-alkanes has been also proposed.

Presenter: Luc Han Tuong

P.6 – Poster, VCTP-44

Spontaneous decay rate and Casimir–Polder interaction of a two-level atom in a Bragg-reflector cylindrical structure

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(1) Institute of Fundamental and Applied Sciences, Duy Tan University, Ho Chi Minh City 700000, Viet Nam; (2) Industrial University of HCM City, 12 Nguyen Van Bao Street, 4th Ward, Go Vap District, Ho Chi Minh City, VietNam

Spontaneous decay rate and Casimir–Polder interaction of an excited two-level atom enclosed in a distributed-Bragg-reflector cylindrical waveguide are studied. Conditions for resonances to exist are established by comparing the distributed-Bragg-reflector-waveguide results with those of a perfectly reflecting hollow waveguide, and taking advantage of the simplicity of the Green tensor of the latter. The Casimir–Polder potential is obtained and found to exhibit a potential well along the cylinder axis. The results remain valid when realistic frequency-dependent permittivities of Si and SiO₂ are used.

Presenter: Nguyen Dung Chinh

P.7 – Poster, VCTP-44

On anisotropic power-law Gauss-Bonnet inflation

Tuan Q. Do, Sonnet Hung Q. Nguyen

Faculty of Physics, VNU University of Science, Vietnam National University, Hanoi

We will present main results of our recent study on anisotropic power-law Gauss-Bonnet inflation. In particular, we will present analytical anisotropic power-law solutions to a scalar-Gauss-Bonnet model with and without the coupling term between scalar and electromagnetic fields. As a result, we will show that large spatial anisotropies appear during an inflationary phase in both studied scenarios.

Presenter: Do Quoc Tuan

P.8 – Poster, VCTP-44

On the derivation of the entropy of ideal quantum gases confined in a three-dimensional harmonic potential

A. T. Nguyen (1,2), Tran Duong Anh-Tai (3), Uyen T. Nguyen (3), Duc Anh Dinh (4), T. V. N. Hao (5), Vinh N. T. Pham (3)

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This study provides a rigorously analytical derivation of the entropy of ideal quantum gases confined in a three-dimensional harmonic trap as functions of the temperature. The numerical calculation is also taken into account for evaluating the applicability of the derived formulas. The results indicate that the entropy of the ideal Bose gas exhibits high consistence between analytical and numerical approaches, the maximum deviation is 7.5% around the vicinity of the critical temperature T_c which is the lowest temperature at which all particles are in the excited state with maximum chemical potential. Nevertheless, in case of Fermi gas, the analytical result fairly departs from numerical one in the interval of $0.3T_F - 0.5T_F$ where T_F is the Fermi temperature associating with Fermi energy level. Besides, the differences between ideal quantum and classical gases in three-dimensional harmonic trap are also presented.

Presenter: Pham Nguyen Thanh Vinh

P.9 – Poster, VCTP-44

Strain and electric field tunable electronic properties and Schottky barrier of Graphene/GaX (X = S, Se) heterostructures

Chuong V. Nguyen (1), Bin Amin (2), Nguyen N. Hieu (3), Le T. P. Thao (4)

(1) Le Quy Don Technical University, Ha Noi, Viet Nam (2) Abbottabad University of Science and Technology, Abbottabad, Pakistan (3) Duy Tan University, Da Nang, Viet Nam (4) University of Education, The University of Da Nang, Da Nang, Viet Nam

Graphene-based two-dimensional materials are recently attracting significant attention because they can preserve novel characteristics of Dirac cone. Here, based on first-principles calculations, we investigate the electronic characteristics of Graphene/GaX (X = S, Se) van der Waals heterostructures (vdWHs). Our results show that the intrinsic electronic properties of both the graphene and GaX monolayer are preserved well in the Graphene/GaX (X = S, Se) vdWHs, and n-type Schottky contacts with a small Schottky barrier height (SBH) are formed at their interfaces. More interestingly, varying the interlayer distance or applying an external electric field can effectively modulate the Schottky barrier and the Schottky contact (n-type and p-type) of the Graphene/GaX vdWHs [1, 2]. Our findings provide insights into the fundamental properties and open up the possibility of vdWHs for designing high-performance optoelectronic nanodevices.

[1] Khang D. Pham, Nguyen N. Hieu, Huynh V. Phuc, A. Fedorov, A. Duque, Bin Amin, Chuong V. Nguyen, Applied Physics Letters, 113 (2018) 171605.

[2] H. Phuc, V. Ilyasov, N. Hieu, Bin Amin, Chuong V. Nguyen, Journal of Alloys and Compounds, 750 (2018) 765-773.

Presenter: Nguyen Van Chuong

P.10 – Poster, VCTP-44

Cyclotron-phonon resonance via one and two-photon absorption in asymmetrical Gaussian potential quantum wells

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In this paper, we study cyclotron – phonon resonance effect via one and two photon absorption processes in quantum wells with asymmetrical Gaussian confined potential subjected by static magnetic field and alternating electric field. The results, calculated for GaAs and Ga_{1-x}Al_xAs materials, show that the characteristics of optical absorption and the half-width are significantly dependent on the well's parameters, the magnetic field, and the temperature. It is also found that in both one and two-photon absorption processes the resonant peaks and the half-width depend monotonically on parameters of the well, external fields and temperature.

Presenter: Le Dinh

P.11 – Poster, VCTP-44

Specific Ion Effects on Static and Dynamic Properties of Aqueous Solution Confined between Uniformly Charged Hydrophobic Plates

Hien Nguyen (1), *Cuong Quoc Doan* (2), *Han Tuong Luc* (3), *Sangmo Kang* (4), *Yong Kweon Suh* (4), *Hai Hoang* (3*)

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Investigation of properties of a aqueous solution confined in nano-pores has one important role not only in the fundamental science, but also in the engineering applications such as the molecular separation or identification processes in the biological and chemical engineering. These properties are strongly affected by various factors, e.g. the confinement gap, the properties of solid wall, ion species etc. In this work, we have developed a FORTRAN molecular dynamics code to study the specific ion effects on the static and dynamic properties of aqueous solution confined in nano-pores that are made of two uniformly charged hydrophobic plates. Two kinds of ion species considered are sodium and chloride ion. The SPC/E model and combination of quaternion coordinates with Euler angles are used to model the water molecules and constraint the structure of water molecules, respectively. The hydrophobic plates are charged uniformly on its inner surface and separated by 2.6 nm. Each of solution consists of 680 water molecules and 20 ions. We employed the modified Ewald summation for the uniformly charged surface following Wen Yang (2006) and the method of PPPM (particle-particle-particle-mesh) to compute long-range interactions. The results show that properties of solution are influenced rather strongly by kind of ion. In particularly, ions and water molecules in the region close to the channel wall is more strongly absorbed on the channel wall for the chloride solution. Otherwise, ions are more hydrated and water molecules are more preferably oriented in the sodium solution. We also compared results obtained the MD simulations with those provided by solving the Poisson-Boltzmann equation

Presenter: Nguyễn Minh Hiền

P.12 – Poster, VCTP-44

Effect of Rigidity on Thermophysical Properties of Lennard-Jones Chains: A Molecular Simulation Study

Phuc Nguyen (1), Vinh Nguyen Thanh Pham (2), Stéphanie Delage Santacreu(3), Hai Hoang (4), Guillaume Galliero (5).

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A simple coarse-grained (CG) molecular model able to simultaneously accurately predict the thermophysical (Thermodynamic + Transport) properties of fluids would be interesting in many fields including chemical and petroleum engineering. There have been a non-negligible number of such GC models proposed in the literature. Among them, it seems that a fully flexible Lennard-Jones (LJ) chain (FF-LJC) model is one of the best options. This model needs only three parameters but able to yield good predictions simultaneously for the thermophysical properties over wide range of thermodynamic condition for various fluids. However, when dealing with fluids containing large molecules at low temperature and high pressure, the FF-LJC model provides good results only for the thermodynamic properties, but not for the transport properties (particularly for shear viscosity). To improve this model, Galliero [Chem. Eng. Res. Des. 92, 3031-3037 (2014)] additionally introduced a bending potential between bonds, leading to the so-called partially Rigid LJC (RLJC) model. It has shown that the RLJC model can provide simultaneously accurate thermophysical properties including the transport properties at low temperatures. Hence, it would be useful to investigate effects of rigidity on thermophysical properties. In this work, we have performed the molecular simulations to compute various thermophysical properties of RLJC fluids over a wide range of values of rigidity. Monte-Carlo molecular method has been used to estimate the thermodynamic properties including liquid-vapor phase equilibrium, direct thermodynamic properties (e.g. density), static structure (e.g. radial distribution function), thermodynamic response functions (e.g. heat capacity) and entropic properties (e.g. chemical potential). In addition, we have employed molecular dynamics method to calculate the transport properties: shear viscosity, thermal conductivity and self-diffusion coefficients. It has been found that the rigidity has a stronger effect on the transport properties, particularly on shear viscosity, than on the thermodynamic properties.

Presenter: Nguyễn Phúc

P.13 – Poster, VCTP-44

Minimal flipped 3-3-1 model

N.T.Duy (1), D.T.Huong (1), D.N.Dinh (1) & P.V.Dong (2)

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University

The flipped 3-3-1 model discriminates lepton families instead of the quark ones often studied. We introduce a minimal setup for the flipped 3-3-1 model which yields novel consequences. Indeed, the model naturally conserves a non-commutative B-L symmetry and subsequent matter parity which prevents unwanted vacuums and interactions, implying dark matter stability. All the fermions get appropriate mass. The lepton flavor changing is governed by Z' . The dark matter and normal matter are manifestly unified by the gauge symmetry.

Presenter: Nguyen Tuan Duy

P.14 – Poster, VCTP-44

Resonance energy transfer rate in the presence of a cylindrical photonic band-gap structure

Nguyen Van Phuoc(1) Nguyen Dung Chinh(2)

(1) Trường ĐH Tôn Đức Thắng (2) Trường ĐH Duy Tân

The resonance energy transfer rate between an excited atom and a ground-state one depends on various factors such as the matching between the donor and acceptor wavelengths, location of the atoms, the environment that surrounds them, etc.. In this research, we investigate the interatomic resonance energy transfer rate in the presence of a cylindrical dielectric multi-layer structure using the Green's tensor formalism. The permittivities of the layers are interchanged periodically between low and high values, so as to create a photonic band-gap system in the radial direction. We present preliminary results for atoms situated in the same cross section normal to the cylinder axis. The number of layers of the cylinder and the contrast between low and high permittivities are varied to elucidate the effect of the band-gap structure. Furthermore, the results are compared with those for atoms located near a perfectly reflecting cylinder.

Presenter: Nguyen Van Phuoc

P.15 – Poster, VCTP-44

The study of neutron star: Nuclear matter Equation of state and Symmetry energy

Ngo Hai Tan (1,2), Dao Tien Khoa (3), Phung Van Dong (2)

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We introduce the study of the equation of state (EOS) of the neutron star (NS) matter. The equation of state (EOS) of asymmetric the nuclear matter has been obtained from the nuclear mean-field potentials in the Hartree-Fock (HF) method. Different in-medium nucleon-nucleon (NN) interaction has been chosen as input for the HF many-body problem: version Sly4 of the Skyrme zero-range interaction; two density-dependent versions of the finite-range M3Y interaction (CDM3Yn and M3Y-Pn), and versions D1S and D1N of the Gogny interaction. Although the considered effective NN interactions were proven to be quite realistic in numerous nuclear structure and/or reaction studies, they give quite different behaviors of the symmetry energy of nuclear matter at supranuclear densities that lead to the soft and stiff scenarios discussed recently in the literature [1, 2].

The EOS of the uniform core inside neutron star has been calculated for the $npe\mu$ composition in

the β equilibrium at zero and finite temperature, without and with spin-polarization of nucleons. Different EOS's of the NS core and the EOS of the NS crust given by the compressible liquid drop model have been used as input of the Tolman-Oppenheimer-Volkov equations to determine the hydrostatic configurations. We study how the nuclear symmetry energy affects the model prediction of different NS properties, like the cooling process as well as the gravitational mass and radius.

[1] Doan Thi Loan, Ngo Hai Tan, Dao T. Khoa, and Jerome Margueron, "Equation of state of neutron star matter, and the nuclear symmetry energy", *Physical Review C* 83, 065809 (2011).

[2] Ngo Hai Tan, Doan Thi Loan, Dao T. Khoa, and Jerome Margueron, "Mean-field study of hot β -stable protonneutron star matter: Impact of the symmetry energy and nucleon effective mass", *Physical Review C* 93, 035806 (2016).

Presenter: Ngo Hai Tan

P.16 – Poster, VCTP-44

Debye model for heat capacity of liquid water at normal condition

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Debye temperature of liquid water is determined from the modified phonon-polariton model. The decrease in the value of Debye temperature with rising temperature is also pointed out. According to the modified phonon-polariton model, the longitudinal sound wave could travel in the system with frequency range from zero to Debye frequency whereas the two transverse acoustic modes propagate on the hydrogen bonding network from Frenkel frequency to the Debye frequency. Using Debye theory, the internal energy of liquid water is given in the explicit form. Therefore, the heat capacity of liquid water can be determined in the similar way which is applied for solid materials. The model shows that the heat capacity of liquid water is almost independently of the temperature in the range from 273.15 K to 373.15 K, in agreement with empirical observation.

Presenter: Tran Thi Nhan

P.17 – Poster, VCTP-44

DFT calculation of electronic and optical properties of quaternary sulfide Cu₂HgSnS₄: a prospective photovoltaic semiconductor

Tuan V. Vu (1,2), A.A. Lavrentyev (3), B.V. Gabrelian (4), Khang D. Pham (1,2), Duy D. Vo (1,2), Phuc Toan Dang (1,2), O.V. Parasyuk (5), O.Y. Khyzhun (6)

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Street, UA-03142 Kyiv, Ukraine

The data of Cu₂HgSnS₄ electronic band-structure was obtained by applying DFT calculation. Different exchange-correlation (XC) approaches were employed to achieve the best total density of states (TDOS) curve in comparison with X-ray photoelectron spectroscopy (XPS). The VB XPS spectrum and TDOS were in good agreement with experimental data when applying MBJ+U+SO technique, in which modified Becke-Johnson (mBJ) was used to describe the XC interaction, the spin-orbit (SO) effect was taken into account, and the strongly correlated electrons of d state was described by the adjusting parameter U. The electronic band structure and optical constant of Cu₂HgSnS₄ were calculated by MBJ+U+SO technique. The Hg 5d and Cu 3d states are the principal contributors to the bottom and the central part of the Cu₂HgSnS₄ valence band, respectively, while its upper part is dominated by S 3p states. Regarding the occupancy of the conduction band, the present APW+lo calculations manifest that its bottom is dominated by the unoccupied Sn 5s states.

Presenter: Vu Van Tuan

P.18 – Poster, VCTP-44

Is the Nonlocal Band-to-Band Tunneling Model Proper for Calculating the Tunneling Current in Tunnel Devices?

Nguyen Dang Chien (1), Chun-Hsing Shih (2)

(1) Dalat University; (2) National Chi Nan university

Based on the assumption of a nonlocal electric field applied in the Kane formalism, the nonlocal band-to-band tunneling (BTBT) model has been successfully applied for a long time to analytically and numerically predict the BTBT current in tunnel devices such as Esaki diodes and tunnel field-effect transistors (TFETs). Although the mixed BTBT model has recently been suggested, the nonlocal BTBT model is still widely used, particularly integrated in the well-known TCAD simulators, for example, Synopsys Sentaurus Devices and Silvaco ATLAS. In this study, we tried to answer the question whether the nonlocal BTBT model is proper to calculate the tunneling current in tunnel devices. To do that, we applied the symmetric principle that if two tunnel devices are completely symmetric, their current-voltage characteristics also have to be strictly symmetric. By using two couples of ideally symmetric devices, including both two and three terminal devices, it is shown that the current-voltage characteristics of each symmetric couple calculated by the mixed model are always symmetric, whereas the symmetric property of those calculated by the nonlocal approach depends on the chosen integrating path. With the fact that the integrating path in the nonlocal model is arbitrarily assumed without definitely physical reasons, it infers that the nonlocal BTBT model is not proper, but the mixed BTBT one is, for calculating the tunneling current in tunnel devices.

Presenter: Nguyen Dang Chien

P.19 – Poster, VCTP-44

Optical absorption coefficients and relative refractive index changes in monolayer silicene

Tran N. Bich (1), Do Muoi (2), Pham T. Vinh (3), Huynh V. Phuc (3), Le Dinh (4)

(1) Quang Binh University; (2) University of Science-VNU.HCM; (3) Dong Thap University; (4) Hue University of Education

In this work, we study the magneto-optical properties of monolayer silicene under a perpendicular magnetic field. We calculate the linear, third-order nonlinear, and total absorption coefficients and relative refractive index changes as functions of the photon energy and the magnetic field. The magneto-optical absorption coefficients and relative refractive index changes appear in two different regimes: the THz and the visible frequency. Our results showed that the resonant peaks are blue-shifted with the magnetic field. The results demonstrate the potential of monolayer silicene as a new two-dimensional material for applications in optical devices as a promising alternative to graphene.

Presenter: Huynh V. Phuc

P.20 – Poster, VCTP-44

Mechanisms of nonsequential double ionization process of argon by near-single cycle laser pulse

Truong Thu D. H. (1), Duc Anh Dinh (2), T. V. N. Hao (3), Vinh N. T. Pham (1)

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In this study, the near-single cycle laser pulse is used to trigger the nonsequential double ionization process of argon atom for decontaminating the secondary recollision processes. The mechanisms and distributions of recollision-ionization channels to the nonsequential double ionization process are comprehensively investigated. Two representative intensities of the laser field are considered for illustrating the nonsequential double ionization process in cases of below and above the recollision-ionization threshold of argon. The results indicate that recollision-induced excitation with subsequent ionization and direct ionization mechanisms are dominant for low and high intensities of laser field, respectively.

Presenter: Truong Dang Hoai Thu

P.21 – Poster, VCTP-44

Controlling the recolliding properties in nonsequential double ionization by orthogonal two-color laser field

Truong Thu D. H. (1), Duc Anh Dinh (2), T. V. N. Hao (3), Vinh N. T. Pham (1)

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As the relative phase between two orthogonal laser fields is varied, the correlated two-electron momentum distribution exhibits strong fluctuation. In this study, we deeply investigate the nonsequential double ionization process of atom to give insight into the microscopic mechanisms of associating recollision process. The results indicate that the strong dependence of two-electron momentum distribution on relative phase of laser fields strongly stems from the different properties of recolliding electrons. All vital characteristic of the returning bunch of electrons such as returning moment, energy, as well as the possibility of energy sharing via the recollision are well controlled by changing the relative phase of laser field. This technique is experimentally straightforward.

Presenter: Truong Dang Hoai Thu

P.22 – Poster, VCTP-44

Band-gap Modulation of Sawtooth Penta-graphene Nanoribbons under Uniaxial Elastic Strain

Le Nhat Thanh (1,2), Tran Yen Mi (1), Le Vo Phuong Thuan (1), and Nguyen Thanh Tien (1)

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The band-gap modulation of sawtooth penta-graphane nanoribbons (SSPGNRs) under uniaxial elastic strain is investigated with the density functional theory method. Our results predict that the band gap of SSPGNRs can be tuned monotonic with strain. The band gap tends to decrease remarkably in both cases of stretching or compression. The value of band gap decrease from 2.71 to 1.75 eV for compression strain and from 2.71 to 2.31 eV for stretching strain when the strain changes from -10.0% to 10.0% , respectively. Moreover, the band gap of the SSPGNRs is more sensitive to the compressive than tensile deformation, which mainly originates from the shift of its valence band edge under strain. Our calculated Young's module of SSPGNR is quite smaller than that of the graphene nanoribbons. Our results imply the great potential of sawtooth penta-graphene nanoribbons in the pressure sensor and optical electronics applications at nanoscale.

Presenter: Thanh Nhật Lê

P.23 – Poster, VCTP-44

Classical interpretation of dynamics of ultracold atoms in the tilted optical lattice

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In this paper, we study the dynamics of ultracold Rb^{87} under the influence of the tilted optical lattice via the Bloch oscillation phenomenon under the single-band approximation. By simulating the intraband dynamics of wave packet in position and momentum spaces, the dependencies of the amplitude and the period of the oscillation on the tilted coefficient and the lattice height are shown and compared with the classical theory under the tight-binding approximation. Therefore, the limit of the single-band approximation where Landau-Zener tunneling is neglected is verified.

Presenter: Pham Nguyen Thanh Vinh

P.24 – Poster, VCTP-44

Effect of spatially modulated magnetic field and spin-orbit coupling in Lieb lattice

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The interplay between the spin-orbit coupling and spatially modulated magnetic field in the Lieb lattice is studied by exact diagonalization. The spin-orbit coupling opens a gap in the single-particle spectra and leads to a topological insulator at third and two thirds fillings, whereas the magnetic field usually destroys the topology of the ground state. It is found at certain conditions of the spin-orbit coupling and the spatially modulated magnetic field the ground state is still paramagnetic and topological despite the presence of the magnetic field. The interplay between the spin-orbit coupling and the spatially modulated magnetic field leads to various exotic ground states.

Presenter: Nguyễn Hồng Sơn

P.25 – Poster, VCTP-44

The formation of magnetization plateaus in the Sastry-Sutherland lattice with disorder.

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We investigate disorder effects using Callen identities on the classical Ising model with anti-ferromagnetic (AF) spin couplings in the Sastry-Sutherland lattice. The simulation results indicate that the field-dependent magnetization curve of the Ising model consists of only one main plateau with a fractional value $m/m_s = 1/3$ (the saturation magnetization m_s) without disorder. In the inclusion of disorder, the fascinating sequence of the magnetization plateaus is surprisingly found with fractional values depending on the disorder probability of the AF exchange interaction between nearest neighbor and next nearest neighbor sites. Our results imply that dynamical mechanism driven by disorder induces multi-steps in the field-dependent magnetization curve which are experimentally observed in many compounds as $\text{SrCu}_2(\text{BO}_3)_2$ and rare-earth tetraborides RB_4 ($\text{R} = \text{Tm}, \text{Ho}, \text{Er}$).

Presenter: Bach Huong Giang

P.26 – Poster, VCTP-44

Molecular dynamics simulation of microstructure and atom-level mechanism of crystallization pathway in iron nanoparticle

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Molecular dynamics simulation is used to study iron nanoparticles containing 5000 atoms at temperatures ranging from 300 K to 900 K. The crystallization and structure evolution was analyzed through pair radial distribution function, angle distribution, transition to different x-types, where x is the bcc, fcc-hcp, ico, 14, 12 and dynamical local structure parameters. The simulation showed that the structure of amorphous NP consists of two parts: the core has the

structure similar to the one of bulk counterpart and the surface has more porous structure. The crystallization occurred when NP was annealed at 750 K, 800 K, 900 K for 40 ns. We found that amorphous NP is crystallized via transformations of amorphous type to bcc-type atoms. Moreover, the crystallization pathway comprises intermediate states between amorphous and crystalline ones. At the early stage a large cluster of Cryst-atom formed is located in a middle layer of NP. Then this cluster grows up and the parameter $\langle \text{fbcc} \rangle$ for it increases rapidly. At the final stage the cluster of Cryst-atom is located in a region covered a major part of NP. The growth of crystal cluster happens parallel with changing its microstructure. We also found that the structure of fully crystalline NP is strongly heterogeneous and consists of three separate regions with amorphous, crystal-like and bcc-crystal structure.

Presenter: Giap Thi Thuy Trang

P.27 – Poster, VCTP-44

A review of using re-quantized classical molecular dynamics simulation method for spectral shape study

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Re-quantized classical molecular dynamics simulation (rCMDS) has been shown as a powerful tool to predict the infrared absorption line shapes of various molecule systems. Comparisons between the rCMDS calculated and experimental spectra of several lines for different linear molecules (such as CO₂, O₂ and HCl) measured in a large pressure range showed very good agreements. This method was also successfully applied to non-linear molecules as for the case of pure H₂O, H₂O in N₂. Note that the rCMDS correctly predicts non-Voigt features of the line shape but it does a poorer job for the pressure-broadening coefficients, especially for the case of CH₄ diluted in N₂. The main purpose of this report is giving an overview of using the re-quantized classical molecular dynamics simulation for molecular spectral shape study. Some discussions and comments about advantages and disadvantages of using this method are also included.

Presenter: Ngo Hoa Ngoc

P.28 – Poster, VCTP-44

Non-equilibrium condensation of Polaritons I: kinetics of the Excitations

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Kinetics of the excitation of a non-equilibrium polariton condensate, called bogolon, is studied by using the quantum Boltzmann equation coupled with the Gross-Pitaevskii equation for polariton and the rate equation for the non-resonant exciton-reservoir which is derived from the non-equilibrium Green functions. The time-, space- and momentum-resolved population of the bogolon and condensate polariton are calculated numerically after the switch-on of a cw non-resonant pump in the exciton-reservoir regime. The bogolon distribution approaching to a thermal equilibrium distribution is studied in detail.

Presenter: Đoàn Trí Dũng

P.29 – Poster, VCTP-44

Sampling the folding transition state ensemble in a tube-like model of protein

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We used the tube model with Go-like potential for native contacts to study the folding transition of a designed three-helix bundle and a designed protein G-like structure. It is shown that both proteins in this model are two-state folders with a cooperative folding transition coincided with the collapse transition. We defined the transition states as protein conformations in a small region around the saddle point on a free energy surface with the energy and the conformational root mean square deviation (rmsd) from the native state as the coordinates. The transition state region on the free energy surface then was sampled by using umbrella sampling technique. We show that the transition state ensemble is broad consisting of different conformations that have different folded and unfolded elements

Presenter: Nguyen Ba Hung

P.30 – Poster, VCTP-44

The geometry of ribosomal exit tunnel affects post-translational escape of nascent proteins

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We study the escape of nascent proteins at the ribosomal exit tunnel by using the Go-like model for proteins and a real atomistic tunnel taken from the PDB structure of a ribosome of archeon *Haloarcula Marismortui*. The full translation and escape process of nascent proteins at the tunnel were simulated by using Langevin dynamics. We show that at the temperature relevant to the physiological conditions, the escape time of protein G (GB1) follows quite well the one-dimensional diffusion model proposed in our earlier works. The escape time distribution of GB1 and the relationship between its folding and the escape obtained for the real exit tunnel is similar to those for simple cylinder model. Compared to an equivalent cylinder tunnel, the real tunnel induces a higher probability of trapping small proteins inside the tunnel and a broader escape time distribution. This probability is shown to be depend on temperature, the friction coefficient and the translation speed. Within a range of translation speed, slower translation leads to less trapped protein.

Presenter: Bui Phuong Thuy

P.31 – Poster, VCTP-44

Study on elastic and nonlinear deformations of BCC interstitial alloy FeC

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Analytic expressions of characteristic nonlinear and elastic deformation quantities such as the elastic modules, the elastic constants, the density of deformation energy, the maximum real stress and the limit of elastic deformation for interstitial alloy AB with body centered cubic at zero pressure are derived from the statistical moment method. The theoretical results are applied numerically to interstitial alloy AB and the calculated results are compared with ones of main metal Fe and experiments.

Presenter: Nguyễn Đức Hiền

P.32 – Poster, VCTP-44

Structural and electronic properties of silicene/gallium selenide van der Waals heterostructure: A first principles study

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Possibilities of different stacking configurations of silicene/gallium selenide (Si/GaSe) van der Waals heterostructure have been proposed and studied by density functional theory. We find that the Si/GaSe heterostructure in all the stacking configurations shows semiconducting behavior with a band gap of about 100 meV and we can control its band gap by strain or external electric field. This gap is much larger than that of graphene/GaSe but is much smaller than MoS₂/GaSe case. In the present work, we focus on the influence of biaxial strain and external electric field on the electronic properties of the most energetically stable configuration of the Si/GaSe heterostructure. Our calculated results indicated that the Si/GaSe heterostructure forms an n-type Schottky contact with a small Schottky barrier height of 0.23 eV and transformation between contacts may occur when strain or an electric field is applied.

Presenter: Nguyen Ngoc Hieu

P.33 – Poster, VCTP-44

Transient super-slow power-law decay of the time-dependent reflection induced by correlations in semi-infinite disordered media

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We investigate numerically the time-dependent reflection properties of a wave packet at a boundary of a semi-infinite medium with long-range correlated disorder. In the absence of the long-range correlation, we reproduce the averaged time-dependent reflectance in such a system decays in time as a power law, $\langle R(t) \rangle \propto t^{-2}$, in the limit of long time. This is a signature of Anderson localization. However, when the long-range correlation is taken into account, the above behavior is significantly modified. In particular, we find that the time evolution of the incident wave

packet undergoes various diffusion regimes ($\langle R(t) \rangle \propto t^{-\alpha}$) with different power-law exponents. Moreover, this behavior strongly depends on the value of the central energy of the incident wave packet.

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Presenter: Ngô Thị Hồng Vy

P.34 – Poster, VCTP-44

Investigation of thermodynamic properties and self-diffusion of AuCu superlattice by an analytic statistical moment method

Cao Huy Phuong (1)

(1) Hung Vuong University

We have investigated the self-diffusion and thermodynamic quantities of AuCu superlattice using the statistical moment method in the statistical physics. The activation energy, diffusion coefficient, pre-exponential factor, lattice parameter, thermal expansion coefficient, etc. . . . , are derived in closed analytic forms within the fourth order moment approximation. The present analytic formulas including the anharmonic effects of the lattice vibration give the predicted values of these quantities.

Presenter: Cao Huy Phuong

P.35 – Poster, VCTP-44

Vibration effect on the elastic differential cross section in the gas-phase electron diffraction within the multiple scattering model

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The gas-phase electron diffraction has been an effective method for determining the structure of molecular [1]. For retrieval of the molecular structure, several simple models such as the independent-atoms model (IAM) [2] and the multiple scattering model (MS) [3] were applied for calculating the electron-molecule differential cross section (DCS). While the IAM is validated sufficiently for an electron-molecule collision at high energy only, the MS also works well at the immediate and low energies [2, 3]. Beside the DCS, the molecular scattering intensity and the radial distribution function, which directly contain the molecular structure, are significant for the molecular structure retrieval [1]. Mainly, due to the contribution of each atomic pair to the diffraction intensity caused by the electron scattering on the molecule, the interatomic separations are clearly shown by the peaks of the radial distribution curve [1]. Within the IAM, molecular vibration distorts the DCS, molecular scattering intensity, and radial distribution function; as a consequence, its inclusion corrects the molecular retrieval structure [4, 5]. However, the MS developed for intermediate and low energies of the electron-molecule collision has not considered the vibration effect [3].

In this report, we show how to include the molecular vibration to the MS. Applying these calculations to some gas-phase molecules, we compare the applicability of the two models, IAM and MS. Furthermore, we analyze the energy region of electron scattering where the MS is highly accurate and, consequently, the included molecular vibration effect can be noticeable. Finally, we investigate the influence of the vibration effect on the molecular structure retrieval.

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Presenter: Nguyen Thi Hien

P.36 – Poster, VCTP-44

Molecular dynamics simulations of structural transformation and mechanical properties in densified MgSiO₃

Le Van Vinh

Phenikaa University

Molecular dynamics simulations of densified MgSiO₃ have been carried out to study the structural and mechanical properties under uniaxial tension. The network structure consists of SiO_x and MgO_y units which link to others by corner-, edge- and face- sharing bonds. The Si-rich and Mg-rich regions exist in densified MgSiO₃. The stress-strain curves exhibit the elastic and plastic characteristics. The transformations of SiO_x and MgO_y units occur with increasing strain, at which the corner-, edge- and face- sharing bonds among SiO_x and MgO_y units change. The Si-rich and Mg-rich regions increase with increasing strain. Under pressure, the transition of units SiO_x, MgO_y occurs from low to high coordination number. The topology of each SiO_x type is less affected than that of each MgO_y type upon compression. With increasing pressure above 20 GPa, oxygen atoms become more ordered to form the distorted oxygen sublattice in fcc, hcp or icosahedral clusters, at which these clusters contain a few ten to hundred atoms. The Young's modulus increases with increasing pressure due to the increasing fraction of high coordination number and the decrease of the volume of each SiO_x and MgO_y types.

Presenter: Le Van Vinh

P.37 – Poster, VCTP-44

A comparative study of the localization properties of eigenstates in conservative and non-conservative systems: Effects of long-range correlation disorder

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We study numerically the effects of long-range correlations in the disorder distribution on the localization properties of the eigenstates in a one-dimensional disordered lattice characterized by a random non-Hermitian Hamiltonian, where the imaginary part of the on-site potential is random. We calculate participation number versus strengths of disorder and correlation. Unlike

in the case of a long-range correlated real random potential, no signature of the localization transition is found in a long-range correlated imaginary random potential. In the region where localization is enhanced in the presence of long-range correlations, we find that the enhancement occurs in the whole energy band, but is strongest near the band center. In addition, we find that the anomalous localization enhancement effect occurs near the band center.

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Presenter: Lieu Thi Kim Thoa

P.38 – Poster, VCTP-44

Elementary excitation in the layered ferroics

*Nguyen Tu Niem, Bach Huong Giang, Nguyen Thuy Trang, Bach Thanh Cong
VNU University of Science*

Temperature and size dependence of the elementary excitation of the layered ferroics (ferro-electrics or ferromagnetics) are calculated using the functional integral method and XZ Heisenberg model within the Gaussian approximation. Basing on this result, the other thermodynamic properties like specific heat, polarization. . . are obtained. A comparision with experimental and other theoretical results for typical ferroics is carried out and discussed.

Presenter: Nguyễn Từ Niệm

P.39 – Poster, VCTP-44

Decay of neutron with participation of the light vector boson X17

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The recently, discovered light vector boson X17 at ATOMKI can bring new decay channels of neutron, which can be used to explain the neutron lifetime puzzle. In this article, we calculate all the possible decay widths and discuss the physical implications

Presenter: Pham Tien Du

P.40 – Poster, VCTP-44

Electric-field-enriched electronic and optical properties of Bernal stacked bilayer graphene nanoribbons

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We investigate the electronic and optical properties of Bernal stacked bilayer graphene nanoribbons under the effect of an external electric field using a combination of tight-binding model and the gradient approximation. Our results demonstrate that the electric field could modify sig-

nificantly the low-energy dispersion, sub-band spacing, bandgap, and band-edge states. These effects are reflected clearly in the density of states and optical spectra. It indicates that the optical absorption spectra are sensitive to both the strength and direction of the electric field. The introduction of the electric field leads to substantial changes in the energy bands and wave functions, and thus creating new optical excitation channels. Additional absorption peaks are therefore explicitly observed.

Presenter: Vu Thanh Tra

P.41 – Poster, VCTP-44

A model to predict the thermal diffusion factors in binary mixtures

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Development of models to predict thermal diffusion factor, or Soret coefficient, of binary fluid mixtures has been the objective of many works in the past [1]. However, the prediction capabilities of the available models are often limited, even for simple binary mixtures, if a large range of thermodynamic conditions is considered. Thus, this work aims at providing a generic model able to quantitatively provide thermal diffusion factors of simple binary mixtures over a wide range of thermodynamic conditions (gas, supercritical and liquid). The proposed model stems from the fact that direct residual transport properties of simple fluids are strongly linked to their so called excess entropy [2,3]. Taking advantage of this link, the model decomposes the thermal diffusion factor into zero-density and residual contributions, in which the former, dominant in gas phases, is computed from the kinetic theory. The latter contribution, dominant in dense phases, is further separated into isotopic and configurational contributions which are both functions of the excess entropy of the two considered species. First, it will be shown that the functional form of the proposed model is fully supported by results coming from molecular dynamics simulations of simple fluids mixtures (e.g. Ar + Kr). Second, the model has been combined with excess entropies deduced from modern equations of states [4] so as to check its ability to predict thermal diffusion factors of various binary mixtures such as those composed of n-alkanes.

Presenter: Nguyen Tu Khai Nam

P.42 – Poster, VCTP-44

Dark matter and flavor changing in the flipped 3-3-1 model

Lê Đức Thiện

Viện vật lý, viện hàn lâm khoa học và công nghệ Việt Nam

The flipped 3-3-1 model discriminates lepton families instead of the quark ones in normal sense, where the left-handed leptons are in two triplets plus one sextet while the left-handed quarks are in antitriplets, under $SU(3)_L$. We investigate a minimal setup of this model and determine novel consequences of dark matter stability, neutrino mass generation, and lepton flavor violation. Indeed, the model conserves a noncommutative $B - L$ symmetry, which prevents the unwanted

vacua and interactions and provides the matter parity and dark matter candidates that along with normal matter form gauge multiplets. The neutrinos obtain suitable masses via a type I and II seesaw mechanism. The nonuniversal couplings of Z' with leptons govern lepton flavor violating processes such as $\mu \rightarrow 3e$, $\mu \rightarrow e\bar{\nu}_\mu\nu_e$, and $h \rightarrow \mu\tau$ as well as the nonstandard interactions of neutrinos with matter.

Presenter: Lê Đức Thiện

P.43 – Poster, VCTP-44

Algebraic relation between bases of the nine-dimensional MICZ-Kepler problem

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Recently, different bases of the wavefunctions of the nonrelativistic MICZ-Kepler problem in the nine-dimensional Euclidean space (9D MICZ-KP) has been investigated analytically by the variable-separation method. In this report, each basis set of the wavefunctions is proved to be eigenfunctions of a corresponding set of 9 algebraically-independent integrals of motion in which they all commute to each other. The existences of such sets expectedly come from $SO(10)$ symmetry and the maximal superintegrability of the 9D MICZ-KP. Also, the relations between different bases are algebraically proposed via the connections between their sets of constants of motion.

Presenter: Le Dai Nam

P.44 – Poster, VCTP-44

Equation of state and thermal expansion of metals Cu, Au, Ag

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The thermodynamic properties of metals are studied using the moment method in the statistical dynamics, which allows us to take into account the anharmonicity of thermal lattice vibrations, going beyond the quasi-harmonic approximation. Applying to Cu, Au, and Ag metals, we determine the equation of state and thermal expansion in dimensionless polynomial form. Numerical results for the thermal expansion coefficient and the lattice spacing of these metals in different temperatures and pressure are in good agreement with experiments. Keywords: moment method, effective pair potential.

Presenter: Pham Duy Tan

P.45 – Poster, VCTP-44

Mott transition in the mass imbalanced ionic Hubbard model at half filling

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(1) Institute of Physics; (2) Hanoi National University of Education; (3) Graduate University of Science and Technology, VAST; (4) Ha Long University

The Mott - Hubbard metal - insulator transition in the half-filled mass imbalanced ionic Hubbard model is investigated using the two-site dynamical mean field theory. We find that for a fixed mass imbalanced parameter r the critical interaction U_c increases when the ionic energy Δ is increased. In the other hand, for a fixed Δ , U_c decreases with increasing the mass imbalance. We also show the existence of a band insulating phase in the system for the case $\Delta \neq 0$, $U = 0$ and calculate the staggered charge density $n_B - n_A$ as a function of the interaction for different values of the mass imbalance. Our results in the limiting cases ($r = 1$, $\Delta \neq 0$ or/and $\Delta = 0$, $r \neq 1$) are in good agreement with those obtained from the full dynamical mean field theory.

Presenter: Nguyen Thi Hai Yen

P.46 – Poster, VCTP-44

Adsorption of Gas Molecules on Sawtooth Penta-Graphene Nanoribbons

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We have studied the adsorption of gas molecules (CO, CO₂, and NH₃) on sawtooth penta-graphene nanoribbons (SPGNRs) 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 SPGNRs show chemical adsorption properties, meanwhile the adsorption of NH₃ shows physical adsorption properties. Gas molecules have little effect on modifying the conductance of SPGNR. We also studied to compare the absorption capacity NH₃ on SPGNR at possible absorption sites. Quantum transport calculations further indicate that NH₃ molecules can be detected by the SPGNRs-based sensor.

Presenter: Vo Van On

P.47 – Poster, VCTP-44

Molecular dynamics simulation of amorphous silica under pressure

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Molecular dynamics (MD) simulation is used to study amorphous silica consisting of 4998 atoms at 500K under pressure from 0 to 100 GPa. The compression was considered through pair radial distribution function, bond-angle distributions, bond length distribution, the geometric units, Voronoi polyhedra and O-particle. We found that in the 0-20 GPa pressure range, the Si-O bond length increases with pressure. At pressure beyond 20 GPa, the Si-O bond length decreases with pressure. This results is due to relate a structural transformation from tetrahedral- to octahedral-network. This is origin of transformation from amorphous to crystalline phase (stishovite) as the pressure higher than 20 GPa.

Presenter: Giap Thi Thuy Trang

P.48 – Poster, VCTP-44

Neutrino mass and mixing in an A4 model with inverse seesaw mechanism

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Masses and mixing of neutrinos from an A4 model with inverse seesaw mechanism are introduced. They are shown to be consistent with the recent experimental data of neutrinos. Effective neutrino masses and Jarlkog invariant parameter predicted by this model are presented.

Presenter: Ngo Minh Ket

P.49 – Poster, VCTP-44

Decay of SM-like Higgs $h \rightarrow \mu\tau$ in an A4 model with inverse seesaw mechanism

Hồ Việt Thắng (1), Nguyễn Thanh Phong (1), Lê Thọ Huệ (2), Đặng Trung Sĩ (3)

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Lepton flavor violating decay of the SM-like Higgs boson (LFVH) $h \rightarrow \mu\tau$ in an A4 model with inverse seesaw mechanism is presented. We will show that the model predicts large branching ratios of this decay that can be detected by the future experiments from LHC.

Presenter: Ho Viet Thang

P.50 – Poster, VCTP-44

Retrieval of structural parameters of monolayer transition-metal dichalcogenides from the exciton energy spectrum

Duy-Nhat Ly (1), Thanh-Truc N. Huynh (2), Ngoc-Hung Phan (1), Van-Hoang Le (1)

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Exciton energy spectra of two-dimensional systems such as graphene, monolayer transition-metal dichalcogenides (TMD) have been investigated actively in the last few years (see, for example [1] and cited therein). It has been found that the interaction between the hole and electron forming an exciton is not Coulombic but instead screened by the reduced dimensionality. This screening potential is well described by Keldysh model [2] which contains some structural parameters such as the exciton effective mass and the screening length related to the polarizability of materials. This report is about an idea of determining the structural parameters from the experimental exciton energy spectrum. Theoretical exciton energies calculated within the Keldysh model by different parameters are compared with the experimental data, and the best fit gives the right structural parameters of the materials. We have applied this idea to very recent experimental data of a monolayer TMD WSe₂ sandwiched by two hBN slabs [1] and published the first results in [3]. Furthermore, we analyze the predicted sizes of the exciton with some excited states and compare them with the experimental data. Finally, we apply the approach for other monolayer TMDs such as MoS₂, MoSe₂, WS₂, and WSe₂ whose experimental exciton energies are available recently.

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[2] L. V. Keldysh, Coulomb interaction in thin semiconductor and semimetal films, JETP Lett. 29 (1979) 658-660.

[3] Duy-Anh P. Nguyen, Duy-Nhat Ly, Dai-Nam Le, Ngoc-Tram D. Hoang, and Van-Hoang. Le, High-accuracy energy spectra of a two-dimensional exciton screened by reduced dimensionality with the presence of a constant magnetic field, Physica E 113 (2019) 152–164.

Presenter: Ly Duy-Nhat

P.51 – Poster, VCTP-44

Magnetic orders of Heisenberg models with arbitrary spin in semi-fermionic representation

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In 1988 Popov and Fedotov (PF) proposed a new method for spin Hamiltonians free of the local constraint problem for spin $S = 1/2$ and $S = 1$. Later, this approach has been extended for arbitrary spin. PF formalism has been used to study magnetic orders in some spin $S = 1/2$ and $S = 1$ Heisenberg models. In this report we show how to study the low temperature phases of quantum Heisenberg models with arbitrary spin by means of PF method. We work out the free energy and the magnetization in one-loop approximation.

Presenter: Pham Thị Thanh Nga

P.52 – Poster, VCTP-44

Nonlocal properties and quantum teleportation in the photon-pair-subtracted and photon-pair-added two-mode squeezed vacuum state

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This paper introduces a new state by adding and subtracting the photons on two-mode squeezed vacuum state called photon-pair-subtracted and photon-pair-added two-mode squeezed vacuum state (PSPATSVS). In this state, the quantitative measures of entanglement by the linear entropy and the Einstein-Podolsky-Rosen correlation as well as quantum steering are investigated. By using the PSPATSVS state as a resource, the quantum teleportation processes are studied by two protocols as the orthogonal quadrature components and the number sum and phase difference. Finally, we propose an experimental scheme for generation of such state by using quantum optical devices.

Presenter: Tran Quang Dat

P.53 – Poster, VCTP-44

Role of pairing in maintaining the constant value of nuclear temperature at low excitation energy

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The nuclear temperature is calculated by using nuclear level density extracted from microscopic EP + IPM approach, which includes exact pairing (EP) for the levels around the Fermi surface in combination with the independent particle (IPM) model for the rest of the single-particle spectrum [1]. It is found that the temperature is almost constant at low excitation energy. This feature explains why the constant-temperature model can describe well the nuclear level density. The validity of this phenomenological model will be clearly analyzed in some nuclei. The results also show that pairing plays an important role in maintaining this nearly constant value of temperature at low excitation energy.

[1] Quang Hung N, Dinh Dang N and Quynh Huong L T (2017) Phys. Rev. Lett. 118 022502

Presenter: Le Thi Quynh Huong

P.54 – Poster, VCTP-44

The effect of external electric fields on the electronic band structure of AA-stacking bilayer graphene ribbons

Nguyen Lam Thuy Duong (1), Dao Thuy Tuong Vi (1), Vu Thanh Tra (2), Tran Van Truong (3)

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Graphene, an isolated single layer of carbon atoms, has attracted huge attention of many scientists due to its unique and intriguing electronic characteristics. Recently, attention has been paid to bilayer structures of graphene where numerous novel phenomena have been observed in the presence of external fields or stacking faults. Although the AB stacking structures have been studied extensively, less attention has been paid to AA-stacking, particularly to bilayers of ribbon structures. In this work, we examine the band structure of AA-stacking bilayer graphene ribbons using a tight binding model. Both armchair and zigzag edge structures are considered. External electric fields are also added into the Hamiltonian. We noticed that the effect of transverse and vertical electric fields is remarkable with some noticeable distinction which is reflected in the change of both the energy bands and the density of states. The electronic properties of these AA-stacking structures, with and without external fields, are also compared to the ones of the AB-stacking systems, providing a more comprehensive understanding of the stacking dependence of the electronic structures in bilayer ribbon structures of graphene.

Presenter: Dao Thuy Tuong Vi

P.55 – Poster, VCTP-44

Electronic structures in armchair silicene nanoribbons

Danh Tan Xuan (1,2), Nguyen Thi Kim Quyen (3), Thai Thanh Lap (4), Vu Thanh Tra (4)

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Nowadays, two dimensional material is the best candidate for the future electronic devices. Armchair silicene nanoribbons is not an exception when its outstanding properties can be comparable with the traditional electronic devices base on silicon. In this paper, we use atomistic Tight binding method and Green 's function formalism to calculate the band structure as well as the density of state (DOS) and the tranmission (T) of this material. The results illustrated that the structure of armchair silicene nanoribbons is the similar to graphene, this means the armchair silicene nanoribbons allways exhibits three groups such as $3p$, $3p+1$ and $3p+2$. However, the natural highest band gap in this material is about 1.4eV , which is smaller than the one in graphene. For this reason, a tunable bandgap would be highly desirable. Consequently, we continue the application of the transverse electric filed to control the energy gap. Our results show that the band gap strongly depends on and modulates as a function of electric field and the width of nanoribbons. With results received, we believe that our study strongly supports write up the picture of the electronic structure and its properties of armchair silicene nanoribbons.

Presenter: Danh Tan Xuan

P.56 – Poster, VCTP-44

Investigation of the magneto-dynamical dielectric function of monolayer phosphorene

Tran Cong Phong (1), Le Thi Thu Phuong (2), Doan Quoc Khoa (3), Bui Dinh Hoi (2)

(1) The Vietnam National Institute of Educational Sciences (2) University of Education, Hue University (3) Quang Tri Teacher Training College

In this investigation, we theoretically address the magnetic field effects on the frequency-dependent dynamical dielectric function, including the refractive index and the absorption coefficient, of phosphorene. An effective Hamiltonian model beyond the continuum approximation is employed to obtain the electronic dispersion energy and the linear response theory is applied to calculate the dynamical dielectric function at a certain temperature along both armchair and zigzag edges. Our numerical calculations show that, independent of the direction, the refraction (absorption) intensity decreases (increases) with the optical frequency at all magnetic field strengths. Moreover, we find out that the refraction and absorption processes along the armchair edge do not change after a critical magnetic field and this critical point increases with the optical frequency stemming from the spin-splitting effects. As for the zigzag edge, however, there is a little to no change for these processes with the magnetic field. Further, we observe that, in average, the dominant contribution to the total magnetic field-dependent dynamical dielectric function comes from the armchair edge originating from the smaller (larger) carrier effective mass (velocity) than the zigzag edge. Tuning the optical responses of phosphorene with the magnetic field is useful for practical spintronic applications.

Presenter: Bui Dinh Hoi

P.57 – Poster, VCTP-44

Metal-insulator phase diagram of the half-filled Anderson-Hubbard model

Hoang Anh Tuan (1), Nguyen Thi Hai Yen (1), Le Duc Anh (2)

(1) Institute of Physics, VAST (2) Faculty of Physics, Hanoi National University of Education

The metal-insulator phase transition diagrams of the Anderson - Hubbard model at half filling with the box and the Gaussian disorder distributions are obtained via typical-medium theory within an approximation to the equation of motion. The equations determining the boundary between the correlated metal, Mott insulator, and Anderson localization phases are derived. Our results are in good agreement with those found by the more sophisticated methods and indicate that on a qualitative level they do not depend on the choice of the above disorder distributions.

Presenter: Hoang Anh Tuan

P.58 – Poster, VCTP-44

Theoretical investigation of quantum beat of excitons in GaAs/AlGaAs quantum dots

Le Thi Ngoc Bao (1,2), Dinh Nhu Thao (1)

(1) Hue University of Education; (2) Hue University of Sciences

In this paper, we studied theoretically quantum beat of excitons in GaAs/AlGaAs spherical quantum dots using renormalized wavefunction formulation. We observed the quantum beat when there is a strong laser coupling two electron quantized levels. Quantum beat is observed at twice the electron Rabi frequency. In addition, we found the dependences of quantum beat absorption on dot radius and pump field detuning.

Presenter: Le Thi Ngoc Bao

P.59 – Poster, VCTP-44

Improved Simulated Annealing Methods for core loading pattern optimization of VVER-1000 reactor

Tran Viet Phu (1), Tran Hoai Nam (2)

(1) Institute for Nuclear Science and Technology, VINATOM (2) Institute of Fundamental and Applied Sciences, Duy Tan University

This work presents the improved simulated annealing (SA) methods for core loading pattern (LP) optimization of VVER-1000 nuclear reactor. Several improvements of the SA method have been investigated, e.g. evolutionary simulated annealing (ESA) method and adaptive simulated annealing (ASA) method, and applied to the problem of in-core fuel management of VVER-1000 reactor. Numerical calculations have been performed to evaluate the performance of the improved SA methods in comparison among them and with the original one. Comparison between the new optimal LP of the VVER-1000 reactor core with the reference one has also been performed. The results show that the ESA method is advantageous over the original SA method. Neutronics performance of the new optimal LP of VVER-1000 core is also better than that of the reference LP.

Presenter: Tran Viet Phu

P.60 – Poster, VCTP-44

A theoretical study of the exciton quantum beats in GaAs/AlGaAs cylindrical

quantum wires*Duong Dinh Phuoc, Dinh Nhu Thao**Hue University of Education*

In this paper we study the exciton quantum beat phenomenon in GaAs/AlGaAs cylindrical quantum wires using renormalized wavefunction theory. We consider an exciton three-level model with a strong pump laser resonating with two exciton excited levels. The results show that exciton absorption intensity is an oscillatory function of time with frequency in the TeraHertz range, which indicates the existence of exciton quantum beats. We also reveal the influence of size effect and laser detuning on amplitude and frequency of those oscillations.

Presenter: Dương Đình Phước

P.61 – Poster, VCTP-44

Dynamical properties of the photon-added two-mode SU(1,1) coherent state in the Jaynes-Cummings-model*Le Thi Hong Thanh, Truong Minh Duc, and Nguyen Ngoc Lam*

(1) Center for Theoretical and Computational Physics, College of Education, Hue University, 34 Le Loi, Hue City, Viet Nam (2) Quang Nam University, 102 Hung Vuong, Tam Ky city, Quang Nam province, Viet Nam

This paper studies the dynamical properties of the photon-added two-mode SU(1,1) coherent state in the Jaynes-Cummings-model. The dynamical behaviors of this state are found to be different compared to that of the corresponding two-mode coherent and two-mode SU(1,1) coherent states. The density operator of the photon-added two-mode SU(1,1) coherent state is presented using the dressed-state representation. By using the linear entropy criterion, the dynamical properties of the entanglement in this state are considered in detail.

Presenter: Le Thi Hong Thanh

P.62 – Poster, VCTP-44

Particle-type Burnable Poison for Improving Neutronics Characteristics and Thermal Conductivity of VVER-1000 Assembly*Hung T.P. Hoang (1), Van-Khanh Hoang (2), Hoai-Nam Tran (3)*

(1) Nuclear Training Center, VINATOM; (2) Institute for Nuclear Science and Technology, VINATOM; (3) Institute of Fundamental and Applied Sciences, Duy Tan University

Application of particle-type burnable poison has been investigated for improving neutronics characteristics and thermal conductivity VVER-1000 fuel assembly. Gadolinia (Gd₂O₃) in form of burnable poison particles (BPPs) have been added in several UO₂ fuel rods of VVER-1000 fuel assembly. The use of BPPs is advantageous due to the increase of thermal conductivity of UO₂-Gd₂O₃ fuel rods compared to the reference design with homogeneous mixture of UO₂-Gd₂O₃. Parametric survey of the BPP parameters such as the number of UO₂-Gd₂O₃ fuel rods, their distribution, diameter and packing fraction of the BPPs has been conducted to improve the neutronics characteristics of the VVER-1000 fuel assembly. Two new models of assembly with 18 UO₂-Gd₂O₃ fuel rods have been considered. The diameter of 300 μm and the packing fraction of 3.33% were determined so that the burnup reactivity curve is approximate that of the reference one, while the power peaking factor can be decreased by about 4.8%. Application of BPPs for compensating the reduction of soluble boron content is also investigated.

Presenter: Tran Hoai Nam

P.63 – Poster, VCTP-44

Method of solving the time-dependent Schrödinger equation and its implementation in strong field physics

Cam-Tu Le (1,2), Ngoc-Loan T. Phan (3), Van-Hoang Le (3)

(1) Atomic Molecular and Optical Physics Research Group, Advanced Institute of Materials Science, Ton Duc Thang University, Ho Chi Minh City, Vietnam; (2) Faculty of Applied Sciences, Ton Duc Thang University, Ho Chi Minh City, Vietnam; (3) Department of Physics, Ho Chi Minh City University of Education, Ho Chi Minh City, Vietnam

We establish a method of numerically solving the time-dependent Schrödinger equation (TDSE) for a linear molecule exposed to a linearly polarized laser. For this purpose, we employ the single-active-electron approximation (SAE) for modeling the molecule as a system with one electron moving in the effective potential. This construction is based on the fact that, basically, only electron in the highest occupied molecular orbital (HOMO) interacts with the laser field. In practice, this TDSE+SAE method saves more computational cost than the others, such as the time-dependent Hartree-Fock (TDHF), multiconfiguration time-dependent Hartree-Fock (MCTDHF), and time-dependent density functional theory (TDDFT) methods. The solving process consists of two stages. First, wave functions of the laser-free system are built by solving the time-independent Schrödinger equation to use them as a basis set. Then, solutions of the TDSE are constructed in an expansion of the basis set functions, where the coefficients are time-dependent and can be obtained by the fourth-order Runge-Kutta method. We use the received wave functions further to investigate some nonlinear optic phenomena, such as the high-order harmonic generation (HHG) and the laser-induced electron diffraction (LIED). In this work, we demonstrate HHG spectra from CO molecule responding to a near-infrared laser. The results are compared with other experimental and theoretical data and used in several physics analyses.

Presenter: Le Thi Cam Tu

P.64 – Poster, VCTP-44

The classical effects of Einstein's GRT for some $f(R)$ modified gravity models in the Sun system

Vo Van On

Group of Computational Physics and Simulation of Advanced Materials – Faculty of Natural Sciences- University of Thu Dau Mot

In the report, we present the calculation results of some classical effects of GRT of Einstein in the Sun system as the perihelion shift of a planet in its orbit, the deflection angle of light ray near the Sun disk for some $f(R)$ modified gravity models as Starobinsky's model, Linder's model and $f(R)$ modified gravity model of polynomial exponential form. The calculation results show that these modified gravity models give very small contributions to GRT's classical effects in the solar system and all are consistent with astronomical observations.

Presenter: Vo Van On

P.65 – Poster, VCTP-44

Temperature-dependent transport properties of two-dimensional hole gas in Ge channel modulation-doped square quantum wells

Tran Thi Hai, Ho Khac Hieu, Le Ba Nam, Trinh Thi Dung

Hong Duc University

We have studied the mobility of a two-dimensional hole gas at high temperature in Ge channel modulation-doped square quantum wells. Within the variational approach, we obtain analytic expressions for the carrier distribution, and autocorrelation functions for various scattering mechanisms. Calculated temperature-dependent hole mobilities of quantum wells with different scattering mechanisms, e.g. acoustic and optical phonon scattering. Our calculation show that the dependence of the mobilities of carriers on the temperature in the square quantum wells.

Presenter: Tran Thi Hai

P.66 – Poster, VCTP-44

Investigation of the frequency shift of microcantilever depends on positions and the correlation between two absorbed mass on the surface.

Le Tri Dat (1,2) and Nguyen Duy Vy (1,2)

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Microcantilever is a crucial tool for determining and measuring sample in various fields such as chemical, physics or biology. Based on the response of the cantilever, such as the deflection or resonance frequency, that one could use to determine tension, temperature or mass. In this work, we theoretically investigate the frequency shift due to two mass attached on the surface of the cantilever. The position of the mass effects on the resonance. Moreover, we show that the correlation between two absorbed objects, such as the position and the attached time, contributes to the characteristic of the dynamics. The results can provide fruitful information for measuring in bio-sensing.

Presenter: Le Tri Dat

P.67 – Poster, VCTP-44

Distributions transition under orthogonal random fluctuations

t.a. chu, n. t. lan

institutue of physics

It is well-known that some famous probability density functions (PDF) of random variables are associated with symmetries of these random variables. The Boltzmann and Gaussian PDFs that are invariant under translation and spherical transformations of their variables, respectively, are obvious and well-studied examples reflecting not only symmetries of many physical phenomena but also their underlying conservation laws. In physics and in many other fields of interests of complexity, the transitions from the Boltzmann PDF to the Gaussian PDF, or at least from Boltzmann-like PDF to the Gaussian-like PDF, i.e from a sharp peak PDF to round peak PDF, are frequently observed. These observed phenomena might provide clues for a phase transition, namely second-order phase transition, where symmetry of given physical quantities in the system under consideration are broken and changed to another one. The purpose of this work is to study this kind of transition in the superconductivity by investigating the transforma-

tion of envelope functions of electron and Cooper pair wave functions in spatial representation which might correspond to the change of symmetrical behavior of the space from its normal to superconducting states near the phase transition critical temperature.

Presenter: Chu Thuy Anh

P.68 – Poster, VCTP-44

Anisotropic magnetoresistance of nickel nanowires with various diameters

Do Ch. Pham (1), V. Thanh Ngo (2), J.-E. Wegrowe (3)

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In this work, we investigate the anisotropic magnetoresistance of single-contacted Ni nano-wires. The samples are grown in a polymer membrane (polycarbonate) using the electrodeposition technique. The resistance of nanowires is measured as a function of external magnetic field. The results show that the magnetovoltic signal is a response to the magnetization but is not a response to the external magnetic field

Presenter: Ngo Van Thanh

P.69 – Poster, VCTP-44

Performance of quantum algorithms on the IBM quantum computers

Tran Minh Duc, Nguyen Van Duy, Nguyen Quoc Hung

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Quantum computation is an emerging technology with the perspective to outperform classical computation in many classes of problem. However, the inaccessibility of a true quantum computer, for reason of both engineering and cost, had been staunching the development of the field for years. In 2016, IBM released the Quantum Experience, an online cloud service for public users to execute quantum algorithms. The quantum computation platform enables researchers and enthusiasts from all over the world to participate and develop the new paradigm of computation. In this work, we execute standard quantum algorithms, specifically Shor's and Grover's, on the IBM Q quantum computers. Shor's algorithm is a quantum algorithm that solves prime factorization - a procedure widely used in public-key cryptography, such as RSA. Employing the power of quantum parallelism to perform quantum Fourier transformation, it requires polynomial time, in comparison to sub-exponential time with a classical algorithm. Grover's algorithm is the foundation of quantum search, a method that could speed up processes such as looking for items in unstructured data. Both algorithm are prominent examples that promise significant improvements in providing solutions for complex computational problems.

Presenter: Nguyen Quoc Hung

P.70 – Poster, VCTP-44

Theoretical study for mid-infrared graphene plasmons

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

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

We propose a theoretical approach to investigate plasmonic properties of mid-infrared graphene-based metamaterials. The artificial structures are composed of periodic arrays of graphene plasmonic resonators on dielectric thin films. Optical resonances are very sensitive to structural parameters and dielectric functions of both substrates and medium. The sensitivity at the mid-infrared regime can be exploited to design biosensors due to the same frequency order as molecular vibrations. Our numerical results are in accordance with previous experiments

Presenter: Do Thi Nga

P.71 – Poster, VCTP-44

Self-assembly of anisotropic colloids with critical Casimir forces: A simulation study

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Recent breakthrough of colloidal synthesis promises new routes for the assembly of colloidal superstructures with critical Casimir forces. However, due to the nature difficulty of near-critical binary solvents, patch-to-patch binding is experimentally challenging. In this presentation, we investigate the bonding morphology changes of single-bonded patchy colloids with effective critical Casimir pair potential using molecular dynamic simulations. For temperatures very close to the coexistence solvent phase diagram, where the attractive Casimir forces dominate, the chain-like colloidal structures stiffen, resulting in a much narrower range of bond angles. These results show qualitative agreement with confocal microscopy observation. This offer new opportunities for assembling single-bonded colloidal chains with temperature-switchable materials.

Presenter: Dang Minh Triet

P.72 – Poster, VCTP-44

Mechanical-thermodynamic responses of 2D penta-graphene materials under applied forces

Nhan Hoang Le (1), Quoc Tuan Truong (1), Trung Phuc Vo (1), Thanh Tien Nguyen (1), Minh Triet Dang (2)

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Recent simulations demonstrate penta-graphene as a promising semiconductor candidate for new optoelectronic properties with quasi-direct band gap of 4.48eV. Penta-graphene can be transitioned from a pentagonal high-energy to a hexagonal low energy level via applied forces or temperature. In this presentation, we demonstrate this sudden but universal transition from pentagon-based to hexagon-based structures by melting or uniaxial yielding these penta-graphene sheets. We provide a direct link between the thermodynamic elastic and plastic deformations and the corresponding transport properties of this interesting material. These results highlight the essential role of conformational changes of 2D penta-graphene materials to applied thermal

and mechanical energy.

Acknowledgement: This research is funded by Vietnam National Foundation for Science and Technology Development (NAFOSTED) under grant number 103.01-2018.308

Presenter: Nhân Hoàng Lê

P.73 – Poster, VCTP-44

Ab initio Study on Adsorption of Volatile Organic Compounds on Germanene

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Lung cancer accounts for 12% of all types of cancers, but has a mortality rate over 28%. In order to diagnosis and staging the lung cancer, cells or tissues is removed then tested by various methods, for example blood tests, chest X-ray, computed tomography (CT), magnetic resonance imaging (MRI) and so on [1]. However, these approaches are time-consuming, expensive, and uncomfortable for patients [2]. Thus there rises a demand of an alternative efficient cancer detector. Electronic nanosensors can detect at early stage breath contains potential biomarkers for lung cancer (volatile organic compounds (VOCs)). 2D materials are strongly expected to be promising candidates for VOC nanosensors. In this work, we study the adsorption of three VOCs (acetone, ethanol and toluene) in the exhaled air from cancer patients on the surface of germanene by using the quantum simulation method based on Density Functional Theory (DFT). The potential adsorption areas and the diffusion path of VOCs on germanene surface are explored by means of Computational DFT-base Nanoscope [3]. The adsorption energy profiles are calculated by three van der Waals functionals: vdW-REV-PBE, vdW-optPBE, and DFT-DF2. Also, we investigate the charge transfer between VOCs and the adsorbent by the Bader charge analysis.

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[2] E. M. Gaspar, A. F. Lucena, J. D. da Costa, and H. C. das Neves. Journal of Chromatography A 2009, 1216, 14, 2749–2756.

[3] Developed by V. A. Dinh, Vietnam Japan University.

Presenter: Duong Thi Diem My

P.74 – Poster, VCTP-44

First-principles study of $\text{Na}_2\text{Fe}_3(\text{SO}_4)_4$: A new material of potential cathodes for the sodium-ion rechargeable batteries

Thien Lan Tran (1,2), Nhu Thao Dinh (1) and Van An Dinh (2,3)

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Recently, there are many sulfate-based polyanion materials suitable for the fabrication of cathode

of Na-ion rechargeable batteries (NIBs), such as $\text{Na}_{2+2x}\text{M}_{2-x}(\text{SO}_4)_3$ ($\text{M} = \text{Fe}$ and Mn) [1,2]. $\text{Na}_2\text{Mn}_3(\text{SO}_4)_4$ was successfully synthesized in 2016 and demonstrated as a promising cathode material for NIBs [3]. Furthermore, Iron is a non-polluting and abundant material in the Earth's crust, leading to the idea of replacement of Mn by Fe to form $\text{Na}_2\text{Fe}_3(\text{SO}_4)_4$ as a new potential material for NIBs. In this work, we propose a new cathode material by using Density Functional Theory method. A systematic study of spatial structure, electronic structure, potential and diffusion mechanisms of ions Na in the material $\text{Na}_2\text{Fe}_3(\text{SO}_4)_4$ using the generalized gradient method with an effective U correction factor (GGA + U) is presented. Applying the simultaneous motion model of vacancy and accompanying polaron proposed by V.A. Dinh et al. [4], we reveal the diffusion mechanism through the exploration of element diffusion processes (EDPs). The diffusion pathways of Na ions along the [100], [010] and [001] directions are demonstrated by combination of EDPs. This material exhibits a wide band gap semiconductor behavior with a band gap of 3.612 eV. The calculated open-circuit voltage is 4.01 V corresponding to the redox pair $\text{Fe}^{+3}/\text{Fe}^{+2}$. Na-ions diffusion along the [100] and [001] directions costs an activation energy of 881 meV for both pathways. In the [010] direction, a pathway with a lower activation energy of 808 meV was also found.

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[4] V. A. Dinh et al., App. Phys. Express 5 (4), 045801 (2012).

Presenter: Tran Thien Lan

P.75 – Poster, VCTP-44

Performance of quantum algorithms on the IBM quantum computers

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Quantum computation is an emerging technology with the perspective to outperform classical computation in many classes of problem. However, the inaccessibility of a true quantum computer, for reason of both engineering and cost, had been stanching the development of the field for years. In 2016, IBM released the Quantum Experience, an online cloud service for public users to execute quantum algorithms. The quantum computation platform enables researchers and enthusiasts from all over the world to participate and develop the new paradigm of computation. In this work, we execute standard quantum algorithms, specifically Shor's and Grover's, on the IBM Q quantum computers. Shor's algorithm is a quantum algorithm that solves prime factorization - a procedure widely used in public-key cryptography, such as RSA. Employing the power of quantum parallelism to perform quantum Fourier transformation, it requires polynomial time, in comparison to sub-exponential time with a classical algorithm. Grover's algorithm is the foundation of quantum search, a method that could speed up processes such as looking for items in unstructured data. Both algorithm are prominent examples that promise significant improvements in providing solutions for complex computational problems.

Presenter: Tran Minh Duc

P.76 – Poster, VCTP-44

Generation of entangled states in Kerr-like nonlinear coupler pumped by external fields

Doan Quoc Khoa (1), Luong Thi Tu Oanh (2), Chu Van Lanh (2), Nguyen Thi Dung (3) and Nguyen Van Hoa (3)

(1) Quang Tri Teacher Training College, Dong Ha, Quang Tri, Viet Nam; (2) Vinh University, Nghe An, Viet Nam; (3) Hong Duc University, Thanh Hoa, Viet Nam

The Kerr-like nonlinear coupler including two nonlinear oscillations is investigated when these oscillations pumped by external classical fields, which are assumed to be decomposed into two parts: a coherent part and a randomly fluctuating chaotic component (white noise). By using nonlinear quantum scissors formalism, we can obtain the truncation of optical states that leads to achieve two-qubit states due to the nonlinear properties of oscillators and their interaction. Solving a set of coupled stochastic integro-differential equations involved in the problem with all initial conditions, we achieve analytical formulae for the complex probability amplitudes of finite n -photon states. Analysis of time evolution of the quantum entanglement shows that maximally entangled states can be generated and they change dramatically when the initial conditions are different.

Presenter: Doan Quoc Khoa

P.77 – Poster, VCTP-44

Dynamics heterogeneity and diffusion mechanism in sodium-silicate melts. Molecular dynamics simulation

Nguyen Thi Thanh Ha, Nguyen Thu Nhan

Hanoi University of Science and Technology

In the present study we use molecular dynamics simulation to investigate sodium-silicate melts with various compositions at 1873 K and ambient pressure. The microstructure and diffusion have been studied with help of simplex and cluster of simplexes. The simulation shows that the simplex contains up to 6 Na and the radius of simplexes varies from 1.4 to 4.5 Å. In the SiO₂-rich melt the majority of simplexes are void-simplexes and simplexes containing 1 Na. As the SiO₂ content of the melt decreases, the fraction of simplexes having 2, 3 and 4 Na monotonously increases. We find that the temporal number density of Na around Si and BO is significantly smaller than that around NBO and FO. The static structure is heterogeneous and comprises Na-poor and Na-rich regions occupied by Si-O subnets and S-clusters, respectively. The simulation also reveals "pockets for sodium" where Na atoms (O and Si) having large number density of Na gather. The structure comprises rigid micro-regions and the dynamics is spatially heterogeneous. The diffusion pathways for sodium consist of simplex-regions of solid-like NBO, FO and liquid type O. Moreover, Na atoms pass more intensively through such pathways than the simplex-regions of solid-like BO and Si.

Presenter: Nguyen Thi Thanh Ha

P.78 – Poster, VCTP-44

Determination of the mass diffusion coefficient of H₂O diluted in N₂ using classical molecular dynamic simulation

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In this work, the auto-correlation function of center of mass velocity has been used to deduce the mass diffusion coefficient (D) of water diluted in nitrogen using the Classical Molecular Dynamics Simulations (CMDs). The calculations have been performed at room temperature (296 K) for different mixtures of H₂O in N₂ and for a larger number of molecules starting a site-site potential. The results show that the auto-correlation functions expected exponential decay behavior and from the decay times we have determined the mass diffusion coefficient. The comparison between the CMDs results and experimental results are presented and discussed.

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[3] J. Lamouroux, R. R. Gamache, A. L. Laraia, Q. Ma, and R. H. Tipping, *J. Quant. Spectrosc. Radiat. Transf.* 113, 951 (2012).

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Presenter: Ngo Hoa Ngoc

P.79 – Poster, VCTP-44

Quantitative measures of entanglement and quantum teleportation in the photon-added and photon-subtracted two-mode pair coherent state

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This paper quantitates the entanglement degree by using linear entropy and Peres-Horodecki inseparability criteria in photon-added and photon-subtracted two-mode pair coherent state (PAPSPCS). The entanglement degree of this state is found to be different compared to that of the pair coherent states. By using the PAPSPCS state as a resource, the quantum teleportation processes are studied by the orthogonal quadrature components and the number sum and phase difference protocols.

Presenter: Hồ Sỹ Chương

P.80 – Poster, VCTP-44

Effects of the gold nanoparticle size on resonance energy transfers in optics system

N. Minh Hoa (1), L. Anh Thi (2), T. V. Nhan Hao (3), D Duc Anh (4), D. Quang Tam (1), D. T. N. Hoa (1), D. Hoang Tung (5)

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Science and Technology, 18 Hoang Quoc Viet Street, Hanoi, Vietnam

We present an analytical model for the fluorescence resonance energy transfer (FRET) between the molecules (donor) and the gold nanoparticles (acceptor). Using a simple model, the dependence of nanoparticle size on the resonance energy transfer's intensity and the energy transfer mechanism has been analyzed. By taking into account the interaction between gold nanoparticles in vivo studies, the mechanism of energy transfer from the excited donors to acceptors has been described by a virtual photon exchange. Also, we suppose that the dipole-dipole interaction dominates in the electronic coupling. The obtained results show that, for small gold nanoparticles the energy transfer is the conventional FRET whereas the surface energy transfer (SET) dominates for the bigger particle size. Email: nmhoa@huemed-univ.edu.vn

Presenter: Nguyễn Minh Hoa

P.81 – Poster, VCTP-44

The quantum Earningshausen effect in parabolic quantum well with in-plane magnetic field in the presence of laser radiation under the influence of confined optical phonon

Nguyen Thi Lam Quynh (1), Nguyen Thu Huong (2), Nguyen Ba Duc (3), Nguyen Quang Bau (1)

(1) Hanoi University of Science; (2) Air Defence - Air Force Academy; (3) Tan Trao University

The quantum Earningshausen effect in a parabolic quantum well subjected to a constant electric field, magnetic field in the presence of laser radiation is studied by using the quantum kinetic equation method. The analytic expressions for conductivity tensors and dynamic tensors as well as the Earningshausen coefficient (EC) are obtained in the case of the confined electron-confined optical phonon (COP) scattering. The EC depends on specific quantities for external field (such as magnetic field, amplitude and frequency of laser radiation), temperature of the system and quantum well length, especially quantum number m - characterizing the confinement of optical phonon (OP). When m is set to zero, we get the results corresponding to the case of unconfined OP. The analytic results are numerically evaluated and graphed for GaAs/AlGaAs parabolic quantum well. When examining the effect of temperature, the EC has greater values due to the COP. Meanwhile, when quantum well length and amplitude of the laser radiation (LR) increase, the EC has greater values without the confinement of OP. Because of the approach of system to bulk semiconductor structure when the quantum well length approaches micrometer-size, the EC reaches constant. The quantum number m leads to the change of resonance peaks position within the change of the magnetic field. In addition, the EC exerts non-linear dependence on the amplitude and frequency of the LE. All results indicated that the COP not only affects qualitatively but also affects the transformation rules of the EC. It provides new insights and contributes to the orientation of research into quantum effects in low-dimensional semiconductor systems (LDS).

Presenter: Nguyễn Thị Lâm Quỳnh

P.82 – Poster, VCTP-44

Effects of pairing correlations on the reactions observables of nucleon-nucleus elastic scattering

N. Hoang Tung (2,3), N. Nhu Le (1), Pham Thi Anh (1), Duc Anh Dinh (4), D. Minh Tuong (1), T. Dieu Thuy (1), T. V. Nhan Hao (1), K. Mizuyama (2)

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Microscopic optical potential [1,2] is one of the most important tools to study the scattering of numerous projectiles from nuclei. In this talk, we make a review of recent progress in developing the microscopic optical potential based on the nuclear structure models. In particular, for the first time, the effects of pairing correlations (in the targets) on the reaction observables are discussed.

[1] T. V. Nhan Hao, B. Minh Loc, and N. Hoang Phuc, Phys. Rev. C 92, 014605 (2015).

[2] T. V. Nhan Hao, N. Nhu Le, Meng-Hock Koh, N. Quang Hung, N. Ngoc Duy, Vinh N. T. Pham and N. Hoang Tung, Int. J. Mod. Phys. E27, 1850052 (2018).

Presenter: Nguyen Hoang Tung

P.83 – Poster, VCTP-44

Proton-nucleus elastic scattering based on microscopic approaches at low-energy

N. Nhu Le (1), P. H. Thao Vy (1), Duc Anh Dinh (4), D. Minh Tuong (1), N. Hoang Tung (2,3), T. N. Quynh Tran (1), T. Dieu Thuy (1), T. V. Nhan Hao (1), K. Mizuyama (2)

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In this talk, we show some preliminary results for a systematic study of the proton-nucleus elastic scattering at low incident energy. A successful account for angular distributions, including analyzing powers, are obtained for all double closed shell nuclei ^{16}O , ^{40}Ca , ^{48}Ca , ^{208}Pb at incident energies up to 50 MeV.

Presenter: Trần Diệu Thùy

P.84 – Poster, VCTP-44

High-pressure melting curves of and phases of iron

Nguyen Thi Hong (1,2), Nguyen Xuan Han (2), Ho Khac Hieu (3)

(1) Hong Duc University, Thanh Hoa, Vietnam (2) VNU University of Science, Hanoi, Vietnam (3) Duy Tan University, Da Nang, Vietnam

Abstract: Statistical moment method (SMM) has been applied in combination with Lindemann melting criterion to investigate pressure effects on melting temperature of iron. Melting curves of phase (with body-centered cubic structure) and phase (with face-centered cubic structure) of iron have been derived up to pressure 13 GPa and 90 GPa, respectively. This work shows that melting curves of these two phases of iron are increasing functions of pressure, and the higher the pressure is the lower the slopes of melting are. Our results are in reasonable agreement with recent published experimental data. The efficiency of the SMM on the investigation of melting

temperatures of and phases of iron allows us to believe that the present SMM scheme can be developed extensively to determine melting temperatures of other materials. Keywords: Melting; High pressure; Iron; Lindemann criterion; Statistical moment method

Presenter: Nguyễn Thị Hồng

P.85 – Poster, VCTP-44

Numerical mean-field solution for the distribution of counterions in a hexagonal DNA lattice

Tuyen T. Tran (1), Toan T. Nguyen (1)

trường THPT quê võ số 3, quê võ, bắc ninh

The mean-field Poisson-Boltzmann and its linearized Debye-Huckel equation for the distribution of counterions in a two-dimensional hexagonal lattice of DNA cylinder is solved numerically. The results are compared to previously published counterion density obtained using Grand Canonical Monte-Carlo simulation. It is shown that mean-field results agrees well at small counterion valence and concentration (large interhelices distance). However, at high concentration or high counterion valence, the strong correlation among counterions cannot be ignored. This is inline with such calculation for single DNA or dimeric DNA systems.

Presenter: Tuyền Thanh Trần

P.86 – Poster, VCTP-44

Dependence of lattice spacing on the temperature and pressure for ordered Cu₃Au alloy.

Pham Duy Tan (1), Pham Dinh Tam (2), Bui Duc Tinh (3)

(1) Research Department, Tank Armour Command (2) Le Qui Don Technical University (3) Hanoi National University of Education

The thermodynamic properties of alloys are studied using the moment method in the statistical dynamics, which allows us to take into account the anharmonicity of thermal lattice vibrations, going beyond the quasi-harmonic approximation. Applying to ordered Cu₃Au alloy, we determine the equation of state and lattice spacing in dimensionless polynomial form. Numerical results for the lattice parameter of this alloy in different temperatures and pressures are in good agreement with experiments. Keywords: moment method, effective pair potential.

Presenter: Pham Duy Tan

P.87 – Poster, VCTP-44

Diverse Electronic Transport of Sawtooth Penta-Graphene Nanoribbons by Substitutional Doping

Pham Thi Bich Thao (1,2), Vo Trung Phuc (1), Tran Thi Ngoc Thao (1), Ngo Vu Hao (1), and Nguyen Thanh Tien (1)

(1) Department of Physics, College of Natural Science, Can Tho University (2) Graduate University of Science and Technology, Vietnam Academy of Science and Technology.

Electronic and transport properties of the sawtooth penta-graphene nanoribbons (SPGNRs) doping by various doped-atoms (Si, N, P) and at various sites are systematically investigated by

using the density-functional theory in combination with the non-equilibrium Green's function formalism. To explore in detail the electronic and transport features, we compute and discuss about the structure properties, band structure, density of states, I-V curve, and transmission spectrum. Our result shows that doping affects dramatically on the electronic feature and the I-V characteristic of samples. The current intensity of N-SSPGNR and P-SSPGNR increase by 8 orders of magnitude compared to that of SSPGNR while the one of Si-SSPGNR has negligible change. Moreover, our results also show that electronic structures and currents of the studied samples will be strongly effected by doping position. Our findings indicate that doping can effectively modulate the electronic and the transport properties of SSPGNRs, which has not been studied so far.

Presenter: Pham Thi Bich Thao

P.88 – Poster, VCTP-44

New analysis characterizing the dynamics heterogeneity and microstructure in liquid silicates

Nguyen Thu Nhan and Pham Khac Hung

Department of Computational Physics, Hanoi University of Science and Technology, Vietnam

We use molecular dynamics simulation to study liquid silicates at ambient pressure and temperature of 3500 K. New analysis on structure and dynamics is carried out using such characteristics as the rate of bond-breaking events, link-cluster function and different subnet types. We found that the structural heterogeneous exists in short and medium length scales. Namely, the local environments of cations are quite different. The parking of SiO_x in the silicate systems is also very different. Further, the simulation shows that during a moderate long time the melt has a two-domain structure consisting of separate immobile domains and a mobile domain. These domain types differ strongly in the atomic mobility and chemical composition. The simulation also gives clear evidences for dynamics heterogeneity (DH) in the melt and that the non-uniform spatial distribution of bond-breaking events is responsible for the DH.

Presenter: Nguyen Thu Nhan

P.89 – Poster, VCTP-44

Biexciton in two dimensional parabolic quantum dots

Nguyen Hong Quang

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In this paper, a biexciton confined in a two dimensional parabolic quantum dot in magnetic field is investigated theoretically by using unrestricted Hartree-Fork method. A numerical calculation of the biexciton energy and binding energy is presented as a function of quantum confinement and magnetic field. For InAs self-assembled quantum dots, the obtained results show that the biexciton binding energy is found to be increased with magnetic fields.

Presenter: Nguyen Hong Quang

P.90 – Poster, VCTP-44

Interaction between two soft-particles with different sizes

Quyen T. L. Bui (1,2), Cam-Tu Mai (1), Hoai T. L. Nguyen (3)

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We calculate the Coulomb-like interaction energy of a system including two viral-like particles (VLPs) immersed in a 1:1 salt suspension. Here, we use the core-shell model for VLPs in which each particle is assumed to consist of a rigid charged core covered by an ion-permeable and negatively charged shell. We consider a specific case where two particles are identical and the general case where two particles are of different sizes. We show that the interaction energy has the form of screened Coulomb energy multiplied with a structural coefficient. The results may give some insight to understand the adhesion process of microbial systems which is an important problem in water treatment studies.

Presenter: Nguyen Thi Lam Hoai

P.91 – Poster, VCTP-44

Non-equilibrium condensation of Polaritons II: luminescence of the Excitations

Harmut Haug (2), Đoàn Trí Dũng (1) and Trần Thoại Duy Bảo (1)

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The frequency- and momentum-resolved luminescence of the excitation of a non-equilibrium polariton condensate, called bogolon, is studied kinetically together with the kinetic of bogolon in the formalism of non-equilibrium Green functions. The numerical results are shown an appearance of the ghost branch of the luminescence connected with the condensation of the polaritons which agrees qualitatively with recent experimental measurement.

Presenter: Đoàn Trí Dũng

P.92 – Poster, VCTP-44

Conceptual design of a small modular reactor with AP1000 fuel assembly

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This work presents the conceptual design of a 300 MWt small modular reactor (SMR) using a partial-height 17x17 fuel assembly of the AP1000® reactor. The active fuel length, fuel enrichment and core loading pattern have been optimized to meet the design criteria. The Doppler, moderator temperature, void and power reactivity coefficients of the SMR core have been evaluated to ensure the feedback coefficients are negative over the core lifetime. Semi-analytical thermal hydraulics analysis was conducted for obtaining radial and axial fuel temperature profiles. The critical heat flux and the nucleate boiling ratio (DNBR) are also calculated. The results show that a 2.2-year cycle length is achievable while the core satisfies the operation and safety-related criteria.

Presenter: Hoang Van Khanh

P.93 – Poster, VCTP-44

Electron-nucleon scatterings in light of ATOMKI'S IPC anomalies

Nguyen Ai Viet (1), Nguyen Van Dat (1)(2), Pham Tien Du (3)

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The observed anomalous IPC of ATOMKI implies the existence of a light vector boson with a mass of 17 MeV. In this article, we compute the electron-nucleon scattering's cross section with this new interaction and discuss the physical consequences.

Presenter: Nguyen Van Dat

P.94 – Poster, VCTP-44

Wave functions: from phenomenological to microscopic approaches

N. Nhu Le (1), N. Hoang Phuc (2), Duc Anh Dinh (3), L. T. Hai Thanh (1), V. Le Uyen (1), T. V. Nhan Hao (1), K. Mizuyama (4)

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We use the R-matrix approach to solve the Schrödinger equation in the optical model (OM) analysis of the elastic nucleon-nucleus scattering using a nonlocal nucleon phenomenological and microscopic optical potential (OP). The phenomenological OP is proposed by Perey and Buck while the microscopic one is proposed by T. V. Nhan Hao et al. [1]. The comparison of the obtained wave functions shows the defects of the phenomenological in the internal region.

[1] T. V. Nhan Hao, B. Minh Loc, and N. Hoang Phuc, Low-energy nucleon-nucleus scattering within the energy density functional approach, *Phys. Rev. C* 92, 014605 (2015).

Presenter: Nguyen Nhu Le

P.95 – Poster, VCTP-44

Quantum computation with cloud services: a new paradigm for physicists

Nguyen Quoc Hung

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The hardware that underly advances in science and technology are computers. They help to model an imaginary representation of almost anything that allow ideas to be examined, ranging from aircraft design to the operation of massive electrical grids. In basic science, computation physics simulates efficiently mechanisms that could lead to the discovery of, for example, new materials, elementary particles, or black hole collisions. An upgrade in computational capabilities means potential breakthroughs in all disciplines. Harnessing the powerful laws of quantum physics, quantum computers not only compute faster, they could perform jobs that no other machine can do. Specifically, the superposition of multiple quantum bits enlarges the programmable memory exponentially. This capability is particularly suit for resource-demanding problems such as optimization, large scale searching and sorting, or machine learning. Through quantum par-

allelism, these important algorithms are calculated with a lower complexity. Quantum simulation is another regime that attracts significant attentions. Directly employing quantum physics, quantum computers are exclusively match to simulate nature. They are expected to solve long-standing problems in molecular biology, quantum chemistry, or material science. In fact, a number of quantum computers that run quantum algorithms using quantum programming languages exist. Being the lead providers, IBM, Rigetti, Google, and Alibaba provide free access through cloud services with their own quantum programming languages. We execute standard quantum algorithm on these platform and compare their performances. Moreover, we show how to use these quantum devices to tackle serious problems in quantum physics. Limited by noise and the number of bits, these quantum computers are not yet practical. However, they are the first light of a bright future for quantum era.

Presenter: Nguyen Quoc Hung

P.96 – Poster, VCTP-44

Lepton mass and mixing in an extension of the standard model based on $\Delta(54)$ discrete symmetry

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We construct a Standard model extension based on $\Delta(54)$ discrete symmetry which accommodates the recent experimental results on neutrino mass and mixing. The Dirac CP violating phase is consistent with the global fit result.

Presenter: Vo Van Vien

P.97 – Poster, VCTP-44

Electrically controlled magnetism in iron thin film

Tran Van Quang

Department of Physics, University of Transport and Communications, Dong Da, Hanoi

The coupling of ferroelectric and ferromagnetic order parameters in low dimension materials have been of great attention due to the potential electronic applications in future technology. In this report, by employing first-principles density-function-theory calculation without including spin-orbital coupling, we demonstrate that the magnetization of iron thin film increases in proportion to the external electric field. This intriguing properties stems from the spin-dependent screening of the electric field which leads to spin imbalance of the excess surface charge. The result is in accordance with a predictive result including spin-orbital coupling published earlier. We suggest that the electrically controlled magnetism might be used in advanced magnetic and electronic devices.

Presenter: Tran Van Quang

P.98 – Poster, VCTP-44

Calculations of beta energies spectra in beta-decay of Rb unstable isotopes

Pham Ngoc Son

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Beta energy spectra in β -decay were calculated for the Rubidium isotopes of Rb-89, Rb-90, Rb-90m, Rb-91 and Rb-93. The beta strength functions used in this calculation were derived from the beta feeding data in the ENSDF evaluated nuclear structure data library. The calculated results are compared with experimental values.

Presenter: Pham Ngoc Son

P.99 – Poster, VCTP-44

Molecular study of interactions of mu-opioid receptor in binding with biased and unbiased ligands by molecular dynamic simulation

Tran Ky Thanh (1), and Toan T. Nguyen (2)

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Mu-opioid receptors (μ OR), members of G-protein coupled receptor (GPCR) family, are the main target of many opioid painkillers. As a biased ligand of μ OR, TRV130 is a new promising pain relief drug due to its higher analgesic and reduced side effects. In this work, to elucidate the mechanism of biased signaling activation of TRV130, molecular dynamics (MD) simulation of two systems of μ OR, each in its binding state with morphine (unbiased ligand) and TRV130 (biased ligand) was carried out. The results show that because of distinct interactions with the two ligands, μ ORs adopt two different conformations. The conformations of transmembrane 6 (TM6) and TM7 of μ OR-morphine complex and μ OR-TRV130 complex are significantly different in direction, fluctuation, and secondary structure. We suggest that the hydrophobic interaction between TRV130 with residue TRP293 (TM6) and TYR326 (TM7) which stabilizes TM6 and TM7 is one of the key factors leading to biased signaling. This result also suggests that the conserved proline and glycine residues play an important role in creating various states of GPCRs. In addition, the hydrophobic property of TRV130 leads to fewer hydrogen bonds with μ OR than morphine; however, binding energy calculated with MM-PBSA method showed that the affinity of TRV130 toward μ OR is higher than that of morphine. Consequently, hydrogen bond may not contribute much to affinity between ligands and μ OR. For the next step – designing biased ligands, our results suggest that much attention should be paid to hydrophobic ligands which can create hydrophobic interaction with TRP293 and TYR326.

Presenter: Tran Ky Thanh

P.100 – Poster, VCTP-44

Multi-scale simulation of low-cost metal-organic framework for hydrogen storage

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Recently, metal-organic frameworks (MOFs) have emerged as a new generation of nano-porous materials with much higher pore volume and accessible surface than any conventional porous materials. However, almost of existing MOFs consist of expensive aromatic linkers which hinder their widespread applications. In this work, we computationally investigated a new MOF for hydrogen storage application basing on MOF-74 using multiscale methods. The original linker, 2,5-dioxidobenzene-1,4-dicarboxylate (DOBDC), was substituted with much cheaper aliphatic linker, 3-dihydroxyfumarate (DHFUMA). Dynamical stability of the new MOF, called DHFUMA-MOF74, was examined via elastic matrix calculated from first principles method. Hydrogen adsorption isotherm was calculated using Grand canonical Monte Carlo (GCMC) method. Classical force field used in GCMC calculations was designed and parametrized on the base of hydrogen – framework interactions observed from first principles simulations. The results showed that DHFUMA-MOF74 is stable up to high temperature (higher than 350K). The gravitational hydrogen uptake of the new MOF is slightly improved but its volumetric hydrogen uptake is much higher than the original.

Presenter: Cao Cong Phuong

P.101 – Poster, VCTP-44

Formation of Two-Dimensional Penta-Germanene by Molecular dynamics (MD) simulation

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We have successfully designed a new two-dimensional (2D) structure of germanene, namely penta-germanene, by using molecular dynamics (MD) simulation. Model containing 6400 atoms Ge is cooled from 3000K to 300K with Stillinger-Weber (SW) potential to obtain pentagon structure. Our simulations suggest that penta-germanene can be flexibly produced by cooling from the melt under high pressure. Evolution of structural and thermodynamic properties upon cooling from the liquid state is investigated in details. The crystallization of penta-germanene exhibits a first-order-like phase transition. Structural properties of penta-germanene obtained at 300K are investigated via analyzing coordination number, ring and bond-angle distribution, 2D visualization of atomic configuration. Moreover, we propose that the penta-germanene would have many important applications in electronics and mechanic devices.

Acknowledgments. This research is funded by Vietnam National University-Ho Chi Minh City (VNU-HCM) under grant number B2018-20-01.

Presenter: Nguyen Hoang Giang

P.102 – Poster, VCTP-44

Composition-dependent microstructural properties of of liquid lead silicate

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Molecular dynamics (MD) simulations investigations of the microstructure of lead-silicate liquid, $x\text{PbO} \cdot (1-x)\text{SiO}_2$, have been undertaken to elucidate the problem of basic structural units and their interconnection. The MD simulations were performed in a wide range of compositions, $x = 0.5-0.75$. The pair correlation function, coordination number are obtained and compared with those of previous works. The microstructures have been analysed detailly via the distribution of V-simplex, O-simplex, T-simplex, SC-particle, and SC-cluster. In particular, it is illustrated how such methods can provide insights into the structural properties of a wide range oxide materials inaccessible by other means. Approaches for further improvements in materials and increased range of applicability are discussed.

Presenter: Mai Van Dung

P.103 – Poster, VCTP-44

Gravitational waves for a central gravitational field in an $f(R)$ -theory of gravitation

Pham Van Ky, Nguyen Thi Hong Van and Nguyen Anh Ky

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While a spherically symmetric vacuum solution of the Einstein equation is always stationary, a spherically symmetric vacuum solution of an $f(R)$ -theory of gravitation is not necessary stationary. This may have interesting consequences. In comparison with the general theory of relativity (GR), a planet's orbital precession or a trajectory deflection of light now get a correction which is a constant for a static central field and varies with time for a non-static central field even from a source of a constant mass, unlike the corresponding Einstein's values in the GR not changing in the same circumstance. In particular, a spherical symmetrical source can radiate gravitational waves. This phenomenon cannot happen in the GR.

Presenter: Nguyen Anh Ky

P.104 – Poster, VCTP-44

Scatterings of proton proton to leptons in the Standard Model

Nguyen Tran Quang Thong

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In this report, based on the Standard Model, we calculate the cross section of proton-proton scatterings into two or four leptons at 13 TeV LHC. The calculation techniques using the helicity amplitude method and Monte Carlo integration are described. Finally, we present some results for the total cross sections and kinematical distributions.

Presenter: Nguyen Tran Quang Thong

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