

**Programs & Abstracts**

**40th National Conference on  
Theoretical Physics**

**&**

**3rd International Workshop on Theoretical and  
Computational Physics**

*Complex Systems and Interdisciplinary Physics*

Dalat Palace Hotel  
Da Lat, 27-30 July 2015



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# Welcome Message

It is a great pleasure to welcome you in the *40th National Conference on Theoretical Physics* (NCTP-40) and the *3rd International Workshop on Theoretical and Computational Physics: Complex Systems and Interdisciplinary Physics* (IWTCP-3) in Da Lat.

With these activities, we celebrate 40 years of the National Conference on Theoretical Physics (NCTP), and also 20 years of research in Interdisciplinary Physics in Vietnam.

The first NCTP was organized in Da Lat in August 1976. Since then, the NCTP has been an annual activity of the Vietnamese Theoretical Physics Society (VTPS), and has become the most well-known scientific forum dedicated to the dissemination of the latest developments in the field of theoretical physics within the country.

The IWTCP-3 workshop is an associated activity of NCTP, with a mission to foster scientific exchanges between the Vietnamese theoretical and computational physics community and world-wide scientists, as well as to promote high-standard level of research and education activities for young physicists in the country.

As the organizers, we have an honor to host more than 140 participants coming from 10 countries, including 15 invited speakers of the workshop and 4 invited speakers of the conference. Thanks to your contributions, a rich scientific program of 89 reports at the conference and 56 reports at the workshop, will be presented.

Thank you for coming. We wish you enjoy the scientific atmosphere at conference and the workshop and have a memorable stay in the beautiful city of Da Lat.

Nguyen Ai Viet  
Chair of NCTP-40 & IWTCP-3

Nguyen Ai Viet is with Institute of Physics, Vietnam Academy of Science and Technology (IOP-VAST), and he is currently President of the Vietnamese Theoretical Physics Society.



# Organizers and Committees

## Conference (NCTP-40)

### Organizers

- Institute of Physics, Vietnam Academy of Science and Technology (IOP-VAST)
- Dalat University (DLU)
- Nuclear Research Institute (NRI)

### Honorary Chair

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

### Chair

- Nguyen Ai Viet (Institute of Physics, VAST, Hanoi)

### Organizing Committee

- Trinh Xuan Hoang (Institute of Physics, VAST, Hanoi), Chair
- Bach Thanh Cong (Hanoi University of Science, VNU, Hanoi)
- Hoang Dzung (Vietnam National University, Ho Chi Minh City)
- Phu Chi Hoa (Dalat University, Da Lat)
- Le Van Hoang (Ho Chi Minh City Pedagogical University, Ho Chi Minh City)
- Nguyen Tri Lan (Institute of Physics, VAST, Hanoi)

### Program Committee

- Hoang Anh Tuan (Institute of Physics, VAST, Hanoi), Chair
- Phung Van Dong (Institute of Physics, VAST)
- Ho Trung Dung (Ho Chi Minh city Institute of Physics)
- Nguyen The Toan (Hanoi University of Science, VNU, Hanoi)
- Vu Ngoc Tuoc (Hanoi University of Technology)

## Secretariat

- Duong Thi Man (Institute of Physics, VAST, Hanoi)

## Workshop (IWTCP-3)

### Organizers

- Institute of Physics, Vietnam Academy of Science and Technology (IOP-VAST)
- Dalat University (DLU)
- Nuclear Research Institute (NRI)

### Honorary Chair

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

### Chair

- Nguyen Ai Viet (Institute of Physics, VAST, Hanoi)

### International Advisory Board

- Tae Soo Chon (Pusan National University, Pusan)
- Mukunda Das (Australian National University, Canberra)
- Hung T. Diep (University of Cergy-Pontoise, Paris)
- Peter Fulde (Asia Pacific Center for Theoretical Physics, Pohang)
- Mai Suan Li (Polish Academy of Sciences, Warsaw)
- Duc Nguyen-Manh (Culham Centre for Fusion Energy, Culham, UK)
- Andreas Savin (CNRS and Sorbonnes Universités, UPMC, Univ Paris 6, Paris)
- Dam Thanh Son (University of Chicago, USA)

### Organizing Committees

- Trinh Xuan Hoang (Institute of Physics, VAST, Hanoi), Chair
- Bach Thanh Cong (Hanoi University of Science, VNU, Hanoi)
- Hoang Dzung (Vietnam National University, Ho Chi Minh City)
- Phu Chi Hoa (Dalat University, Da Lat)
- Hoang Anh Tuan (Institute of Physics, Hanoi)



## Program Committee

- Nguyen Tri Lan (Institute of Physics, VAST, Hanoi), Chair
- Trinh Xuan Hoang (Institute of Physics, VAST, Hanoi)
- Nguyen Manh Duc (Culham Center for Fusion Energy, Culham, UK)
- Truong Minh Duc (Hue University, Hue)
- Nguyen Toan Thang (Institute of Physics, VAST, Hanoi)
- Vu Ngoc Tuoc (Hanoi University of Science and Technology, Hanoi)

## Secretariat

- Duong Thi Man (Institute of Physics, VAST, Hanoi)

## Sponsors

- Vietnam National Foundation for Science and Technology Development (NAFOSTED) – *for workshop only*
- Asia Pacific Center for Theoretical Physics (APCTP) – *for workshop only*
- Institute of Physics, Vietnam Academy of Science and Technology (IOP-VAST)
- Vietnam Academy of Science and Technology (VAST)

The IWTCP-3 workshop is also an external activity of the Asia Pacific Center for Theoretical Physics (APCTP).



# General Information

## Conference Venue

The NCTP-40 conference and the IWTCP-3 workshop take place in:

Dalat Palace Hotel  
12 Tran Phu Street, Da Lat  
Lam Dong Province, Viet Nam.



The Dalat Palace Hotel is a historic luxury hotel located in the Da Lat city center, overlooking the Xuan Huong lake. Originally called the Lang-Bian Palace Hotel, the hotel was built under French Governor, and first opened in 1922.

The hotel is of about 30 km from Dalat Airport (DLI), also known as Lien Khuong Airport, and can be reached in about 30-40 minutes from the airport by shuttle bus or taxi.

## About Da Lat

Đà Lạt, the capital of Lâm Đồng Province, is located 1,500 m (4,900 ft) above sea level, on the Langbian Plateau in the southern part of Vietnam's Central Highlands.

Founded by explorers (including Swiss-French physician and bacteriologist Alexandre Yersin) in 1890s, with its distinctive temperate climate, surrounded by hills, pine forests, lakes and waterfalls, Đà Lạt was developed as a resort center by the French in the early 1900s. The French

endowed the city with villas and boulevards, and its Swiss charms remain today.

Da Lat is also known for nuclear research with a nuclear reactor, the first ever built in Vietnam (in 1962-1963 with American support), now belonging to Nuclear Research Institute of the Vietnam Atomic Energy Institute.

## 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 presentation is 30 and 35 minutes in the conference and the workshop, respectively. This includes 25 and 30 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. No overhead projectors will be made available.

## Instructions for Posters

Two poster sessions of the NCTP-40 will be held during 14:00 PM - 15:30 PM in the afternoons of 27 July and 29 July, respectively.

One poster session of the IWTCP-3 will be held during 08:30 AM - 10:00 AM in the morning of 28 July.

Poster should be prepared as one page of size A0 (841 mm x 1189 mm) in portrait mode. Please hang your poster on the poster standee with a correct presentation code as given in the abstract book. 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 (for the conference) first warning at 25 minutes, second warning at 30 minutes (for the workshop).
- Regular talk: first warning at 15 minutes, second warning at 17 minutes (for both the conference and the workshop).

## Meeting Rooms

- **Cezanne 1:** conference sessions on day 1 and day 2, workshop sessions on day 3, VTPS meeting on day 1.
- **Cezanne 2:** workshop sessions on day 1 and day 2, conference sessions on day 3.

## Program Schedule

### Conference (NCTP-40)

Time	Monday 27 July	Tuesday 28 July	Wednesday 29 July
08:30 – 10:00	Registration Opening (9:00)	Poster Session 2 (Chair: N. Q. Hung)	Dao Vong Duc (O.10) Nguyen Quang Hung (O.11) Tran Viet Nhan Hao (O.12) (Chair: N. A. Ky)
10:00 – 10:30	Coffee break		
10:30 – 12:00	Nguyen Viet Hung (I.1) Nguyen Tien Cuong (O.1) Nguyen Mai Chung (O.2) Pham Khac Hung (O.3) (Chair: B. T. Cong)	Hoang Ngoc Cam (I.3) Nguyen Quang Bau (O.7) Giang Huong Bach (O.8) Pham Nguyen Thanh Vinh (O.9) (Chair: L. V. Hoang)	Nguyen Anh Ky (I.4) Tran Minh Hieu (O.13) Dang Trung Si (O.14) Phi Quang Van (O.15) (Chair: D. V. Duc)
12:00 – 14:00	Lunch time		
14:00 – 15:30	Poster Session 1 (Chair: V. N. Tuoc)	Excursion	Vu Ngoc Tuoc (O.16) Le Van Vinh (O.17) Vo Van Tai (O.18) Ngo Thi Phuong (O.19) (Chair: P. K. Hung)
15:30 – 16:00	Coffee break		Coffee break
16:00 – 17:30	Vo Van Vien (I.2) Vo Van On (O.4) Nguyen Thi Kim Ngan (O.5) Phan Ngoc Hung (O.6) (Chair: H. N. Long)		Ho Trung Dung (O.20) Bach Thanh Cong (O.21) Le Duy Manh (O.22) (Chair: N. Q. Bau)
from 17:30	VTPS meeting	Gala Dinner (18:00)	Closing

### Workshop (IWTCP-3)

Time	Monday 27 July	Tuesday 28 July	Wednesday 29 July
08:30 – 10:00	Registration	Gerhard Hummer (I.6) Tae-Soo Chon (I.7) Danh-Tai Hoang (O.5) (Chair: A. Liwo)	Poster Session (Chair: N. T. Lan)
10:00 – 10:30	Coffee break		
10:30 – 12:00	Opening Mukunda Das (I.1) Nguyen Van Hieu (I.2) (Chair: N. A. Viet)	Rudolf Podgornik (I.8) Masaki Sasai (I.9) Trinh Xuan Hoang (O.6) (Chair: G. Hummer)	Robert B. Best (I.10) Edward O'Brien (I.11) Chuong Nguyen (O.7) (Chair: M. Sasai)
12:00 – 14:00	Lunch time		
14:00 – 15:30	Adam Liwo (I.3) Antonio Trovato (I.4) Trung D. Nguyen (O.1) (Chair: M. S. Li)	Excursion	Toan T. Nguyen (I.12) Que-Huong Nguyen (I.13) Nguyen Thuy Hang (O.8) (Chair: R. Podgornik)
15:30 – 16:00	Coffee break		Coffee break
16:00 – 17:30	Viet-Hung Nguyen (I.5) Tran Cong Phong (O.2) Truong Minh Duc (O.3) Nguyen Dang Chien (O.4) (Chair: M. Das)		Sihyun Ham (I.14) Mai Suan Li (I.15) Quy Vo (O.9) (Chair: R. B. Best)
from 17:30	VTPS meeting	Gala Dinner (18:00)	Closing

## Excursion

Tours around Da Lat or to nearby attractions are available in the afternoon of Tuesday, 28 July, at the cost of individuals. Please register for tours at Travel Desk near the conference rooms.

Popular tourist attraction points in Da Lat include: Truc Lam Monastery, The Palace of Bao Dai King, Dreamlike Hill (Mộng Mơ Hill), Langbiang Peak, Prenn Waterfall, Valley of Love, Dalat Cathedral, Golden Stream Lake, Bidoup - Núi Bà National Park (cover image).

## Gala Dinner

All participants are invited to Gala Dinner:

BBQ with International Buffet Menu

Time: 28 July 2015, from 18:00 PM

Place: Le Rabelais Restaurant, Dalat Palace Hotel.

## VTPS Meeting

A regular meeting of the Vietnamese Theoretical Physics Society (VTPS) will be held during the NCTP-40 conference:

Time: 27 July 2015, 17:30 - 18:30 PM

Place: Room Cezanne 1, Dalat Palace Hotel.

The meeting program includes announcement and delivery of the VTPS's Young Research Award to Dr. Vo Van Vien (Tay Nguyen University).

# Conference Program

## Monday, 27 July 2015

08h30 - 09h30      Registration

09h00 - 10h00      Opening

10h00 - 10h30      Coffee Break

### **Oral Session 1:** *Condensed Matter Theory and Simulation*

**Chair: Bach Thanh Cong**

- 10h30 - 11h00      I.1 – Invited  
Strain effects on the electronic properties of devices made of twisted graphene layer  
**Viet-Hung Nguyen** (Université Paris-Sud & Institute of Physics)
- 11h00 - 11h20      O.1 – Oral  
Density functional studies of gas molecules adsorbed on Graphene Nanoribbons  
**Nguyen Tien Cuong** (VNU University of Science)
- 11h20 - 11h40      O.2 – Oral  
Transport gap in strained graphene heterochannels  
**Nguyen Mai Chung** (Université Paris-Sud & Institute of Physics)
- 11h40 - 12h00      O.3 – Oral  
The study of dynamics heterogeneity and slow down of network-forming liquid computer simulation  
**Phạm Khắc Hùng** (Đại học Bách Khoa Hà Nội)
- 12h00 - 14h00      Lunch Break

### **Poster Session 1**

**Chair: Vu Ngoc Tuoc**

- 14h00 - 15h30      P.1 – Poster  
Calculation of Etingshausen coefficient in Quantum Well in the presence of Electromagnetic Wave  
**Dao Thu Hang** (People's Police University of Technology and Logistics)
- 14h00 - 15h30      P.2 – Poster

An analytical description for the ground state energy of two dimensional exciton in a magnetic field

**Hoang-Do Ngoc-Tram** (Ho Chi Minh City University of Education)

14h00 - 15h30

P.3 – Poster

Energy spectrum inverse problem of q-deformed harmonic oscillator and WKB approximation

**Nguyễn Ánh Sáng** (Vocational Training and comprehensive technical center of Phu Tho province)

14h00 - 15h30

P.4 – Poster

Calculating the current density of the radioelectrical effect in parabolic cylindrical quantum wires

**Hoang Van Ngoc** (Truong Dai hoc Khoa hoc tu nhien Ha Noi)

14h00 - 15h30

P.5 – Poster

Phonon-assisted cyclotron resonance in AlGaAs-GaAs hyperbolic quantum well via two-photon absorption process

**Pham Tuan Vinh** (Dong Thap University)

14h00 - 15h30

P.6 – Poster

Plasmon resonance absorption of core-shell nanoparticles

**Do Chi Nghia** (Hanoi Pedagogical University 2)

14h00 - 15h30

P.7 – Poster

The ordered phase in the Spin -1 Heisenberg model with strict single occupancy.

**Pham Thi Thanh Nga** (Thuy loi University)

14h00 - 15h30

P.8 – Poster

probing nuclear vibration of  $H_2^+$  using high-order harmonic generation

**Lê Thị Thanh Thủy** (HCM city University of Education)

14h00 - 15h30

P.9 – Poster

The crystallization of iron nanoparticles

**Nguyen Thi Thao** (Hanoi national university of education)

14h00 - 15h30

P.10 – Poster

Search for doubly charged Higgs at  $e^+e^-$  colliders

**Thao Huy Nguyen** (Hanoi University of Education No 2)

14h00 - 15h30

P.11 – Poster

q-Phonon

**Nguyen Thi Ha Loan** (Hanoi Pedagogical University No.2)

14h00 - 15h30

P.12 – Poster

Rotation of induced vortex-antivortex pair in microcavity polaritons

**Doan Tri Dung** (Ho Chi Minh City Institute of Physics)

14h00 - 15h30

P.13 – Poster



- Numerical study of whispering gallery mode in photonic crystal H2 defect nanocavity  
**LÊ Hải Mỹ Ngân** (HCM city University of Pedagogy)
- 14h00 - 15h30 P.14 – Poster  
 Simple model for optical modes of graphene nano ribbons  
**Đào Thị Thúy Nga** (Bac Ninh Department of Education and Training)
- 14h00 - 15h30 P.15 – Poster  
 Thermodynamic Property of Interstitial Double Alloy with BCC Structure: Dependence on Temperature and Concentration of Interstitial Atoms  
**Nguyễn Đức Hiền** (Sở GD&ĐT Gia Lai)
- 14h00 - 15h30 P.16 – Poster  
 INVESTIGATION OF NONSEQUENTIAL DOUBLE IONIZATION PROCESS OF HELIUM BY LINEARLY POLARIZED LASER FIELD AT HIGH INTENSITY  
**Tran Lan Phuong** (Ho Chi Minh University of Pedagogy)
- 14h00 - 15h30 P.17 – Poster  
 Effective method for retrieval of interatomic separation of molecule CO<sub>2</sub> based on the theoretical analysis of molecular transition dipole zero-points  
**Le Cam Tu** (HCMC University of Science)
- 14h00 - 15h30 P.18 – Poster  
 Influence of phonon confinement on the optically detected electrophonon resonance line-width in quantum wells.  
**Nguyen Dinh Hien** (Center for Theoretical and Computational Physics, Hue University)
- 14h00 - 15h30 P.19 – Poster  
 On the fluctuation induced mass enhancement  
**Le Van Xuan** (Truong cao dang cong nghe va kinh te Ha noi)
- 14h00 - 15h30 P.20 – Poster  
 AUTOIONIZATION WITH FANO PROFILE AND BROAD-BAND CHAOTIC LIGHT - PHOTOELECTRON SPECTRA  
**Doan Quoc Khoa** (Quang Tri Teacher Training College)
- 14h00 - 15h30 P.21 – Poster  
 A perturbative solution to an f(R)-gravity theory  
**Nguyễn Anh Kỳ** (Institute of physics)
- 14h00 - 15h30 P.22 – Poster  
 Transport properties of the Hubbard model on a honeycomb lattice  
**Nguyen Thi Hai Yen** (Institute of Physics)
- 14h00 - 15h30 P.23 – Poster  
 Higgs sector of 3-3-1 model with three lepton singlets  
**Duong Van Loi** (Tay Bac University)

- 14h00 - 15h30 P.24 – Poster  
Mott transitions in the ionic Hubbard model on a honeycomb lattice  
**Nguyễn Thị Hương** (Đại học sư phạm Hà Nội)
- 14h00 - 15h30 P.25 – Poster  
Unified Spinor Fields in Space-time with Extradimensions  
**Dao Vong Duc** (Institute of Physics, Vietnam Academy of Science and Technology)
- 14h00 - 15h30 P.26 – Poster  
Effect of scattering from potential-barrier roughness on the linewidth of intersubband optical absorption in symmetric rectangular quantum wells: Non-local representation for scattering form factors  
**Toan Ngoc Huynh** (Đại học Duy Tân)
- 14h00 - 15h30 P.27 – Poster  
Phonon-scattering-limited electron mobilities in zincblende and wurtzite Al-GaN/GaN quantum-well heterostructures.  
**Võ Văn Tài** (College of Technology and Industrial Management (CTIM))
- 14h00 - 15h30 P.28 – Poster  
EFFECT OF TEMPERATURE ON ELECTRON EFFECTIVE MASS AND BAND-GAP IN SEMICONDUCTOR CARBON NANOTUBES  
**Tan Van Le** (Ho Chi Minh City Institute of Physics Vietnam Academy of Science and Technology)
- 14h00 - 15h30 P.29 – Poster  
Surface optical phonon-assisted cyclotron resonance in graphene on a h-BN substrate  
**Huynh Vinh Phuc** (Dong Thap University)
- 14h00 - 15h30 P.30 – Poster  
Temperature dependence of electron-hole pair condensation driven by exciton-phonon interaction  
**Do Thi Hong Hai** (Department of Physics, Hanoi University of Mining and Geology)
- 14h00 - 15h30 P.31 – Poster  
Effects of pairing reentrance on the inverse nuclear level density parameter of hot rotating nuclei  
**Le Thi Quynh Huong** (Department of Natural Sciences, Nha Trang College of Education, Nha Trang City, Vietnam)
- 14h00 - 15h30 P.32 – Poster  
Surface Properties of TiO<sub>2</sub> from Self-Consistent-Charge Density Functional Tight Binding  
**Viên Tuấn Anh** (Can Tho University)
- 15h30 - 16h00 Coffee Break

**Oral Session 2: Particle Physics and Cosmology****Chair: Hoang Ngoc Long**

- 16h00 - 16h30 I.2 – Invited  
Lepton mass and mixing in the 3-3-1 models based on discrete symmetries  
**Vo Van Vien** (Tay Nguyen University)
- 16h30 - 16h50 O.4 – Oral  
Some new cosmological implications in polynomial exponential  $f(R)$  modified gravity model  
**On Van Vo** (University of Thu Dau Mot)
- 16h50 - 17h10 O.5 – Oral  
Phenomenology of the simple 3-3-1 model  
**Nguyễn Thị Kim Ngân** (Đại học Cần Thơ)
- 17h10 - 17h30 O.6 – Oral  
Parameterization of  $SO(8)$  group and its Schwinger representation.  
**Phan Ngọc Hưng** (HCMC university of Education)
- 17h30 - 18h30 VTPS Meeting

**Tuesday, 28 July 2015****Poster Session 2****Chair: Nguyen Quang Hung**

- 08h30 - 10h00 P.33 – Poster  
Dynamics Simulation of Backward Diffusion Based on Random Walk Theory  
**Bui Huu Nguyen** (Hanoi University of Mining and Geology)
- 08h30 - 10h00 P.34 – Poster  
Connection between  $q$ -deformed harmonic oscillator and aharmonic symmetric aharmonic potential  
**Ngô Gia Vĩnh** (Bac Ninh Department of Education and Training)
- 08h30 - 10h00 P.35 – Poster  
Second quantization model for surface plasmon polariton for spherical shape of metallic nano particles  
**Đào Thị Thúy Nga** (Bac Ninh Department of Education and Training)
- 08h30 - 10h00 P.36 – Poster  
Cooper pair of superconductivity in the coordinate representation and  $q$ -deform harmonic oscillator  
**Man Van Ngu** (Hung Yen Industrial Colleague)
- 08h30 - 10h00 P.37 – Poster  
Influence of phonon confinement on the optically detected magnetophonon resonance line-width in parabolic quantum wells

**Tran Cong Phong** (Vietnam Institute of Educational Sciences)

08h30 - 10h00

P.38 – Poster

High-pressure thermodynamic properties of  $\epsilon$ -Fe

**Ho Khac Hieu** (Duy Tan University)

08h30 - 10h00

P.39 – Poster

Nonclassical properties and entanglement of even and odd nonlinear charge coherent states

**Truong Minh Duc** (Hue University of Education)

08h30 - 10h00

P.40 – Poster

Second quantization model for surface plasmon polariton in metallic nano wires

**Nguyen Thi Phuong Lan** (Hanoi Pedagogical University 2)

08h30 - 10h00

P.41 – Poster

NOISE REDUCTION IN RAMAN RING LASER BY TWO-TELEGRAPH PREGAUSSIAN PUMP

**Doan Quoc Khoa** (Quang Tri Teacher Training College)

08h30 - 10h00

P.42 – Poster

One loop corrections to decay  $\tau \rightarrow \mu\gamma$  in the economical 3-3-1 model

**Thuc Trong Truong** (Trường THPT Phú Hưng, Xã Phú Hưng, huyện Cái Nước, tỉnh Cà Mau)

08h30 - 10h00

P.43 – Poster

The muon anomalous magnetic moment in the supersymmetric economical 3-3-1 model

**Dinh T Binh** (Institute of Physics)

08h30 - 10h00

P.44 – Poster

Study of magnetic properties in core/shell Fe<sub>98</sub>B<sub>2</sub> nanoparticle

**Nguyen Thu Nhan** (Hanoi University of Science and Technology)

08h30 - 10h00

P.45 – Poster

Nonlocal correlations in a correlated Chern insulator

**Nguyen Hong Son** (Trade Union University)

08h30 - 10h00

P.46 – Poster

Effect of combined uniaxial – torsional strain on electronic properties of armchair graphene nanoribbons

**Nguyen Ngoc Hieu** (Duy Tan University)

08h30 - 10h00

P.47 – Poster

Molecular dynamics simulation of the mechanical properties of CrN/AIBN/CrN systems

**Nguyen Thi Trang** (Ha noi University of Sciences and Technology)

08h30 - 10h00

P.48 – Poster

- Controlled joint remote preparation of an arbitrary two-qubit state via non-maximally entangled quantum channels  
**Nguyen Van Hop** (Physics Department, Hanoi National University of Education, 136 Xuan Thuy, Hanoi)
- 08h30 - 10h00 P.49 – Poster  
 Mott transition in the asymmetric Hubbard model at half-filling: Equation of motion approach  
**Tran Thi Thu Trang** (Halong University)
- 08h30 - 10h00 P.50 – Poster  
 THE INFLUENCE OF SPIN POLARIZABILITY AND THE TEMPERATURE ON THE COMPRESSIBILITY IN THE SEMICONDUCTOR QUANTUM WELL-WIRES  
**Tan Van Le** (Ho Chi Minh City Institute of Physics Vietnam Academy of Science and Technology)
- 08h30 - 10h00 P.51 – Poster  
 Dependence of the Hall Coefficient on a length of rectangular quantum wires with infinitely high potential under the influence of a Laser Radiation  
**Nguyen Thu Huong** (air defence and air force Academy)
- 08h30 - 10h00 P.52 – Poster  
 Ginzburg-Landau functional for three-order parameter problem  
**Nguyen Van Hinh** (Hanoi University of Industry)
- 08h30 - 10h00 P.53 – Poster  
 New-physics effects in the 3-3-1-1 model  
**Duong Van Loi** (Tay Bac University)
- 08h30 - 10h00 P.54 – Poster  
 Critical behavior near the Mott transition in the half-filled asymmetric Hubbard model  
**Hoang Anh - Tuan** (Institute of Physics - VAST)
- 08h30 - 10h00 P.55 – Poster  
 On the applications of non extensive statistical mechanics to studying ecological diversity  
**Le Van Xuan** (Truong cao dang cong nghe va kinh te Ha noi)
- 08h30 - 10h00 P.56 – Poster  
 CONTROLLED TELEPORTATION WITH PARTIALLY ENTANGLED QUANTUM CHANNEL: DETERMINISM AND POWER OF THE CONTROLLER  
**Nguyen Van Hop** (Physics Department, Hanoi National University of Education, 136 Xuan Thuy, Hanoi)
- 08h30 - 10h00 P.57 – Poster  
 Production and decay of radion and Higgs boson  $h_0$  in Randall - Sundrum model  
**Bui Thi Ha Giang** (Hanoi university of Education)

- 08h30 - 10h00 P.58 – Poster  
Hypercharge  $Y$  and gauge couplings in 3-3-1 models with  $\beta$  arbitrary  
**Ha Thanh Hung** (Ha Noi University of Education No.2)
- 08h30 - 10h00 P.59 – Poster  
Sphaleron electroweak phase transition in the economical 3-3-1 Model  
**Vo Quoc Phong** (The University of Science-Ho Chi Minh City)
- 08h30 - 10h00 P.60 – Poster  
Hawking radiation and black hole evaporation  
**Nguyen Hoang Vu** (Institute of physics)
- 08h30 - 10h00 P.61 – Poster  
The ab-plane complex conductivity in type-II superconductor  
**Nguyễn Đức Hiền** (Sở GD&ĐT Gia Lai)
- 08h30 - 10h00 P.62 – Poster  
The Radioelectric effect in doped superlattices under the influence of confined phonon  
**Nguyen Quang Bau** (Faculty of Physics, Hanoi University of Science, Vietnam National University)
- 08h30 - 10h00 P.63 – Poster  
Quasi-bound states in circular graphene quantum dots  
**To Duy Quang** (Center for Computational Physics - Institute of Physics)
- 10h00 - 10h30 Coffee Break
- Oral Session 3: Condensed Matter Theory**  
**Chair: Le Van Hoang**
- 10h30 - 11h00 I.3 – Invited  
Microscopic model for scattering of ultracold paraexcitons in cuprous oxide  
**Hoang Ngoc Cam** (Institute of Physics)
- 11h00 - 11h20 O.7 – Oral  
Influence of an electromagnetic wave on the Hall effect in two-dimensional semiconductor systems  
**Nguyen Quang Bau** (Faculty of Physics, Hanoi University of Science, Vietnam National University)
- 11h20 - 11h40 O.8 – Oral  
Negative charge transfer to the surface in the electron-hole asymmetric models.  
**Giang Huong Bach** (VNU University of Science)
- 11h40 - 12h00 O.9 – Oral  
Investigating the ionization process of noble gas atoms in a static electric field  
**Pham Nguyen Thanh Vinh** (Ho Chi Minh University of Pedagogy)

12h00 - 14h00	Lunch Break
14h00 - 18h00	Excursion

## Wednesday, 29 July 2015

### **Oral Session 4: *Particle and Nuclear Physics***

**Chair: Nguyen Anh Ky**

08h30 - 08h50	O.10 – Oral Tachyons of cosmological origin in general relativity <b>Dao Vong Duc</b> (Institute of Physics, Vietnam Academy of Science and Technology)
08h50 - 09h10	O.11 – Oral The pygmy dipole resonance in neutron-rich nuclei <b>Nguyen Quang Hung</b> (Tan Tao University)
09h10 - 09h30	O.12 – Oral A particle-number conserving microscopic approach to octupole deformation of even-even nuclei <b>Tran Viet Nhan Hao</b> (Department of Physics, College of Education, Hue University)
10h00 - 10h30	Coffee Break

### **Oral Session 5: *Particle Physics***

**Chair: Dao Vong Duc**

10h30 - 11h00	I.4 – Invited Was the H boson discovered? <b>Nguyen Anh Ky</b> (Institute of physics)
11h00 - 11h20	O.13 – Oral Seesaw-deflected anomaly mediation and the 125GeV Higgs boson <b>Trần Minh Hiếu</b> (Hanoi University of Science and Technology)
11h20 - 11h40	O.14 – Oral Minimal 3-3-1-1 model <b>Dang Trung Si</b> (NCS, Viện Vật lý, Viện Hàn lâm KHCVN)
11h40 - 12h00	O.15 – Oral A general scenario of a model with A4 discrete symmetry <b>Phí Quang Văn</b> (Institute of physics)
12h00 - 14h00	Lunch Break

### **Oral Session 6: *Condensed Matter Theory and Simulation***

**Chair: Pham Khac Hung**

14h00 - 14h20	O.16 – Oral
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Density functional theory based tight binding study on theoretical prediction of low-density nanoporous phases from II-VI semiconductor materials

**Vu Ngoc Tuoc** (Hanoi univ. of Science and Technology)

14h20 - 14h40

O.17 – Oral

Structure correlation and mechanical properties in Al<sub>1-x</sub>Si<sub>x</sub>N materials under densification

**Le Van Vinh** (Hanoi University of Science and Technology)

14h40 - 15h00

O.18 – Oral

Electron mobility in MgZnO/ZnO heterojunctions: Effect of phonon scattering in wurtzite structures.

**Võ Văn Tài** (College of Technology and Industrial Management (CTIM))

15h00 - 15h20

O.19 – Oral

High quality factor in 2D photonic crystal L3 nanocavities on silicon-on-insulator

**Ngô Thị Phương** (HCM city University of Pedagogy)

15h30 - 16h00

Coffee Break

**Oral Session 7:** *Condensed Matter Theory*

**Chair:** Nguyen Quang Bau

16h00 - 16h20

O.20 – Oral

Born-series approach to the spontaneous decay near a realistically sized cylinder: second-order correction

**Ho Trung Dung** (Theoretical Physics Research Group, Ton Duc Thang University)

16h20 - 16h40

O.21 – Oral

Spin wave in ultra-thin film in presence of interfacial Dzyaloshinskii-Moriya and anisotropy interactions

**Bach Thanh Cong** (VNU University of Science)

16h40 - 17h00

O.22 – Oral

Analysis of Ventricular Tachycardia and Fibrillation by Bivariate Data Analysis

**Le Duy Manh** (Institute of Physics, Hanoi)

17h00 - 17h10

Closing



# Workshop Program

Monday, 27 July 2015

08h30 - 10h00      Registration

10h00 - 10h30      Coffee Break

10h30 - 10h40      Opening

**Oral Session 1:** *Condensed Matter Theory*

**Chair:** **Nguyen Ai Viet**

10h40 - 11h15      I.1 – Invited

Density Functional Theory and Fermi Surfaces

**Mukunda P. Das** (The Australian National University)

11h15 - 11h50      I.2 – Invited

Quantum field theory of interacting plasmon-photon-phonon system

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

12h00 - 14h00      Lunch Break

**Oral Session 2:** *Methods in Molecular Modeling and Simulation*

**Chair:** **Mai Suan Li**

14h00 - 14h35      I.3 – Invited

A rigorous approach to the derivation of analytical potentials in physics-based coarse-grained force fields

**Adam Liwo** (Faculty of Chemistry, University of Gdansk)

14h35 - 15h10      I.4 – Invited

Improved prediction of protein complex binding affinities: the role of entropy

**Antonio Trovato** (University of Padua)

15h10 - 15h30      O.1 – Oral

Coarse-grained models for the formation of self-limited supraparticle assemblies

**Trung D. Nguyen** (Institute of Mechanics, Vietnam Academy of Science and Technology)

15h30 - 16h00      Coffee Break

**Oral Session 3: *Condensed Matter Theory*****Chair: Mukunda Das**

- 16h00 - 16h35 I.5 – Invited  
Thermoelectric effects in graphene nanostructures  
**Viet-Hung Nguyen** (Université Paris-Sud & Institute of Physics)
- 16h35 - 16h55 O.2 – Oral  
Nonlinear optically detected magnetophonon resonance via two-photon process in parabolic quantum wells  
**Tran Cong Phong** (Vietnam Institute of Educational Sciences)
- 16h55 - 17h15 O.3 – Oral  
Entanglement and teleportation in the even and odd photon-added charge coherent states  
**Truong Minh Duc** (Hue University of Education)
- 17h15 - 17h35 O.4 – Oral  
Theoretical evaluation of maximum electric field approximation of direct band-to-band tunneling Kane model for low bandgap semiconductors  
**Nguyen Dang Chien** (Faculty of Physics, University of Da Lat)

**Tuesday, 28 July 2015****Oral Session 4: *Living Systems*****Chair: Adam Liwo**

- 08h30 - 09h05 I.6 – Invited  
Energy transduction and dissipation in biomolecular motors and pumps  
**Gerhard Hummer** (Max Planck Institute of Biophysics)
- 09h05 - 09h40 I.7 – Invited  
Defining behavior states of indicator animals under stressful or conflict conditions in a confined area  
**Tae-Soo Chon** (Pusan National University)
- 09h40 - 10h00 O.5 – Oral  
Cellular Organization and Synchronization of Pancreatic Islets  
**Danh-Tai Hoang** (Asia Pacific Center for Theoretical Physics (APCTP))
- 10h00 - 10h30 Coffee Break

**Oral Session 5: *Macromolecular Assembly*****Chair: Gerhard Hummer**

- 10h30 - 11h05 I.8 – Invited  
Electrostatics in viruses  
**Rudolf Podgornik** (J. Stefan Institute and University of Ljubljana)
- 11h05 - 11h40 I.9 – Invited

	Eukaryotic chromatin folding and gene regulation <b>Masaki Sasai</b> (Nagoya University)
11h40 - 12h00	O.6 – Oral Modeling DNA condensates with generalized elastic potential <b>Trinh Xuan Hoang</b> (Institute of Physics, Vietnam Academy of Science and Technology)
12h00 - 14h00	Lunch Break
14h00 - 18h00	Excursion

## Wednesday, 29 July 2015

### Poster Session

Chair: **Nguyen Tri Lan**

08h30 - 10h00	P.1 – Poster Studies on interactions between Ebola viral protein 35 and dsRNA using steered molecular dynamics approach <b>Nguyen Quy Ngan</b> (Department of Theoretical Physics, Faculty of Physics and Engineering Physics, University of Science)
08h30 - 10h00	P.2 – Poster Modeling the interactions between putative anticancer bacteriocins and the p53 DNA-binding domain <b>Pham Thoa</b> (Department of Theoretical Physics, Faculty of Physics, University of Science, Vietnam National University, Ho Chi Minh City, Vietnam)
08h30 - 10h00	P.3 – Poster Estimation of partial atomic charges of calcite (CaCO <sub>3</sub> ) by Electrostatic Potential Fitting method <b>Phan Van Cuong</b> (Nha Trang University, Vietnam)
08h30 - 10h00	P.4 – Poster Fission Product Decay Heat Calculations for Neutron Fission of <sup>232</sup> Th <b>Pham Ngoc Son</b> (Nuclear Research Institute)
08h30 - 10h00	P.5 – Poster Binding of F-19848 A and Natural Compounds to CD44: Implications to Breast Cancer <b>Nguyen Trung Tin</b> (Institute of Computational Science and Technology ( <a href="http://www.icst.org.vn/">http://www.icst.org.vn/</a> ))
08h30 - 10h00	P.6 – Poster Thermal neutron radiative capture cross-section of <sup>186</sup> W(n,g) <sup>187</sup> W reaction <b>Pham Ngoc Son</b> (Nuclear Research Institute)
08h30 - 10h00	P.7 – Poster Effect of Taiwan mutation (D7H) on structures of amyloid beta peptides:

- replica exchange molecular dynamics study  
**Phan Minh Trường** (Institute for Computational Science and Technology)
- 08h30 - 10h00 P.8 – Poster  
Calculation of Etingshausen coefficient in Quantum Well in the presence of Electromagnetic Wave  
**Dao Thu Hang** (People’s Police University of Technology and Logistics)
- 08h30 - 10h00 P.9 – Poster  
Transient super-ballistic spreading of wave packets in hybrid ordered-quasiperiodic lattices  
**Nguyen Ba Phi** (Mien Trung University of Civil Engineering)
- 08h30 - 10h00 P.10 – Poster  
First Principles Study on Nickel carbonophosphate  $\text{Li}_3\text{NiPO}_4\text{CO}_3$  for Cathode Materials of rechargeable Li-ion batteries.  
**Dương Thị Diễm My** (Khoa Vật lý, Trường Đại học Sư phạm)
- 08h30 - 10h00 P.11 – Poster  
Alzheimer’s Amyloid- $\beta$  Sequesters Caspase-3 via its C-terminal Tail  
**Nguyen Hoang Linh** (Institute for Computational Science and Technology (ICST))
- 08h30 - 10h00 P.12 – Poster  
Preformed template fluctuations promote fibril formation: Insights from lattice and all-atom models  
**Nguyen Truong Co** (Institute for Computational Science and Technology)
- 08h30 - 10h00 P.13 – Poster  
Improved thermoelectric properties of graphene devices by strain and doping engineering  
**Mai Chung Nguyen** (Université Paris-Sud & Institute of Physics)
- 08h30 - 10h00 P.14 – Poster  
Interactions between small molecules and amyloid beta peptides: Implications for Alzheimer’s disease  
**Ngo Son Tung** (Institute of Physics, Polish Academy of Sciences)
- 08h30 - 10h00 P.15 – Poster  
A New Model for the Collective Behavior of Animals  
**Nguyễn Phước Thế** (Duy Tan University)
- 08h30 - 10h00 P.16 – Poster  
A model of optical trapping cold atoms using a metallic nano wire with surface plasmon effect  
**Nguyen Thi Phuong Lan** (Hanoi Pedagogical University 2)
- 08h30 - 10h00 P.17 – Poster  
Dependence of Effective Diffusivities on Boron impurity Concentration in Simultaneous Diffusion Process in Silicon

- Vu Ba Dung** (Physics Faculty, Hanoi University of Mining and Geology, Ha Noi, Viet Nam)
- 08h30 - 10h00 P.18 – Poster  
THE DEPENDENCE OF MELTING RATE IN HEATING PROCESS OF BORON NITRIDE NANORIBBONS  
**Nguyen Thi Thuy Hang** (Ho Chi Minh City University of Technology)
- 08h30 - 10h00 P.19 – Poster  
Generalized Bogoliubov polariton model with distribution functions for complex systems. Application to stock exchange market  
**Chu Thuy Anh** (Institute of Physics, VAST)
- 08h30 - 10h00 P.20 – Poster  
Pi-plasmon model for carbon nano structures. Application to porphyrin  
**Chu Thuy Anh** (Institute of Physics, VAST)
- 08h30 - 10h00 P.21 – Poster  
On the time-dependent spatial dimension in six dimensional space-time  
**Phan Hong Lien** (Military Technical Academy)
- 08h30 - 10h00 P.22 – Poster  
Prediction of inhibitors of LSD1 protein using molecular modeling and simulation methods  
**Nguyen Quy Truong** (University of Science, HCM city)
- 08h30 - 10h00 P.23 – Poster  
Folding and escape of nascent proteins at ribosomal exit tunnel  
**Bui Phuong Thuy** (Namdinh University of Technology Education)
- 08h30 - 10h00 P.24 – Poster  
Non-additive effects of crowding and confinement on folding stability of proteins  
**Bui Phuong Thuy** (Namdinh University of Technology Education)
- 08h30 - 10h00 P.25 – Poster  
Identification of Potential Drugs for Alzheimer’s Disease by in Silico and in Vitro Experiments  
**Nguyen Quoc Thai** (Dong Thap University)
- 08h30 - 10h00 P.26 – Poster  
First-principles Study on Controlling Energy Gap of Graphene using Hybrid Armchair-Zigzag Structures  
**Nguyen Tien Cuong** (VNU University of Science)
- 08h30 - 10h00 P.27 – Poster  
PROTEIN REFOLDING UNDER AN EXTERNAL MECHANICAL FORCE  
**Pham Dang Lan** (ICST)
- 08h30 - 10h00 P.28 – Poster

A New Method for Determination of Optimal Pulling Direction for ligand from Binding Pocket: Application to Ranking Binding Affinity by Steered Molecular Dynamics

**Vuong Van Quan** (The Institute for Computational Science and Technology (ICST))

08h30 - 10h00 P.29 – Poster

Analysis of Binding Affinity of Derivatives of Vitamin K3 to Fibrils of A $\beta$  peptides

**Vu Thi Mui** (Institute for Computational Science and Technology)

08h30 - 10h00 P.30 – Poster

pH-dependence of UV-visible Spectra of human-Neuroglobin, a sign of structural and dynamical properties based on Two-Level Model

**Nguyễn Minh Hoa** (Đại học Y Dược Huế)

08h30 - 10h00 P.31 – Poster

Study of amyloid fibrillation in a simple model

**Nguyen Ba Hung** (Vietnam Military Medical University & Institute of Physics)

08h30 - 10h00 P.32 – Poster

Simple model for gold nano particles GNPs concentration dependence of Resonance Energy Transfer intensity

**Nguyễn Minh Hoa** (Đại học Y Dược Huế)

10h00 - 10h30 Coffee Break

### Oral Session 6: *Protein Folding and Protein Binding*

**Chair: Masaki Sasai**

10h30 - 11h05 I.10 – Invited

One-dimensional diffusion models for protein folding – how good can they be?

**Robert B. Best** (National Institute of Diabetes and Digestive and Kidney Diseases, National Institutes of Health)

11h05 - 11h40 I.11 – Invited

Codon positions that strongly influence cotranslational folding are far from equilibrium: A framework for controlling nascent-protein folding

**Edward O'Brien** (Pennsylvania State University)

11h40 - 12h00 O.7 – Oral

Studies on interactions between Ebola virus protein VP35 and its partners using molecular simulation approach

**Chuong Nguyen** (Ton Duc Thang University)

12h00 - 14h00 Lunch Break

### Oral Session 7: *DNA Dynamics, Nano Materials*

**Chair: Rudolf Podgornik**

- 14h00 - 14h35 I.12 – Invited  
DNA looping in the presence of divalent counterions, a simulation study using a coarse-grained model of DNA  
**Toan The Nguyen** (VNU University of Science)
- 14h35 - 15h10 I.13 – Invited  
Emission in Maganese-Doped Semiconductor Nanocrystals  
**Que-Huong Nguyen** (Marshall University)
- 15h10 - 15h30 O.8 – Oral  
THE EVOLUTION OF MELTING PROCESS OF GRAPHENE NANORIBBONS  
**Nguyen Thi Thuy Hang** (Ho Chi Minh City University of Technology)
- 15h30 - 16h00 Coffee Break
- Oral Session 8: *Protein Aggregation, Molecular Simulation of Protein***  
**Chair: Robert B. Best**
- 16h00 - 16h35 I.14 – Invited  
Protein Misfolding and Aggregation Revealed by Fluctuating Thermodynamics Analysis  
**Sihyun Ham** (Sookmyung Women’s University)
- 16h35 - 17h10 I.15 – Invited  
Protein aggregation: Key principles and applications  
**Mai Suan Li** (Institute of Physics, Polish Academy of Science & Institute for Computational Science and Technology at Ho Chi Minh City)
- 17h10 - 17h30 O.9 – Oral  
Molecular Modelling of Alcohol Dehydrogenase from *Lactobacillus Brevis* in Organic Solvent  
**Quy Vo** (University of Stuttgart)
- 17h30 - 17h40 Closing





# Conference Abstracts

I.1 – Invited, NCTP-40

## Strain effects on the electronic properties of devices made of twisted graphene layer

*V. Hung Nguyen (1,2), H. Viet Nguyen (2), J. Saint-Martin (1), P. Dollfus (1)*

*(1) Institute of Fundamental Electronics, CNRS, Univ. of Paris-Sud, Orsay, France; (2) Center for Computational Physics, Institute of Physics, VAST, Hanoi, Vietnam*

Graphene is one of the most attractive materials for beyond-CMOS electronics because of its specific electronic properties, which are a consequence of its two-dimensional honeycomb lattice and relativistic-like charge carriers at low energy [1]. To enlarge its range of applications, the modulation of electronic structure of graphene nanomaterials has been the subject of intense research. Recently, the interest of the graphene community has also been oriented toward the investigation of twisted graphene multilayer lattices, a specific type of Van der Waals structures of graphene. These lattices appear as promising materials providing various possibility of modulating their electronic properties by changing the twist angle [2,3]. In this work, we investigate the effects of uniaxial strain on the electronic properties of twisted graphene bilayer (T-GBL) systems [4,5]. First, we explore the effects of strain on the low-energy bands of twisted graphene bilayer. Second, we demonstrate that the strain engineering is an efficient technique to open finite transport gaps in vertical devices made of stack of twisted graphene layers. Regarding the first topic, we find that the bandstructure of T-GBLs is dramatically deformed and the degeneracy of the bands around the Dirac points is broken by strain. As a consequence, the number of valleys in the bandstructure can double and the van Hove singularity points are separated in energy. The effects are shown to be strongly dependent on the magnitude of strain, its applied direction and the twist angle. As an important result, we demonstrate that the position of van Hove singularities can be modulated by strain, suggesting the possibility of observing this peculiar feature of the bandstructure at low energy in a large range of twist angles (i.e., larger than 10 degrees). For the second topic, we find that because of the different orientations of the two layers in the vertical devices made of twisted graphene layers, their Dirac points can be displaced and separated in the k-space by the effects of strain. Hence, a finite conduction gap as large as a few hundred meV can be obtained in the device with a small strain of only a few percent. On this basis, the strong modulation of conductance and significant improvement of Seebeck coefficient are shown. The suggested devices therefore may be very promising for improving applications of graphene, e.g., as transistors or strain and thermal sensors.

References: [1] A. C. Ferrari et al., *Nanoscale* 7, 4598 (2015) [2] G. Li et al., *Nat. Phys.* 6, 109 (2010) [3] W. Yan et al., *Nat. Commun.* 4, 2159 (2013) [4] V. H. Nguyen and P. Dollfus (2015); arXiv:1412.7583 [5] V. H. Nguyen et al., *Nanotechnol.* 26, 115201 (2015)

**Presenter: Viet-Hung Nguyen**

I.2 – Invited, NCTP-40

### **Lepton mass and mixing in the 3-3-1 models based on discrete symmetries**

*V. V. Vien*

*Department of Physics, Tay Nguyen University, 567 Le Duan, Buon Ma Thuot, DakLak, Vietnam*

We present non-Abelian discrete groups, which play an important role for the model building in particle physics that beyond the Standard model. We discuss about constructing the 3-3-1 models based on some non-Abelian discrete symmetry groups such as  $S_3$ ,  $S_4$ ,  $A_4$ ,  $T_7$ ,  $T_{13}$  and  $D_4$  which accommodates lepton mixing with non-zero  $\theta_{13}$  and CP violation phase that consistent with the most recent experimental data on neutrino masses and mixing.

**Presenter: Vo Van Vien**

I.3 – Invited, NCTP-40

### **Microscopic model for scattering of ultracold paraexcitons in cuprous oxide**

*Hoàng Ngọc Cẩm, Ngô Đức Thiện*

*Institute of Physics, VAST*

With their unique properties, paraexcitons in high-purity cuprous oxide have been considered an attractive candidate for observing excitonic Bose Einstein condensation (BEC). Despite a lot of experimental effort to create a state of quantum degeneracy in the system, conclusive evidence for an excitonic BEC has not been obtained. The main reason for this failure is proved to be an efficient collision-induced loss process, whose nature still remains an open question. To gain insight into the mechanism of the decay, we develop a microscopic model for the para-para scattering at ultralow temperatures. In connection with the existence of the orthoexciton along with the paraexciton as internal states of the  $1s$  exciton and their coupling by the exchange interaction, the para-para scattering is a two-channel problem. That is, two orthoexcitons, which are 24 meV higher than the threshold energy of two incoming paraexcitons, form for the latter a closed channel. Employing a reasonable approximation for the nonlocal exchange exciton-exciton interaction, we calculate the scattering potential in the open and closed channels as well as the coupling potential up to the third order in the small mass ratio. This allows us to compute the background s-wave scattering length, which entirely describes the entrance para-para collision at ultralow temperatures. Further, applying a localization procedure to the obtained ortho-ortho interaction potential, we compute the position of the quasibiexciton level in the closed channel, at which a resonance scattering of the incoming paraexcitons takes place. As any resonance scattering includes an inelastic component, the resonance paraexciton scattering is probably associated with the particles loss in experiments on BEC in cuprous oxide. Along with an empirical parameter for the lifetime of the metastable biexciton state, the computed quasibiexciton position makes it possible to calculate the rate of the decay process as well as the total s-wave scattering length of paraexcitons. These theoretical results are considered in relation to recent experiments on excitonic BEC.

**Presenter: Hoang Ngoc Cam**

I.4 – Invited, NCTP-40

## Was the H boson discovered?

*Dinh Nguyen Dinh, Nguyen Anh Ky, Nguyen Thi Hong Van and Phi Quang Van*

*Institute of Physics, Vietnam Academy of Science and Technology, 10 Dao Tan, Ba Dinh, Hanoi, Vietnam*

The standard model has postulated the existence of a scalar boson, named the Higgs boson. This boson plays a central role in a symmetry breaking scheme called the Brout-Englert-Higgs mechanism (or the Brout-Englert-Higgs-Guralnik-Hagen-Kibble mechanism, for completeness) making the standard model realistic. However, until recently at least, the 50-year-long-sought Higgs boson had remained the only particle in the standard model not yet discovered experimentally. It is the last but very important missing ingredient of the standard model. Therefore, searching for the Higgs boson is a crucial task and an important mission of particle physics. For this purpose, many theoretical works have been done and different experiments have been organized. It may be said in particular that to search for the Higgs boson has been one of the ultimate goals of building and running the LHC, the world's largest and most powerful particle accelerator, at CERN, which is a great combination of science and technology. Recently, in the summer of 2012, ATLAS and CMS, the two biggest and general-purpose LHC collaborations, announced the discovery of a new boson with a mass around 125 GeV. Since then, for over two years, ATLAS, CMS and other collaborations have carried out intensive investigations on the newly discovered boson to confirm that this new boson is really the Higgs boson (of the standard model). It is a triumph of science and technology and international cooperation. Here, we will review the main results of these investigations following a brief introduction to the Higgs boson within the theoretical framework of the standard model and Brout-Englert-Higgs mechanism as well as a theoretical and experimental background of its search. This paper may attract interest of not only particle physicists but also a broader audience.

**Presenter: Nguyen Anh Ky**

O.1 – Oral, NCTP-40

## Density functional studies of gas molecules adsorbed on Graphene Nanoribbons

*Nguyen Tien Cuong and Nguyen Manh Tien*

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

We present first-principles studies on adsorption of CO<sub>2</sub> and NH<sub>3</sub> gas molecules on pristine and modified graphene nanoribbons (GNRs). Electronic properties and transport properties are calculated using density functional theory and non-equilibrium Green's function method, respectively. Adsorption energy, density of states, and charge transfer are examined. It is found that both CO<sub>2</sub> and NH<sub>3</sub> molecules show physical adsorption on pristine GNRs with low adsorption energies and small charge transfer. In contrast, the adsorptions of the molecules on modified GNRs are chemical adsorption. The analysis of electron density deformation and charge transfer demonstrate that NH<sub>3</sub> and CO<sub>2</sub> adsorbed on GNRs exhibit donor-like and acceptor-like behavior, respectively. We also calculated transmission spectra and current-voltage characteristics for the GNRs with and without adsorption of gas molecules. The obtained results suggest that the sensitivity and selectivity of designed GNR-based gas sensors could be significantly improved by introducing the modified electronic structures of the GNR systems

**Presenter: Nguyen Tien Cuong**

O.2 – Oral, NCTP-40

### Transport gap in strained graphene heterochannels

*M. Chung Nguyen (1,2), V. Hung Nguyen (1,2), H. Viet Nguyen (1) and P. Dollfus (2)*

*(1) Center for Computational Physics, Institute of Physics, VAST, Hanoi, Vietnam; (2) Institut d'Electronique Fondamentale, Université Paris Sud, Orsay, France*

Due to its unusual electronic structure and excellent physical properties, graphene has become an attractive material in several research fields [1]. However, applications of graphene in electronic devices are still questionable due to its gapless character. Hence, many nanostructuring techniques (e.g., graphene nanoribbons [2], graphene bilayer with a perpendicular electric field [3], graphene nanomesh lattices [4], channels based on vertical stack of graphene layers [5], graphene/hexagonal boron nitride [6], nitrogen-doped graphene [7], and so on), to open a bandgap in this material have been suggested. However, each method still has its difficulties in the fabrication and need to be further confirmed by experiments. Recently, strain has been shown to be an alternative/promising approach to modulating the electronic properties of this material.

In current works [8,9], we found that though it can not change the gapless character of 2D graphene channel, a small strain (i.e., a few percent) can lead to a significant deformation of graphene's bandstructure. In graphene strain junctions, this results in a misalignment of Dirac cones of different graphene sections in the k-space and hence a large energy-gap (i.e., a few hundred meV) of transmission can be achieved. Moreover, it has been shown that the effect is strongly dependent not only on the strain magnitude but also on the strain direction and lattice orientation. On this basis, such strain heterochannels have been demonstrated to be very promising for enlarging the applications of graphene devices as in transistors or strain and thermal sensors.

References: [1] A. C. Ferrari et al., *Nanoscale* 7, 4598 (2015); [2] M. Y. Han et al., *Phys. Rev. Lett.* 98, 206805 (2007); [3] Y. Zhang et al., *Nature* 459, 820 (2009); [4] J. Bai et al., *Nat. Nanotechnol.* 5, 190 (2010); [5] L. Britnell et al., *Science* 335, 947 (2012); [6] N. Kharche et al., *Nano Lett.* 11, 5274 (2011); [7] A. Zabet-Khosousi et al., *J. Am. Chem. Soc.* 136, 1391 (2014); [8] V. H. Nguyen et al., *Nanotechnology*. 25, 165201 (2014); [9] M.C. Nguyen et al., *Semicond. Sci. Technol.* 29 115024 (2014); *Physica E* (2015) in press (<http://arxiv.org/abs/1505.06474>)

**Presenter: Nguyen Mai Chung**

O.3 – Oral, NCTP-40

### The study of dynamics heterogeneity and slow down of network-forming liquid computer simulation

*P. K. Hùng (1), L. T. San (1), H. V. Huệ (2)*

*(1) Hà Nội University of Science and Technology (2) Tay Nguyen University*

We have numerically studied the diffusion in silica liquid following an approach that the particles mobility is evaluated via the  $\text{SiO}_x \text{SiO}_x - 1$  and  $\text{OSiy OSiy} - 1$  reactions. Four models at temperatures from 2600 to 3500 K have been constructed by molecular dynamic simulation. The simulation reveals that the liquid has a tetrahedral network structure with a small amount of defect-cells. Moreover, defect-cells do not uniformly distribute in the liquid, but they have a tendency to form clusters. Further, we found two distinct clusters. First cluster contains the particles on which no reaction happens. The second cluster consists of particles where the reactions frequently happen. The mobility of atoms in the none-reaction cluster is significantly

smaller than in the reaction cluster. This clearly indicates the coexistence of slow and fast mobility regions. The size of two mention clusters strongly depends on the temperature. The dynamics slowdown near glass transition point is interpreted by the percolation of none-reaction cluster.

**Presenter: Phạm Khắc Hùng**

O.4 – Oral, NCTP-40

### **Some new cosmological implications in polynomial exponential $f(R)$ modified gravity model**

*Vo Van On*

*Department of Physics- Faculty of Natural Science - University of Thu Dau Mot*

In the paper, first we present shortly to the polynomial exponential  $f(R)$  modified gravity model in which Einstein – Hilbert action of  $R$  replaced by a  $f(R)$  function of polynomial exponential form, then we show some new cosmological implications in the model as: cosmological dynamics, some scenarios of cosmological evolutions, some constraints from experimental of Sun system upon the model. Results point that the model is a good candidate for researching cosmological revolution.

**Presenter: On Van Vo**

O.5 – Oral, NCTP-40

### **Phenomenology of the simple 3-3-1 model**

*N. T. K. Ngan (1), D. V. Soa (2) and P. V. Dong (3)*

*(1) Cantho University; (2) Hanoi National University of Education; (3) Institute of Physics, Vietnam Academy of Science and Technology*

We construct the simple 3-3-1 model for solving the inappropriate problems of the reduced 3-3-1 model. We introduce new fermion mass terms, identify the masses of fermion, gauge and scalar bosons. The Dark matter candidates are also studied through different Higgs sectors included in the model.

**Presenter: Nguyễn Thị Kim Ngân**

O.6 – Oral, NCTP-40

### **Parameterization of $SO(8)$ group and its Schwinger representation.**

*Phan Ngọc Hưng(1), Dương Nhật Huy(2), Nguyễn Thanh Sơn (3), Lê Văn Hoàng (1)*

*(1) HCMC University of Education; (2) HCMC University of Science; (3) HCMC University of Architecture*

A parameterization of  $SO(8)$  is proposed using seven angles that allows us to describe explicitly the  $SO(8)$  monopole field in the nine-dimensional space. The Schwinger representation of  $SO(8)$  is also constructed so that the algebraic method can be used for the nine-dimensional MICZ-Kepler problem.

**Presenter: Phan Ngọc Hưng**

O.7 – Oral, NCTP-40

### **Influence of an electromagnetic wave on the Hall effect in two-dimensional semiconductor systems**

*Nguyen Quang Bau(a, \*), Nguyen Dinh Nam(a), Bui Dinh Hoi(b)*

*(a) Faculty of Physics, Hanoi University of Science, Vietnam National University, Hanoi, Vietnam (b) Department of Physics, National University of Civil Engineering, Hanoi, Vietnam*

The Hall effect in some two-dimensional semiconductor systems under the influence of an electromagnetic wave (EMW), is theoretically studied using the quantum kinetic equation for electrons. The magnetic field is applied perpendicularly to the plane of free motion of electrons. The magnetoresistance and conductivity are calculated in parabolic quantum wells, square quantum wells and compositional superlattices taking account the electron – phonon interaction. For the electron – acoustic phonon interaction at low temperature, numerical results for the magnetoresistance are in good agreement with available experimental data. For the electron – optical phonon interaction at high temperature, the magneto-phonon resonance effect is observed in the case of absence of the EMW and optically detected magneto-phonon resonance effect is observed in the case of presence of EMW.

**Presenter: Nguyen Quang Bau**

O.8 – Oral, NCTP-40

### **Negative charge transfer to the surface in the electron-hole asymmetric models.**

*Giang Huong Bach*

*VNU University of Science*

Ising-like dynamic Hubbard model describes a single electronic band model with an auxiliary spin-1/2 degree of freedom in order to capture physics of a solid with hydrogen-like atoms. This type of models proves that electrons becomes more strongly correlated when the number of electrons increase, which is presented by the inversely proportional to electron number filling of quasi-particle weight in a bulk system. Dynamical mean field theory calculations show that electrons in the surface are even more strongly correlated since electrons prefer residing in the surface in order to take advantage of lowering kinetic energy in the interior. The negative charge transfer to the surface is investigated in detail under the effect of parameters, for example on-site  $U$  Coulomb potential,  $g$  coupling between auxiliary field with the electronic band...

**Presenter: Giang Huong Bach**

O.9 – Oral, NCTP-40

### **Investigating the ionization process of noble gas atoms in a static electric field**

*Pham Nguyen Thanh Vinh (1)*

*(1) Ho Chi Minh University of Pedagogy*

We investigate the ionization process of noble gas atoms in a static electric field by using Siegert state approach. All the observable quantities of the ionized electrons such as the energy shift, ionization rate, and transverse momentum distribution in the out-going flux can be expressed in term of Siegert states that are the solutions to the stationary Schrödinger equation satisfying the regularity and out-going wave boundary conditions. The method is illustrated by calculations of

the energy, ionization width, and transverse momentum distribution as functions of the electric field with arbitrary strength for the outer  $p$  shells of Ne, Ar, Kr, and Xe. Comparison of the numerical results with the prediction of perturbation theory for the energy, with weak-field asymptotic theory for the ionization rate and transverse momentum distribution is discussed. The failure of these approximation theories for strong electric field underlines the indispensable role of our numerical approach.

**Presenter: Pham Nguyen Thanh Vinh**

O.10 – Oral, NCTP-40

### **Tachyons of cosmological origin in general relativity**

*Dao Vong Duc (1) and Phu Chi Hoa (2)*

*(1) Institute of Physics, VAST; (2) Dalat University*

The results presented in this report are mainly based on our work recently published [D. V. Duc, P. C. Hoa, J. Mod. Phys., vol.5, p.2106 (2014)]. The concept of generally covariant duality is treated within the framework of vierbein formalism. The equations for associated scalar fields are derived from vierbein postulate. The existence of scalar tachyons is predicted with the masses completely determined by Einstein cosmological constant.

**Presenter: Dao Vong Duc**

O.11 – Oral, NCTP-40

### **The pygmy dipole resonance in neutron-rich nuclei**

*Nguyen Quang Hung (1), Huynh Ngoc Duc (2), and Hoang Anh Tuan Kiet (1)*

*(1) School of Engineering, Tan Tao University, Duc Hoa, Long An Province, Vietnam; (2) Graduate School, University of Pedagogy, An Duong Vuong, Ho Chi Minh City, Vietnam*

The pygmy dipole resonance (PDR), which has been observed via the enhancement of the electric dipole strength  $E1$  of atomic nuclei, is studied within a microscopic collective model. The latter employs the Hartree-Fock method with realistic nucleon-nucleon interactions of the Skyrme types plus the random-phase approximation (RPA). The results of the calculations obtained for various even-even nuclei such as  $^{16-28}\text{O}$ ,  $^{40-58}\text{Ca}$ ,  $^{100-120}\text{Sn}$ , and  $^{182-218}\text{Pb}$  show that the PDR is significantly enhanced when the number of neutrons outside the stable core of the nucleus is increased, that is, in the neutron-rich nuclei. It is found that the relative ratio between the total  $E1$  strengths in the low energy region (the PDR region) and the high energy one (the giant dipole resonance – GDR region) does not exceed 4.5 percent. The collectivity of the PDR states will be also discussed.

**Presenter: Nguyen Quang Hung**

O.12 – Oral, NCTP-40

### **A particle-number conserving microscopic approach to octupole deformation of even-even nuclei**

*T. V. Nhan Hao (1, 2), Aloys Nizigama (3)*

*(1) Department of Physics, College of Education, Hue University, 34 Le Loi Street, Hue City, Vietnam (2) Center for Theoretical and Computational Physics, College of Education, Hue Uni-*

*versity, 34 Le Loi Street, Hue City, Vietnam (3) University of Bordeaux, CENBG, UMR5797, F-33170, Gradignan, France*

Octupole deformation description of medium and heavy nuclei regions has been systematically carried out by using the particle-number-conserving microscopic approach [1, 2]. The commonly used effective interaction Skyrme energy density functional has been used for particle-hole channel. The low multipole components of the pairing-plus-multipole two-body interaction have been neglected, whereas the high multipole components are approximately represented by a density independent  $\delta$  interaction to describe the pairing correlations. The obtained results are compared with previous HF+BCS ones.

[1] T. V. Nhan Hao, J. Le Bloas, M. H. Koh, L. Bonneau, and P. Quentin, *Int. J. Mod. Phys. E* 21 (2012) 1250051. [2] T. V. Nhan Hao, P. Quentin, and L. Bonneau, *Phys. Rev. C* 86 (2012) 064307.

**Presenter: Tran Viet Nhan Hao**

O.13 – Oral, NCTP-40

### Seesaw-deflected anomaly mediation and the 125GeV Higgs boson

*Tran Minh Hieu (1), Nobuchika Okada (2)*

*(1) Hanoi University of Science and Technology; (2) University of Alabama*

We investigate the phenomenology of a class of model that at the same time solves the tachyonic slepton problem originated from the pure anomaly mediated supersymmetry breaking (AMSB) model and generates neutrino masses. The heavy fields in seesaw mechanism play the role of messengers in the deflected AMSB scenario. Taking into account various theoretical and phenomenological constraints, especially the measured limits for the Higgs mass, we specify the viable parameter regions and depict the properties of dark matter candidate. We point out that the type III seesaw with three generations of 24-messenger is excluded, while the type II seesaw and type III seesaw with two generations of 24-messenger are still allowed. Even though the sparticle masses are too heavy to be directly detected at the LHC, results on the spin-independent cross-section of the scattering between the lightest neutralino and proton show the possibility to see evidences of new physics from future dark matter search experiments. In these models, lepton flavor violation is indispensable due to the Yukawa couplings between the seesaw messenger sector and MSSM fields (Yukawa mediation). Interestingly, we find that such dangerous FCNC effects are indeed suppressed because of the upper limit on the messenger scale induced by the electroweak symmetry breaking condition.

**Presenter: Trần Minh Hiếu**

O.14 – Oral, NCTP-40

### Minimal 3-3-1-1 model

*P. V. Dong (1), D. T. Si (2), T. T. Thuc (3), and N. T. Phong (4)*

*(1) Institute of Physics, (2) Institute of Physics, (3) Institute of Physics, (4) Department of Physics, Cantho University*

We argue that the weak, electromagnetic and  $B - L$  interactions can be unified similarly to the electroweak theory. The fermion content that is anomaly free is minimally introduced. The trivial representations of the gauge symmetry can act as dark matter candidates. The small neutrino masses as well as the electric charge quantization are naturally emerged. We identify



the particles in the standard model, the interaction of fermions with gauge bosons and predict the new physics with the masses in the TeV scale.

**Presenter: Dang Trung Si**

O.15 – Oral, NCTP-40

### **A general scenario of a model with $A_4$ discrete symmetry**

*Dinh Nguyen Dinh(1), Nguyen Anh Ky(1), Phi Quang Van(1), Nguyen Hong Van(1)*

*(1) Institute of physics*

In this research, an extended version of the standard model (SM) with  $A_4$  discrete symmetry is considered. Two SM-like Higgs doublets are added to the SM one to form an  $A_4$  Higgs triplet, whose vacuum expectation value  $(v_1, v_2, v_3)^T$  satisfies the relation  $m_e : m_\mu : m_\tau = v_1 : v_2 : v_3$ . A light active neutrino mass matrix is generated through the type-I see-saw mechanism by adding 4 right-handed neutrino multiplets, which are one  $A_4$  triplet and three  $(1, 1', 1'')$   $A_4$  singlets. The PMNS matrix obtained after fitting with the current experimental data is checked by applying it to calculating some physical quantities, such as  $|\langle m_{ee} \rangle|$  and  $J_{CP}$ .

**Presenter: Phí Quang Văn**

O.16 – Oral, NCTP-40

### **Density functional theory based tight binding study on theoretical prediction of low-density nanoporous phases from II-VI semiconductor materials**

*Vu Ngoc Tuoc,(1), Tran Doan Huan(1,2), Nguyen Viet Minh(1), Nguyen Thi Thao(1,3)*

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Polymorphs or phases - different inorganic solids structures of the same composition usually have widely differing properties and applications, thereby synthesizing or predicting new classes of polymorphs for a certain compound is of great significance and has been gaining considerable interest. Herein, we perform a density functional theory based tight binding (DFTB) study on theoretical prediction of several series of II-VI semiconductor material (ZnO, ZnS, CdS, CdSe, CdTe) nanoporous phases from their bottom-up building blocks. Among these, three phases are reported for the first time, which may greatly extended the family of II-VI compound nanoporous phases. We also show that they are all generally can be categorized similarly to the aluminosilicate zeolites inorganic open-framework materials. The hollow cage structure of the corresponding building block AkBk (A=Zn,Cd B=O,S,Se,Te) is well preserved in all of them, which leads to their low-density nanoporous and high flexibility. Additionally the electronic wide-energy gap of the individual AkBk is also retained. Our study reveals that they are all semiconductor with a large band gap. Further, this study is likely to be the common for II-VI semiconductor compounds and will be helpful for extending their range of properties and applications

Keywords: Nanoporous phases, DFT, II-VI semiconductor

**Presenter: Vu Ngoc Tuoc**

O.17 – Oral, NCTP-40

## Structure correlation and mechanical properties in Al<sub>1-x</sub>Si<sub>x</sub>N materials under densification

*N. T. Trang, N. T. Giang, N. T. Thao, N. M. Hung, L. V. Vinh\**

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

Molecular dynamics simulations of Al<sub>1-x</sub>Si<sub>x</sub>N materials under densification were carried out to investigate their structure and mechanical properties. Such effects on other microscopic characteristics, such as bond-length distance, bond-angles and coordination number distribution have been observed. Based on the common neighbour analysis, we found that AlN and Si<sub>3</sub>N<sub>4</sub> samples have amorphous state, whereas the remained Al<sub>1-x</sub>Si<sub>x</sub>N samples show the structure of crystalline AlN mixed amorphous AlN which segregated with amorphous Si<sub>3</sub>N<sub>4</sub>. The strengthening enhancement is clearly observed in the sample with rich crystalline AlN and denser amorphous Si<sub>3</sub>N<sub>4</sub>.

**Presenter: Le Van Vinh**

O.18 – Oral, NCTP-40

## Electron mobility in MgZnO/ZnO heterojunctions: Effect of phonon scattering in wurtzite structures.

*Vo Van Tai (1), Nguyen Quoc Khanh (2)*

*(1) College of Technology and Industrial Management (CTIM). (2) University of Science Ho Chi Minh City.*

Mobility of a two-dimensional electron gas at MgZnO/ZnO heterojunctions for temperatures  $T < 300$ (K) is studied in detail. The electrons, assumed to be confined to the lowest subband, are considered to be scattered by interface charges, interface roughness, background impurities, acoustic phonons via deformation potential and piezoelectric fields, and polar LO phonons. Our work encompasses three physically distinct temperature ranges with respect to phonon scattering: the Block-Gruneissen (BG), equipartition (EP), and inelastic regimes. We carry out calculations in the BG regime and compare the results with corresponding ones in the EP regime. We also compute the first order perturbation distribution by directly solving the linearized Boltzmann equation by an iterative method, and compare with the low-temperature relaxation-time approximation and the high-energy relaxation-time approximation. Good agreement with recent low temperature mobility data is obtained.

**Presenter: Võ Văn Tài**

O.19 – Oral, NCTP-40

## High quality factor in 2D photonic crystal L3 nanocavities on silicon-on-insulator

*Thi-Phuong Ngo, Anh-Nguyet T. Nguyen, Tieu-Khanh Ngo*

*HCM University of Pedagogy*

We report on the numerical and experimental analysis of high-quality factor (Q) two-dimensional photonic crystal L3 nanocavities. Ge/Si quantum dots are embedded as active internal sources inside the photonic crystal slab. Cavities in this configuration operate around 1550 nm, i.e. telecommunication wavelength. A strong luminescence signal enhancement by two orders of magnitude associated with the islands embedded in the nanocavities is observed. We focus on

optimizing the quality factor of L3 nanocavities by modifying the hole position at the edges of the nanocavity. High  $Q > 75000$  is obtainable by optimization of structural parameters based on the FDTD calculation. The maximum Q-factor measured is limited by the spectrometer resolution. We conclude by outlining the mix of optical properties and structure parameters needed to open up the further research directions.

**Presenter: Ngô Thị Phương**

O.20 – Oral, NCTP-40

**Born-series approach to the spontaneous decay near a realistically sized cylinder: second-order correction**

*Ho Trung Dung*

*Theoretical Physics Research Group Ton Duc Thang University*

The Born series has recently proved to be quite useful in many problems of the matter-electromagnetic field interaction. Singularities may arise, however, when the field point or the source point coincides with the scattering point, or when the scattering points coincide with each other. Even though the integrals are expected to converge, the singularities have to be eliminated before any physically meaningful analytical or numerical results can be derived. We show how to tackle the singularity in the second-order term in the Born series of the atomic decay rate near a realistically sized cylinder and obtain an estimation of the second-order correction as a result. We also show that by using the bulk Green tensor instead of the vacuum Green tensor as the unperturbed term in the Born series, one can avoid the singularity in the first-order term, which arises when the atom is embedded in the medium.

**Presenter: Ho Trung Dung**

O.21 – Oral, NCTP-40

**Spin wave in ultra-thin film in presence of interfacial Dzyaloshinskii-Moriya and anisotropy interactions**

*Nguyen Tu Niem, Bach Thanh Cong*

*Computational Materials Science Laboratory, Faculty of Physics, VNU University of Science*

In this report we examine spin wave in thin magnetic films at finite temperature using double time temperature dependent Green function method for the Heisenberg Hamiltonian with additional interfacial Dzyaloshinskii- Moriya and anisotropy interactions. It is shown during RPA that, interfacial Dzyaloshinskii- Moriya interaction leads to the un-symmetric propagation of spin wave in opposite directions and the anisotropy is responsible for the gap of spin wave at center of Brillouin zone.

**Presenter: Bach Thanh Cong**

O.22 – Oral, NCTP-40

**Analysis of Ventricular Tachycardia and Fibrillation by Bivariate Data Analysis**

*Le Duy Manh (1), A. V. Dvornikov (2), C. K. Chan (3,4), Pik-Yin Lai (3)*

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ogy, Loyola University School of Medicine 2160 South First Ave., Maywood, IL 60153, USA. (3) Department of Physics and Center for Complex Systems, National Central University Chungli, Taiwan 320, R.O.C. (4) Institute of Physics, Academia Sinica - Nankang, Taipei, Taiwan 115, R.O.C.

Heart is a complex dynamical system that contains many components worked rhythmically in a coordinated manner to produce rhythmic activity for effectively pumping blood, feeding activities of the whole living body with nutrition and oxygen. Under fast electrical pacing, heart shows rich dynamical behaviors due to its instability, such as alternans, tachycardia and fibrillation. Ventricular tachycardia (VT) is the disease that the heart beats much faster than the normal rhythm. If VT lasts for long time, it may develop into much more serious problems such as ventricular fibrillation or even the sudden cardiac death. Ventricular fibrillation (VF) is an extremely serious arrhythmia which is known to be the major cause of sudden cardiac death, and thus the research to understand its mechanism as well as clinical treatments is very important. In our study, VT and VF in isolated rat hearts perfused in the Langendorff system are induced by fast electrical pacing. Electrical signals from right atrium (a site very close to sinoatrial node) and left ventricle are recorded simultaneously. We find that when there is strong component of ventricular signal detected in the atria one during VT & VF, the induced VT & VF is usually not self-terminating. Quantitative criteria for the prediction of self-terminating VF are proposed based on the analysis of bivariate time series (atrial and ventricular signals) by the cross-wavelet and cross-Fourier power spectra methods. The success rate of our prediction is about 80-90

**Presenter: Le Duy Manh**

P.1 – Poster, NCTP-40

### **Calculation of Ettingshausen coefficient in Quantum Well in the presence of Electromagnetic Wave**

*Dao Thu Hang and Nguyen Quang Bau*

*Faculty of Physics, Hanoi University of Science, Vietnam National University, 334 Nguyen Trai, Thanh Xuan, Hanoi, Vietnam.*

The analytic expressions for Ettingshausen coefficient in the Quantum Well with parabolic potential in the presence of Electromagnetic wave are calculated by using the quantum kinetic equation for electrons. The dependence of Ettingshausen coefficient on the frequency of Electromagnetic wave, the Quantum Well parameters and especially the dependence of Ettingshausen coefficient on temperature gradient are obtained. The results are numerically calculated and discussed for AlGaAs/GaAs/AlGaAs Quantum Well

**Presenter: Dao Thu Hang**

P.2 – Poster, NCTP-40

### **An analytical description for the ground state energy of two dimensional exciton in a magnetic field**

*Nguyen Phuong Duy Anh (1), Hoang Do Ngoc Tram (2)*

*(1) Thu Dau Mot University (2) Ho Chi Minh City University of Education*

The article presents an analytical expression describing the dependence of the ground state energy on magnetic field intensity for a two-dimensional exciton in a magnetic field. The special

feature of the obtained expression is its very high accuracy with error less than 1% for the whole range of the magnetic field intensity.

**Presenter: Hoang-Do Ngoc-Tram**

P.3 – Poster, NCTP-40

### **Energy spectrum inverse problem of q-deformed harmonic oscillator and WKB approximation**

*Nguyen Anh Sang, Nguyen Thi Ha Loan, Nguyen Tri Lan, Do Thi Thu Thuy, Nguyen Ai Viet Vocational Training and Comprehensive technical center of Phu Tho province; Ha Noi Pedagogical University 2; Institute of Physics - VAST; Cam Pha Industrial College; Institute of Physics - VAST.*

Using the connection between q-deformed harmonic oscillator and Morse-like aharmonic potential we investigate the energy spectrum inverse problem. Consider some energy levels of energy spectrum of q-deformed harmonic oscillator are known, we construct the corresponding Morse-like potential then find out the deform parameter q. The application possibility of using the WKB approximation in the energy spectrum inverse problem was discussed for the cases of parabolic potential (harmonic oscillator), Morse-like potential (q-deformed harmonic oscillator), and some other.

**Presenter: Nguyễn Ánh Sáng**

P.4 – Poster, NCTP-40

### **Calculating the current density of the radioelectrical effect in parabolic cylindrical quantum wires**

*Hoang Van Ngoc (1), Nguyen Vu Nhan (2), Nguyen Quang Bau (1)*

*(1) Faculty of Physics, Hanoi University of Sciences, Vietnam National University; (2) Air Defence - Air Force Academy*

The density of the current of the radioelectrical effect associated with the drag of the charge carriers in a parabolic cylindrical quantum wire by a linearly polarized electromagnetic wave, a dc electric field, a laser radiation is calculated. By using the quantum kinetic equation for electrons interacting with acoustic phonon at low temperatures, the dependence of the current density on the temperature, the frequency of the laser radiation, the frequency of the linearly polarized electromagnetic wave, the frequency of the parabolic potential is obtained. The analytic expression of current density is numerically evaluated and plotted for a specific quantum wires, GaAs/AlGaAs, to show clearly the dependence of the current density of charge carriers on above parameters. The results of current density in this case are compared with bulk semiconductors to show the difference.

**Presenter: Hoang Van Ngoc**

P.5 – Poster, NCTP-40

### **Phonon-assisted cyclotron resonance in AlGaAs-GaAs hyperbolic quantum well via two-photon absorption process**

*Le Dinh (1), Luong Van Tung (2), Pham Tuan Vinh (1,2)*

(1) *Department of Physics and Center for Theoretical and Computational Physics, Hue University's College of Education, Hue, Viet Nam;* (2) *Department of Physics, Dong Thap University, Dong Thap, Viet Nam.*

Phonon-assisted cyclotron resonance (PACR) in AlGaAs-GaAs hyperbolic quantum well is investigated via two-photon absorption process when electrons are scattered by longitudinal optical phonons (LO-phonons). Using the Green's function method, we obtain the expression of absorption power in the case of two-photon absorption. The dependence of absorption power on photon energy with different values of magnetic field, diffusion length and well width is indicated. The results are compared those to the quantum well models with different types of confined potentials.

**Presenter: Pham Tuan Vinh**

P.6 – Poster, NCTP-40

### **Plasmon resonance absorption of core-shell nanoparticles**

*Do Chi Nghia (1), Do Thi Nga (2)*

(1) *Hanoi Pedagogical University 2;* (2) *Institute of Physics, VAST*

Core-shell nanoparticles have exciting applications in different areas and biomedical field based on their optical properties. Metallic nanoparticles support plasmon resonances, where the resonance wavelengths and the local field enhancements (LFEs) depend sensitively on the geometrical shapes. In this work, we propose a core-shell nanoparticle consisting of Fe<sub>3</sub>O<sub>4</sub> core and Ag shell (Fe<sub>3</sub>O<sub>4</sub>@Ag nanoparticle). We theoretically study absorption properties of Fe<sub>3</sub>O<sub>4</sub>@Ag nanoparticles based on the Mie theory. There are two maxima at around 380 nm and near-infrared regime in the absorption spectrum of the nanoparticle.

**Presenter: Do Chi Nghia**

P.7 – Poster, NCTP-40

### **The ordered phase in the Spin -1 Heisenberg model with strict single occupancy.**

*Pham Thi Thanh Nga (1), Nguyen Toan Thang (2)*

(1) *Thuy loi University, 175 Tay Son St., Hanoi;* (2) *Institute of Physics, Vietnamese Academy of Science and Technology, 10 Dao Tan, Hanoi.*

In 1988 Popov and Fedotov proposed a new approach for spin - 1/2 and spin -1 systems. The Popov-Fedotov method has been applied for various problems of strongly correlated physics for the case of 1/2-spin. In this report we present a study of ordered phases in the fermionized spin-1 Heisenberg models when the constraint of strict single particle site occupation is taken into account by Popov-Fedotov trick. We discuss the quantum and thermal fluctuations at one-loop level for the partition function obtained by means of saddle point approximation in functional integral approach.

**Presenter: Pham Thi Thanh Nga**

P.8 – Poster, NCTP-40

### **probing nuclear vibration of $H_2^+$ using high-order harmonic generation**

*Le Thi Thanh Thuy (1), Phan Thi Ngoc Loan (2), Nguyen Ngoc Ty (3)*

*(1) student at Ho Chi Minh City University of Education, (2) (3) Lecturer at Ho Chi Minh City University of Education, Department of Physics, 280 An Duong Vuong Street, District 5, Ho Chi Minh City*

From the numerical solution of the time-dependent Schrödinger equation, we calculate the high-order harmonic generation (HHG) spectra of  $H_2^+$ , interacting with ultrashort intense laser pulses. Molecular nuclei vibrate with a superposition of individual vibrational states populated according to Franck-Condon distribution. We point out the possibility of probing the nuclear vibration using HHG. The results show that the intensity of HHG is correlated with the time delay, and it is strongly determined not only by the molecular configuration but also by the initial velocity of nuclei. When the internuclear separation takes the equilibrium value and nuclei are moving closer together, intensity of HHG is enhanced. But, with the same initial internuclear separation with the opposite direction of nuclear velocity, the intensity of HHG is reduced.

**Presenter: Lê Thị Thanh Thủy**

P.9 – Poster, NCTP-40

### The crystallization of iron nanoparticles

*Nguyen Thi Thao (1), Le Van Vinh (2), Nguyen Thi Thanh Ha (2)*

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Using molecular dynamics simulation, we have studied the crystallization of iron nanoparticles. The crystallization is analyzed through the potential energy and number of different type atoms. The simulation results indicated that when the amorphous sample is annealed at 900 K, it is crystallized into bcc phase. The influence of temperature on crystallization is clarified through the samples with different temperature. When the crystal cluster has a size larger than some critical value, the crystal growth occurs. Further, this cluster is stable and tends to have a nearly spherical shape. The fully crystallized sample consists of the core with crystalline structure and surface shell with amorphous porous structure.

**Presenter: Nguyen Thi Thao**

P.10 – Poster, NCTP-40

### Search for doubly charged Higgs at $e^+e^-$ colliders

*N. H. Thao (1), K. D. Thang (2), Tran Dinh Tham (3)*

*(1, 2) Department of Physics, Hanoi University of Education No 2, Vinh Phuc, Vietnam; (3) Pham Van Dong University, 986 Quang Trung Street, Quang Ngai City, Vietnam.*

A study of searching for doubly charged Higgs (DCHs) is performed in the supersymmetric reduced minimal 3-3-1 (SUSYRM331) model. We find that DCHs and the cross section of creating DCHs at  $e^+e^-$  colliders depend on five unknown parameters. For searching for the signals of

DCHs, we require that,  $\frac{(m_{A_1}^2 + m_W^2)c_{2\gamma}}{m_V^2} < c_{2\beta} < \frac{m_W^2 c_{2\gamma}}{m_V^2} < 0$  to avoid tachyon DCHs at tree level. Moreover, when the value of  $m_{A_1}$  is close to  $m_V$  there will exist a light DCH.

**Presenter: Thao Huy Nguyen**

P.11 – Poster, NCTP-40

### **q-Phonon**

*Nguyen Thi Ha Loan (1), Do Thi Thu Thuy (2), Nguyen Thi Lan Huong (3)*

*(1) Hanoi Pedagogical University No.2; (2) Cam Pha Industrial College; (3) 17th Master student of Physics Dept., Hanoi Pedagogical University No.2*

In this paper, a q-deformed crystal lattice vibration for generic atomic string is suggested. Energy spectrum of this vibration is calculated. We have obtained the expression for frequency of q-deformed crystal lattice vibration depends on amplitude and a concept of q-phonon is introduced.

**Presenter: Nguyen Thi Ha Loan**

P.12 – Poster, NCTP-40

### **Rotation of induced vortex-antivortex pair in microcavity polaritons**

*Doan Tri Dung and Tran Thoai Duy Bao*

*Ho Chi Minh City Institute of Physics, Vietnam Academy of Science and Technology, 1 Mac Dinh Chi, Dist. 1, Ho Chi Minh City, Vietnam*

Spontaneous pattern formation and the connected superfluid current patterns of microcavity polaritons due to nonresonant pumping are studied by using nonequilibrium Gross-Pitaevskii equation in the form recently derived [H. Haug et al., Phys. Rev. B 89, 155302 (2014)]. Under a Laguerre-Gauss laser beam which is used as a resonant pumping, these patterns are shown to rotate or oscillate depending on power of resonant pumping.

**Presenter: Doan Tri Dung**

P.13 – Poster, NCTP-40

### **Numerical study of whispering gallery mode in photonic crystal H2 defect nanocavity**

*Le Hai My Ngan, Nguyen Thi Anh Nguyet, Tran Ngoc Huy*

*HCM University of Pedagogy*

We present a numerical analysis of whispering gallery mode (WGM) in photonic crystal H2 defect. Using plane-wave expansion and finite-difference time-domain calculations, we investigate WGM of photonic-crystal-slab triangular H2-defect nanocavity structures as a good candidate for a high-quality factor (Q) and small-mode volume (V) resonant mode. We show a strong WG mode dependence on 12 nearest air-holes around the nanocavity. The ideal symmetric nature of the WG mode profile reduces the out-of-slab radiation and allows us to achieve a high Q. These results show a possible way to realize an optical resonator of the optoelectronic oscillator and practical silicon-based light emitting devices.

**Presenter: LÊ Hải Mỹ Ngân**

P.14 – Poster, NCTP-40

### **Simple model for optical modes of graphene nano ribbons**

*Dao Thi Thuy Nga (1), Phuong Thi Phuong Lan (2), Duong Thi Ha (2), Can Thi Thuy Thuy(2),*



*Do Thi Nga (2), Nguyen Ai Viet (2)*

*(1) Bac Ninh Department of Education and Training; (2) Institute of Physics, 10 Dao Tan, Ba-Dinh, Hanoi*

At present, graphene nano ribbons have drawn great attention due to many applications in nano technology, but their theory is quite complicated. We propose a simple model for approximate calculation of some main optical parameters of graphene nano ribbons. Several fitting schemes for optical transition energy versus width of graphene nano ribbons were investigated: Coulomb and Coulomb with screening forms, Pade and generalized Pade forms. The collective mechanism of pi-plasmon in graphene nano ribbons is also discussed.

**Presenter: Đào Thị Thúy Nga**

P.15 – Poster, NCTP-40

### **Thermodynamic Property of Interstitial Double Alloy with BCC Structure: Dependence on Temperature and Concentration of Interstitial Atoms**

*Nguyen Quang Hoc(1), Nguyen Thi Hoa(2), Dinh Thi Thanh Thuy(1), Bui Duc Tinh(1), Dinh Quang Vinh(1) and Nguyen Duc Hien(3)*

*(1)Hanoi National University of Education, 136 XuanThuy, CauGiay District, Hanoi (2) University of Transport and Communications, 3 CauGiay, Dong Da District, Hanoi (3)Mac Dinh Chi Secondary School, Chu Pah District, Gia Lai Province*

ABSTRACT. The thermodynamic quantities such as the mean nearest neighbor distance, the free energy, the isothermal and adiabatic compressibilities, the isothermal and adiabatic elastic modulus, the thermal expansion coefficient, the heat capacities at constant volume and at constant pressure, the entropy of interstitial double alloy with bcc structure with the concentration of interstitial atoms is very small are derived by the statistical moment method. The obtained expressions of these quantities depend on temperature and concentration of interstitial atoms. The theoretical results are applied to interstitial alloys FeX (X = Si, Li, H) and the numerical results are compared with the experimental data.

**Presenter: Nguyễn Đức Hiền**

P.16 – Poster, NCTP-40

### **INVESTIGATION OF NONSEQUENTIAL DOUBLE IONIZATION PROCESS OF HELIUM BY LINEARLY POLARIZED LASER FIELD AT HIGH INTENSITY**

*Tran Lan Phuong (1), Truong Dang Hoai Thu (1), Huynh Van Son (2), Le Hoang Dong Phuong (1), Pham Nguyen Thanh Vinh (1)*

*(1) Ho Chi Minh University of Pedagogy, 280 An Duong Vuong Ward 4 District 5 Ho Chi Minh City (2) Ho Chi Minh University of Science, 227 Nguyen Van Cu Ward 4*

By using the classical three-dimensional ensemble model, we investigate the nonsequential double ionization process of helium by 800-nm laser pulses at 2.0 PW/cm<sup>2</sup>. The results show that a pronounced V-like structure is exhibited in the two-electron momentum distribution along the laser polarization axis. At high laser intensity, this structure which was observed experimentally [Phys. Rev. Lett. **99**, 263003 (2007)] can be explained by the asymmetric energy sharing of two electrons during the recollision process. This asymmetric energy sharing process also embeds in the transverse momentum spectra, which provide insight into the microscopic dynamics of the

three-body interactions.

**Presenter: Tran Lan Phuong**

P.17 – Poster, NCTP-40

**Effective method for retrieval of interatomic separation of molecule CO<sub>2</sub> based on the theoretical analysis of molecular transition dipole zero-points**

*Le Thi Cam Tu (1), Vu Tran Dinh Duy (2), Hoang Van Hung (2), Le Van Hoang (2)*

*(1) HCMC University of Science (2) HCMC University of Pedagogy*

By the theoretical analysis of zero-points of the transition dipole of CO<sub>2</sub>, we obtain very accurate formulae describing a connection between three quantities: interatomic separation, electron kinetic energy in the continuum region, angle between electron direction and molecular axis. These formulae are very similar to the Bragg's equations for the electron interference effect and allow us to obtain the interatomic separation from the high-order harmonic spectra. Therefore, an effective method for retrieval of interatomic separation of CO<sub>2</sub> from high-order harmonic generation is proposed. This method can be applied for other molecules having two centers of emitting electrons.

**Presenter: Le Cam Tu**

P.18 – Poster, NCTP-40

**Influence of phonon confinement on the optically detected electrophonon resonance line-width in quantum wells.**

*Nguyen Dinh Hien (1), Le Dinh (1), Vo Thanh Lam (2), Tran Cong Phong (3)*

*(1) Hue University's College of Education, 34 Le Loi Str., Hue City, Viet Nam. (2) Department of Physics, Sai Gon University, 273 An Duong Vuong Str., District 5, Ho Chi Minh City, Viet Nam. (3) Vietnam Institute of Educational Sciences, 101 Tran Hung Dao Str., District Hoan Kiem, Ha Noi, Viet Nam.*

We investigate the effect of phonon confinement on the optically-detected electrophonon resonance (ODEPR) effect and ODEPR line-width in GaAs quantum wells. The ODEPR conditions as functions of the well's width and the photon energy are also obtained. The shifts of ODEPR peaks caused by the confined phonon are discussed. The numerical result for the specific GaAs quantum well shows that in the two cases of confined and bulk phonons, the line-width (LW) decreases with increasing well's width and increases with increasing temperature. Furthermore, in the small range of the well's width the influence of phonon confinement plays an important role and cannot be neglected in reaching the ODEPR line-width.

**Presenter: Nguyen Dinh Hien**

P.19 – Poster, NCTP-40

**On the fluctuation induced mass enhancement**

*Nguyen Van Hoa (1), Vu Ngọc Tuan (2), Lê Văn Xuân (3), Nguyen Tri Lan (4) and Nguyen Ai Viet (4)*

*Ha Noi College of Technology and Economy, Ha Noi, Viet Nam*

The effective mass induced by the background fluctuation on particles is considered. The ana-

lytical results show that the effective mass depends only on the properties of fluctuation, and takes non-zero value when and only when fluctuation mean value is non-zero. The possible applications of the obtained results to complex systems such as biology and ecology where environmental factors change the information exchange ranges from long to short one are discussed, i.e. the possibility of using physical modelling techniques to investigate macroscopic behaviours of some complex systems under consideration.

**Presenter: Le Van Xuan**

P.20 – Poster, NCTP-40

### **AUTOIONIZATION WITH FANO PROFILE AND BROAD-BAND CHAOTIC LIGHT - PHOTOELECTRON SPECTRA**

*Doan Quoc Khoa (1), Cao Long Van (2,3), Hoang Xuan Tam (4)*

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Fano profiles which with their asymmetric character have many potential applications in technology: The design of Fano profiles into optical systems may create new non-linear and switchable metamaterials, high-quality optical waveguides, ultrasensitive media for chemical or biosensing etc. Recently the Fano model has been considered in the cases of electromagnetically induced transparency for Lambda systems with degenerate and non-degenerate autoionizing levels. In this paper, we consider an external field driven double Fano model introduced by Leoński and his coworkers. We assume that the external electromagnetic field can be decomposed into two parts: coherent part and white noise. This assumption corresponds to the case of the real multimode laser operating without any correlation between the modes. We solve a set of coupled stochastic integro-differential equations involving the Fano model with two discrete levels and two levels of the same energy. We derive an exact formula by determining the photoelectron spectrum and detail it to two interesting physical limits: weak and strong fluctuations and compare it with the results obtained earlier.

**Presenter: Doan Quoc Khoa**

P.21 – Poster, NCTP-40

### **A perturbative solution to an $f(R)$ -gravity theory**

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

*Institute of physics, Vietnam academy of science and technology, 10 Dao Tan, Ha Noi, Viet Nam*

A perturbative solution to an  $f(R)$ -gravity model with a spherical symmetry is obtained and discussed. The solution is given for an arbitrary  $f(R)$  as a function of the scalar curvature. This solution can be reduced to particular cases including that of Einstein gravity.

**Presenter: Nguyễn Anh Kỳ**

P.22 – Poster, NCTP-40

## Transport properties of the Hubbard model on a honeycomb lattice

*N. T. H. Yên(1), H. A. Tuấn(1), N. T. Hương(2), L. D. Ánh(2)*

*(1) Institute of Physics; (2) Ha Noi University of Education*

We study a two-component Dirac fermion mixtures loaded into an optical lattice. The system is modeled by the Hubbard model on a honeycomb lattice. The local lattice Green function of the model is obtained within the coherent potential approximation. The critical value for the Mott transition at zero temperature is evaluated. The transport properties such as the electronic resistivity, the thermal conductivity, and the thermal power are calculated at finite temperature. The results reveal the key feature of Dirac fermion on a honeycomb lattice, which differs from that of casual fermion.

**Presenter: Nguyen Thi Hai Yen**

P.23 – Poster, NCTP-40

## Higgs sector of 3-3-1 model with three lepton singlets

*Hoang Ngoc Long (1), Bui Hong Nhung (1), Duong Van Loi (2), Vo Quoc Phong (4)*

*(1) Institute of Physics, Vietnam Academy of Science and Technology; (2) Physics Division, Mathematics-Physics-Informatics faculty, Tay Bac University, SonLa, Vietnam; (3) Department of Theoretical Physics, Ho Chi Minh City University of Science, Vietnam*

The most general scalar sector of the 3-3-1 model with three lepton singlets, where one scalar carrying lepton number 2 has a vacuum expectation value (VEV)  $n_2$ , is considered. We show that the new VEV  $n_2$  leads to new constraint among Higgs self-coupling constants. The Higgs sector contains 6 massless fields: two in the charged sector, three in pseudoscalar sector and one/three in neutral scalar sector. This number is enough for massive gauge bosons.

**Presenter: Duong Van Loi**

P.24 – Poster, NCTP-40

## Mott transitions in the ionic Hubbard model on a honeycomb lattice

*N. T. Hương, L. D. Ánh, N. T. H. Yên, H. A. Tuấn*

*Institute of Physics*

We study a two-dimensional ionic Hubbard model on a honeycomb lattice as a simple basis for describing the electronic structure of silicone in the presence of an electric field induced by the substrate. The local lattice Green function of the model is obtained within the coherent potential approximation. Two transitions from the band insulator via a metallic state to a Mott insulator are found with increasing  $U$ . The values of the critical correlation-driven metal-insulator transitions are estimated. Results of the calculated charge density wave and double occupation reveal the nature of the two transitions .

**Presenter: Nguyễn Thị Hương**

P.25 – Poster, NCTP-40

## Unified Spinor Fields in Space-time with Extradimensions

*Dao Vong Duc (1), Nguyen Mong Giao (2), and Tran Thanh Dung (3)*

(1) *Institute of Physics, VAST*; (2) *Hung Vuong University*; (3) *Thu Dau Mot University*

This work is based on the results recently published /D.V.Duc, N.M.Giao, T.T.Dung, J. Phys. Sci. Appl. (USA), vol.4, p.60 (2014); Intern. J. Theor. Phys. vol.54, p.1071 (2015)/. The mass spectrum for spinor fields is considered within the framework of the mass creation mechanism proposed in our previous works. It is shown that a single spinor field in the whole multidimensional space-time corresponds to a set of multiplets of effective spinor fields in ordinary 4-dimensional space-time with the masses obeying the sum rule expressed in terms of metric for extradimensions and parameter functions dictated by the periodicity conditions. The existence of spinor tachyons having negative square mass is also predicted, it is closely related to the presence of time-like extradimensions.

**Presenter: Dao Vong Duc**

P.26 – Poster, NCTP-40

**Effect of scattering from potential-barrier roughness on the linewidth of intersubband optical absorption in symmetric rectangular quantum wells: Non-local representation for scattering form factors**

*Huynh Ngoc Toan (1) Nguyen Thanh Tien (2)*

(1) *Đại học Duy Tân, K7/25 Quang Trung, Đà Nẵng, Việt Nam* (2) *Đại học Khoa học, Đại học Cần Thơ, đường 3/2, Cần Thơ, Việt Nam*

We develop a theory for study of the effect due to scattering from barrier roughness (BR), i.e., interface roughness-induced fluctuations in the potential-barrier position on the intersubband optical absorption linewidth in actual rectangular quantum wells (RQWs). In difference from the previous theory, within the wave-function-based approach to BR scattering, we derived properly a formula for the form factors for the scattering in terms of non-local quantities (integrals) of the envelope wave functions involved in intersubband transition. We found that for flat-band symmetric RQWs, the normal subband-energy-based approach and the wave-function-based approach with the non-local representation give the equal BR form factors. However, this non-local representation must be applied for the analysis of intersubband absorption in bent-band and/or asymmetric RQWs.

**Presenter: Toan Ngoc Huynh**

P.27 – Poster, NCTP-40

**Phonon-scattering-limited electron mobilities in zincblende and wurtzite AlGa<sub>N</sub>/Ga<sub>N</sub> quantum-well heterostructures.**

*Vo Van Tai (1), Nguyen Quoc Khanh (2)*

(1) *College of Technology and Industrial Management (CTIM)*. (2) *University of Science Ho Chi Minh City*.

We present calculations of phonon scattering in zincblende (ZB) and wurtzite (WZ) AlGa<sub>N</sub>/Ga<sub>N</sub> quantum-well heterostructures. In the Block-Gruneissen (BG) and equipartition (EP) regimes, we take into account many-body effects. Dependences of the mobility on the temperature and the electron density for both ZB and WZ Ga<sub>N</sub> are presented, and it is shown that the WZ mobility is higher than the ZB mobility.

**Presenter: Võ Văn Tài**

P.28 – Poster, NCTP-40

## EFFECT OF TEMPERATURE ON ELECTRON EFFECTIVE MASS AND BAND-GAP IN SEMICONDUCTOR CARBON NANOTUBES

*Le Van Tan and Cao Huy Thien*

*Ho Chi Minh City Institute of Physics Vietnam Academy of Science and Technology*

The effect of temperature on the self-energy of electron in semiconductor carbon nanotubes are studied by Matsubara Green function approach. Numerical results show a large influence of the temperature and electron density on the band-gap and electron effective mass in semiconductor carbon nanotube

**Presenter: Tan Van Le**

P.29 – Poster, NCTP-40

## Surface optical phonon-assisted cyclotron resonance in graphene on a h-BN substrate

*Huynh Vinh Phuc (1), Luong Van Tung (1), Le Dinh (2)*

*(1) Dong Thap University, Dong Thap, Viet Nam (2) College of Education, Hue University, Hue, Viet Nam*

In this work, the influence of surface optical (SO) phonons on the phonon-assisted cyclotron resonance (PACR) effect has been theoretically studied in a single-layer graphene on h-BN substrates via both one and two-photon absorption processes. The two-photon absorption process gives a significant contribution to magneto-optical absorption coefficient (MOAC) compared to one-photon process. The shifts of the absorption peaks are larger for h-BN substrate than those in graphene on nonpolar substrates, where only the intrinsic optical phonons of graphene contribute. Effects of temperature, graphene-substrate separation, and magnetic field on the MOAC and the half width are discussed. Our results show that the h-BN substrate strongly influence on the magneto-optical absorption spectra not only in the magnitude but also in the position of the resonant peaks due to electron-SO phonon scattering.

**Presenter: Huynh Vinh Phuc**

P.30 – Poster, NCTP-40

## Temperature dependence of electron-hole pair condensation driven by exciton-phonon interaction

*Do Thi Hong Hai (1), Nguyen Thi Giang (2), Nguyen Huu Nha (3), Phan Van Nham (4).*

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A stability of the electron-hole pair condensation at low temperature has been addressed by involving the coupling of exciton to vibrational degrees of freedom in two-dimensional two-band  $f - c$  electron system. By mean of the unrestricted Hartree-Fock approximation, we find a formation of the insulating state typifying an excitonic condensate accompanied by a finite lattice distortion if the exciton-phonon coupling is large enough. As functions of temperature

both excitonic condensation order parameter and lattice distortion behave in a same way which manifests the continuous transition in analogy to the superconductivity in the BCS theory. Inspecting to the microscopic properties in momentum space we strongly specify the BCS type of the excitonic condensation driven by the exciton-phonon interaction at low temperature.

**Presenter: Do Thi Hong Hai**

P.31 – Poster, NCTP-40

### **Effects of pairing reentrance on the inverse nuclear level density parameter of hot rotating nuclei**

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Angular momentum dependence of the inverse level density parameter  $K$  in the excitation-energy region of about 30 – 40 MeV is studied within the finite-temperature Bardeen-Cooper-Schrieffer (FTBCS) theory that takes into account the noncollective rotation of the nucleus at nonzero values of  $z$ -projection  $M$  of the total angular momentum. The comparison between the results obtained within the FTBCS as well as the case without pairing correlations and the experimental data for several medium-mass nuclei such as  $^{108}\text{Cd}$ ,  $^{109}\text{In}$ ,  $^{112}\text{Sn}$ ,  $^{113}\text{Sb}$ ,  $^{122}\text{Te}$ ,  $^{123}\text{I}$ ,  $^{127}\text{Cs}$ , shows that by including the pairing corrections the FTBCS reproduces quite well all experimental data, whereas the non-pairing case overestimates the data. As the result, within the FTBCS, there appears an effect that pairing correlations is first small at a given value of angular momentum  $M$ , which is close to its critical value  $MC$ , where pairing is completely disappeared, and zero temperature ( $T = 0$ ), increases with increasing  $T$ , and then decreases to vanish at high  $T$ . This effect is called the pairing reentrance.

**Presenter: Le Thi Quynh Huong**

P.32 – Poster, NCTP-40

### **Surface Properties of TiO<sub>2</sub> from Self-Consistent-Charge Density Functional Tight Binding**

*Huynh Anh Huy (1), Vien Tuan Anh (1), Nguyen Vy Khuong (1), Le Thi Cam Loan (2)*

*(1) Can Tho University, (2) Tra Vinh University*

Anatase and rutile TiO<sub>2</sub> surfaces have been investigated with a computationally efficient semiempirical tight binding method: self-consistent-charge density functional tight binding (SCC-DFTB). SCC-DFTB predicts a band gap of anatase TiO<sub>2</sub> surface of 2.3 eV comparing with one of rutile TiO<sub>2</sub> surface of 1.9 eV. The OH group has been found when hydrogen adsorbed on the anatase (001) surface and water molecules on rutile (110) surface.

**Presenter: Viên Tuấn Anh**

P.33 – Poster, NCTP-40

### **Dynamics Simulation of Backward Diffusion Based on Random Walk Theory**

*Vu Ba Dung and Bui Huu Nguyen*

*Ha Noi University of Mining and Geology - Duc Thang ward, Bac Tu Liem district, Hanoi, Vietnam*

Some results of diffusion study in silicon showed that diffusion of the self-interstitial and vacancy could be backward diffusion and their diffusivity could be negative [1]. The backward diffusion process and negative diffusivity is contrary to the fundamental laws of diffusion such as Fick's law and Onsager's law, namely the diffusive flux of backward diffusion goes from regions of low concentration to regions of high concentration. Backward diffusion could be explained that the thermal velocity of molecules in low concentration is greater than two times. Moreover, based on the thermodynamics and random walk theory the backward diffusion process are be simulated. Results of simulation is corresponding to theory. They also showed that when thermal velocity of molecules in low concentration area is greater than two times in high concentration area, the backward diffusion is occurred.

**Presenter: Bui Huu Nguyen**

P.34 – Poster, NCTP-40

### **Connection between q-deformed harmonic oscillator and aharmonic symmetric aharmonic potential**

*Ngo Gia Vinh (1), Man Van Ngu (2), Nguyen Tri Lan (3), Luu Thi Kim Thanh (4), Nguyen Ai Viet (3)*

*(1) Bac Ninh Department of Education and TrainingHung; (2) Yen Industrial Colleague; (3) Institute of Physics, 10 Dao Tan, Ba-Dinh, Hanoi; (4) Hanoi Pedagogical University No. 2*

In our previous article, the connection between q-deformed harmonic oscillator and Morse-like asymmetric potential is investigated. In this work we explore a possibility of a connection between q-deformed harmonic oscillator and aharmonic symmetric potential. For simplicity we take the inverse square cosine form of potential. The relation between the deformation parameter q and the set of parameters of aharmonic symmetric potential was found. The corresponding of two types of connections between q-deformed harmonic oscillator with asymmetric and symmetric potentials are discussed.

**Presenter: Ngô Gia Vịnh**

P.35 – Poster, NCTP-40

### **Second quantization model for surface plasmon polariton for spherical shape of metallic nano particles**

*Can Thi Thuy Thuy (1), Dao Thi Thuy Nga (2). Chu Thuy Anh (1), Dao Thu Ha (1), Tran Thi Thanh Van (1), Nguyen Ai Viet (Belarus) (1)*

*(1) Institute of Physics, 10 Dao Tan, Ba-Dinh, Hanoi; (2)Bac Ninh Department of Education and Training;*

It is well known that surface plasmon polaritons exhibit both wave and particle properties. Like photons, the second quantization formalism can be established for surface plasmon polaritons. The case of planar geometry with Kretschmann configuration of excitation surface plasmon was studied in our previous article. In this work we continue to investigate surface plasmon polariton modes in a spherical metal nano particle. A model effective Hamiltonian with interaction parameters is proposed in second quantization representation for system of surface plasmons and photon. Using the Bogoliubov transformation technique, the dispersion relations of surface



plasmon polariton were calculated. The surface plasmon – photon vertexes also are found for spherical geometry. The conditions for excitation surface plasmon of the cases of spherical and planar geometries were compared, and a possible existence of Plasmon radiation modes is also discussed.

**Presenter: Đào Thị Thúy Nga**

P.36 – Poster, NCTP-40

### **Cooper pair of superconductivity in the coordinate representation and q-deform harmonic oscillator**

*Man Van Ngu (1), N.G. Vinh (2), Nguyen. T. Lan (3), L.T.K. Thanh (4), and N.A. Viet(3)*

*(1) Hung Yen Industrial College; (2) Bac Ninh Department of Education and Training; (3) Institute of Physics, 10 Dao Tan, Ba-Dinh, Hanoi; (4) Hanoi Pedagogical University No. 2*

In this work we study the similarity between the wave functions of q-deformed harmonic oscillator and wave functions of Cooper pair. The wave functions of Cooper pairs in coordinate-space have an “onion-like” layered structure with exponent decay (Boltzmann) envelope modulation. The ground state wave function of q-deform harmonic oscillator has the form of oscillate functions with Gaussian decay envelope modulation. The corresponding between Boltzmann and Gaussian forms of envelope functions and their quantum similarity are discussed.

**Presenter: Man Van Ngu**

P.37 – Poster, NCTP-40

### **Influence of phonon confinement on the optically detected magnetophonon resonance line-width in parabolic quantum wells**

*Vo Thanh Lam (1), Nguyen Dinh Hien (2), Tran Cong Phong (3)*

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We investigate the influence of phonon confinement on the optically detected magneto-phonon resonance (ODMPR) effect and ODMPR line-width in parabolic quantum wells (PQW). The ODMPR conditions as functions of the confinement frequency of PQW and the photon energy are also obtained. The shifts of ODMPR peaks caused by the confined phonon are discussed. The numerical result for the quantum well shows that in the two cases of confined and bulk phonons, the line-width (LW) increases with increasing both confinement frequency and temperature. Furthermore, in the large range of the confinement frequency, the influence of phonon confinement plays an important role and cannot be neglected in reaching the ODMPR linewidth

**Presenter: Tran Cong Phong**

P.38 – Poster, NCTP-40

### **High-pressure thermodynamic properties of $\epsilon$ -Fe**

*Ho Khac Hieu (1), Phan Thi Thanh Hong (2), Nguyen Ngoc Ha (1)*

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*versity No 2., Xuan Hoa, Vinhphuc, Vietnam*

$\epsilon$ -Fe is a hexagonal close-packed phase of iron which is stable only at very high pressure. In this work, we studied the thermodynamic properties of  $\epsilon$ -Fe under high pressure by using the empirical method. The expressions of high-pressure melting temperature, Gruneisen parameter, Debye frequency and Debye temperature have been derived analytically. Numerical calculations have been performed for  $\epsilon$ -Fe up to pressure 100 GPa. Our results are compared with those of shock-compression and static-compression X-ray diffraction experiments as well as previous calculations showing the good agreements.

**Presenter: Ho Khac Hieu**

P.39 – Poster, NCTP-40

### **Nonclassical properties and entanglement of even and odd nonlinear charge coherent states**

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*(1) Center for Theoretical and Computational Physics, College of Education, Hue University, 32 Le Loi, Hue City (2) University of Transport and Communications, Campus 2, 450 Le Van Viet, 9 District, Ho Chi Minh City*

We study the higher-order nonclassical properties and the intermodal entanglement of the even and odd nonlinear charge coherent states. We derive the analytic expressions of the higher-order antibunching, higher-order squeezing and higher-order entanglement. We show that these states exhibit antibunching to all orders and the antibunching exists depending on the variables, especially on the nonlinear functions. We also show that in such states, the higher-order squeezing appears only in the even orders and the degree of squeezing depends on the nonlinear functions. Furthermore, it is proved that these states are two-mode entangled.

**Presenter: Truong Minh Duc**

P.40 – Poster, NCTP-40

### **Second quantization model for surface plasmon polariton in metallic nano wires**

*Nguyen Thi Phuong Lan (1), Dao Thi Thuy Nga (2), Do Thi Nga (3), Nguyen Ai Viet (3)*

*(1) Hanoi Pedagogical University 2; (2) BacNinh department of Education and training; (3) Institute of Physics, VAST*

A model of effective Hamiltonian is proposed in second quantization representation for system of surface plasmons and photon (polariton) in metallic nano wires. The dispersion relation curves of surface plasmon polariton was calculated by mean the Bogoliubov diagonalization method. The surface plasmon – photon vertexes are considered. The conditions for excitation surface plasmon, existence plasmon radiate modes, and a possible application of metallic nano wires also discussed.

**Presenter: Nguyen Thi Phuong Lan**

P.41 – Poster, NCTP-40

### **NOISE REDUCTION IN RAMAN RING LASER BY TWO-TELEGRAPH PREGAUSSIAN PUMP**

*Doan Quoc Khoa (1), Cao Long Van (2,3), Le Huu Vuong (4)*

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We consider Raman Ring Laser (RRL) by modeling the laser pump light by a classical time-dependent random process, namely a pregaussian process introduced by Wódkiewicz and his coworkers. It is composed of a finite number of independent so-called telegraphs. The strength of the pregaussian formalism derives from the exact solubility of wide classes of the stochastic equations. Even in the case of one random telegraph signal one can obtain several interesting results. In particular we also observed the so-called noise reduction in RRL: the Stokes output of this laser tends to stabilize under the influence of the broad-band one-telegraph pregaussian pump as it has been discovered sometimes ago for the chaotic pump Gaussian noise. In this communication, we will extend our model to the case of two-telegraph pregaussian noise. We will compare obtained results with that obtained previously. It will be shown that new results tend to the results for the case of Gaussian chaotic noise.

**Presenter: Doan Quoc Khoa**

P.42 – Poster, NCTP-40

### **One loop corrections to decay $\tau \rightarrow \mu\gamma$ in the economical 3-3-1 model**

*T.T. THUC (1), D.P. KHOI (2), L. T. HUE (3) AND N.T. PHONG (4)*

*(1) Truong THPT Phu Hung (2) Vinh University (3) Institute of Physics (4) Cantho University*

Lepton flavor violating (cLFV) decays of charged leptons such as  $\tau \rightarrow \mu\gamma$ ,  $\tau \rightarrow e\gamma$ ,  $\mu \rightarrow e\gamma, \dots$ , are now the subjects of experiments as signals of new Physics beyond the Standard Model (SM). In the limit of the unitary gauge, we prove that contributions from one loop corrections to the above decays are very small in the framework of the economical 3-3-1 model.

**Presenter: Thuc Trong Truong**

P.43 – Poster, NCTP-40

### **The muon anomalous magnetic moment in the supersymmetric economical 3-3-1 model**

*D. T. Binh, D. T. Huong, H. N. Long, K. H. Viet*

*Institute of Physics, Vietnam Academy of Science and Technology. Thai Nguyen University*

We investigate the muon anomalous magnetic moment in the context of the supersymmetric version of the economical 3-3-1 model. We compute the 1-loop contribution of super-partner particles. We show that the contribution of superparticle loops become significant when  $\tan \gamma$  is large. We investigate for both small and large values of  $\tan \gamma$ . We find the region of the parameter space where the slepton masses are of a few hundreds GeV is favoured by the muon  $g - 2$  for small  $\tan \gamma$  ( $\tan \gamma \sim 5$ ). Numerical estimation gives the mass of supersymmetric particle, the mass of gauginos  $m_G \sim 700$  GeV and light slepton mass  $m_{\tilde{L}}$  is of order  $\mathcal{O}(100)$  GeV. When  $\tan \gamma$  is large ( $\tan \gamma \sim 60$ ), the mass of charged slepton  $m_{\tilde{L}}$  and the mass of gauginos  $m_G \sim \mathcal{O}(1)$  TeV while the mass of sneutrino  $\sim 450$  GeV is in the reach of LHC.

**Presenter: Dinh T Binh**

P.44 – Poster, NCTP-40

### **Study of magnetic properties in core/shell Fe98B2 nanoparticle**

*Nhan N.T(1), Ngan D.T.T(1,2), Ha N. T. T(1)*

*(1) Hanoi University of Science and Technology (2) Vietnam National University, Hanoi*

Core/shell Fe98B2 nanoparticle has been constructed by molecular dynamics with pair Pak-Doyama potential under free boundary condition. The core/shell Fe98B2 nanoparticles with different crystallized fractions were prepared by annealing from amorphous core/shell nanoparticle sample. The magnetic properties as magnetization moment, energy, heat capacity and magnetic susceptibility have been investigated by Ising model show the dependence of magnetic behaviors on shell thickness, on exchange interaction.

**Presenter: Nguyen Thu Nhan**

P.45 – Poster, NCTP-40

### **Nonlocal correaltions in a correlated Chern insulator**

*Nguyen Hong-Son and Tran Minh-Tien*

*Department of Occupational Safety and Health, Trade Union University, 169 Tay Son, Hanoi, Vietnam, and Institute of Physics, Vietnam Academy of Science and Technology, 10 Dao Tan, Hanoi, Vietnam*

Effect of nonlocal correlations in a correlated Chern insulator is investigated within the cellular dynamical mean-field theory. The correlated Chern insulator is described by the Haldane model and the electron correlations are incorporated by introducing the local interaction between the itinerant electrons and localized fermions. In the homogeneous phase, the electron correlations drive the itinerant electrons from the Chern topological insulator to a metallic phase, and then to a Mott nontopological insulator. Nonlocal correlations do not affect the phase transition qualitatively.

**Presenter: Nguyen Hong Son**

P.46 – Poster, NCTP-40

### **Effect of combined uniaxial – torsional strain on electronic properties of armchair graphene nanoribbons**

*Nguyen Ngoc Hieu (a), Le Cong Nhan (b)*

*(a) Institute of Research and Development, Duy Tan University, Vietnam (b) Department of Environmental Sciences, Saigon University, Vietnam*

In the present work, we study the effect of the combined uniaxial – torsional strain on electronic properties of armchair graphene nanoribbons by using the tight-binding approximation. Our calculations show that under the combined uniaxial – torsional strain, the semiconductor-metal-semiconductor transition occurs in 8-AGNR. In addition, we can control the band gap of the armchair graphene nanoribbon by its strain. The sensitivity of nanoribbon band gap due to the combined strain makes nanoribbon becoming a promising component for applications in nanoelectromechanical devices.

**Presenter: Nguyen Ngoc Hieu**

P.47 – Poster, NCTP-40

### **Molecular dynamics simulation of the mechanical properties of CrN/AlBN/CrN systems**

*Nguyen Thi Trang, Le Van Vinh, Pham Khac Hung*

*Ha noi University of Sciences and Technology*

Abstract: We presented the simulation of CrN/AlBN/CrN multilayered systems with different structures of AlBN layer. The elastic and plastic properties of these materials were investigated by applying uniaxial deformation. The simulation results confirmed that the fraction of hexagonal crystal AlBN embedded in an amorphous AlBN and the thickness of AlBN layer influence significantly on the mechanical behavior of CrN/AlBN/CrN systems. Keywords: Molecular dynamics simulation, CrN/AlBN/CrN systems, mechanical properties.

**Presenter: Nguyen Thi Trang**

P.48 – Poster, NCTP-40

### **Controlled joint remote preparation of an arbitrary two-qubit state via non-maximally entangled quantum channels**

*Cao Thi Bich (1), Nguyen Van Hop (2) and Nguyen Ba An (1)*

*(1) Center for Theoretical Physics, Institute of Physics, 10 Dao Tan, Hanoi (2) Physics Department, Hanoi University of Education No. 1, 136 Xuan Thuy, Hanoi*

Remote preparation of quantum states only by means of local operation and classical communication is highly favorable for global quantum information processing and distributed quantum computation. Because security is the most highlighted issue remote state preparation was extended to joint remote state preparation whose security can be further enhanced by adding a third powerful party, a controller, who reserves the right to push the "launch button" for an intended task. This is called joint remote state preparation under control or controlled joint remote state preparation. Here we consider preparation of a general two-qubit state using nonmaximally entangled quantum channels in the forms of (i) two four-qubit states, (ii) one four-qubit state plus one three-qubit GHZ state and (iii) a single seven-qubit state. We design schemes to generate all the three types of the quantum channel whose parameters are on-purpose given to the controller (not to the receiver as in most previous protocols) so that only he/she is able to correctly manage the operation on his/her qubits. By arranging the preparers to follow the adaptive measurement strategy all our three protocols succeed deterministically.

**Presenter: Nguyen Van Hop**

P.49 – Poster, NCTP-40

### **Mott transition in the asymmetric Hubbard model at half-filling: Equation of motion approach**

*Tran Thi Thu Trang (1), Le Duc Anh (2), Hoang Anh Tuan (3)*

*(1) Ha Long University; (2) Ha Noi National University of Education (3) Institute of Physics, VAST*

We investigate the Mott metal-insulator transition in the asymmetric Hubbard model, which may describe the ground state of fermionic atoms trapped in optical lattice. We use the dynamical mean field theory and the equation of motion approach to calculate the density of states at the

Fermi level and the double occupation for various values of on-site interaction  $U$  and hopping asymmetry  $r$ . The critical interaction is also obtained as a function of hopping asymmetry. Our results are in good agreement with the ones obtained by the full dynamical mean field theory using exact diagonalization and quantum Monte Carlo techniques.

**Presenter: Tran Thi Thu Trang**

P.50 – Poster, NCTP-40

### **THE INFLUENCE OF SPIN POLARIZABILITY AND THE TEMPERATURE ON THE COMPRESSIBILITY IN THE SEMICONDUCTOR QUANTUM WELL-WIRES**

*Le Van Tan and Cao Huy Thien*

*Ho Chi Minh City Institute of Physics Vietnam Academy of Science and Technology*

We formulated for the inverse compressibility of spin up and down electrons as a function of spin polarizability, temperature and carrier's density in the parabol lateral barrier quantum well-wires. Numerical calculations are performed for different sizes of GaAs quantum well-wires.

**Presenter: Tan Van Le**

P.51 – Poster, NCTP-40

### **Dependence of the Hall Coefficient on a length of rectangular quantum wires with infinitely high potential under the influence of a Laser Radiation**

*Nguyen Thu Huong (1), Dao Manh Hung (1), Nguyen Quang Bau (2), Le Thai Hung (3)*

*(1)Academy of Air Defense and Air Force , Son Tay, Hanoi, Vietnam (2)Faculty of Physics, Hanoi University of Sciences, Vietnam National University 334 - Nguyen Trai, Thanh Xuan, Hanoi, Viet Nam (3) Hanoi National University of Education, Hanoi*

The Hall coefficient is theoretically studied in a rectangular quantum wires with infinitely high potential subjected to a crossed dc electric field and magnetic field in the presence of a high frequency electromagnetic wave (EMW). By using the quantum kinetic equation for electrons interacting with optical phonons, analytical expressions for the conductivity tensor as well as the Hall coefficient in a rectangular quantum wires is obtained. The results are numerically evaluated and graphed for GaAs/GaAsAl rectangular quantum wire to show clearly the dependence of Hall coefficient (HC) on a length rectangular quantum wires with different temperature values. We can see the length of the small increase in the value domain Hall coefficient increased, further increasing the length of the Hall coefficient continues to increase and reaches a constant value.

**Presenter: Nguyen Thu Huong**

P.52 – Poster, NCTP-40

### **Ginzburg-Landau functional for three-order parameter problem**

*Nguyen Van Hinh (1, 2) and Nguyen Tri Lan (2)*

*(1) Faculty of Fundamental Science, Ha Noi University of Industry, Minh Khai, Bac Tu Liem, HaNoi (2) Institute of Physics, Vietnam Academy of Science and Technology, 10 Dao Tan, Ba Dinh, Hanoi*

A model is presented utilizing a generic Hamiltonian with equal pairings in channels based on

quantum field theory and functional integral formalism, to show the correlation among the order parameters which are described in multi-component Ginzburg-Landau functional. In the vicinity of the phase transition, the further perturbative expansions of the functional around the mean-field theory in the auxiliary fields are carried out with the aim of leading to a possible solution for the coexistence of many phases. The work is motivated by the recent theoretical researches and experimental evidences of the coexistence of superconductivity and ferromagnetism in U and Ce compounds.

**Presenter: Nguyen Van Hinh**

P.53 – Poster, NCTP-40

### **New-physics effects in the 3-3-1-1 model**

*D. V. Loi, N. T. Thuy, H. T. Hung, D. T. Huong, and P. V. Dong*

*Institute of Physics, Vietnam Academy of Science and Technology*

We give a brief review of the 3-3-1-1 model. The new physics results such as neutrino masses, dark matter, leptogenesis, and inflation are subsequently investigated. The CPT symmetry, CKM unitarity, FCNCs, and LEP-II searches are also discussed.

**Presenter: Duong Van Loi**

P.54 – Poster, NCTP-40

### **Critical behavior near the Mott transition in the half-filled asymmetric Hubbard model**

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

*(1) Institute of Physics - VAST (2) Hanoi National University of Education*

We study the half-filled asymmetric Hubbard model within the two-site dynamical mean field theory. At zero temperature, explicit expressions of the critical interaction  $U_c$  for the Mott transition and the local self-energy are analytically derived. Critical behavior of the quasi-particle weights and the double occupancy is also obtained analytically as functions of the on-site interaction  $U$  and the hopping asymmetry  $r$ . Our results are in good agreement with the ones obtained by much more sophisticated theory.

**Presenter: Hoang Anh - Tuan**

P.55 – Poster, NCTP-40

### **On the applications of non extensive statistical mechanics to studying ecological diversity**

*Le Van Xuan (1), Nguyen Tri Lan (2) and Nguyen Ai Viet (2)*

*(1) Hanoi College of Technology and Economy, Dong Xuan, Soc Son, Ha Noi, Viet Nam (2) Institute of Physics, Vietnam Academy of Science and Technology, 10 Dao Tan, Ha Noi, Viet Nam*

Several indices have been proposed to estimate diversity, and the most well-known are the Shannon-Wiener ( $H$ ) and Simpson ( $D$ ) indices along with the number of species ( $S$ ) and evenness ( $E$ ). It is not clear which index is more effectively applicable in a certain context. However, a non extensive entropy (Tsallis entropy) has probably potential to explore insights of these problems.

In this work, a family of diversity indices ( $S_q$  where  $q$  is the Tsallis index) and evenness ( $E_q$ ), based on Tsallis entropy that incorporates the most used indices is explored. In addition, the ecological properties of  $E_q$  and  $S_q$  are also discussed.

**Presenter: Le Van Xuan**

P.56 – Poster, NCTP-40

### CONTROLLED TELEPORTATION WITH PARTIALLY ENTANGLED QUANTUM CHANNEL: DETERMINISM AND POWER OF THE CONTROLLER

*Nguyen Van Hop (1), Cao Thi Bich (2), and Nguyen Ba An (2)*

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Nonlocal correlation inherent in entangled channel enables transmission of quantum states between two remote locations without actually carrying the states through space. This process is named teleportation which always succeeds if the channel is maximally entangled. This work studies controlled teleportation (i.e., teleportation under supervision of a controller) of a general two-qubit state via a quantum channel of the form  $|Q\rangle_{1233'45} = \sum_{m=0}^1 \sum_{n=0}^1 x_{mn} |B_{mn}\rangle_{12} |m, n\rangle_{33'} \otimes |B_{00}\rangle_{45}$ , where  $\sum_{m=0}^1 \sum_{n=0}^1 |x_{mn}|^2 = 1$  and  $|B_{mn}\rangle_{12} = \sum_{j=0}^1 (-1)^{mj} |j, j \oplus n\rangle_{12}$ , while qubits 1 and 4, 2 and 5 and 3 and 3' belong to the sender, the receiver and the controller, respectively. We show in detail that, not only for  $|x_{mn}| = 1/2$  but even for  $|x_{mn}| \neq 1/2$  (i.e.,  $|Q\rangle_{1233'45}$  is not maximally entangled), any unknown two-qubit state can be teleported deterministically (i.e., with unit success probability). We also prove that if  $|x_{00}| \geq 1/2$  then the teleported state's average fidelity  $F_{av}$  obtained without the controller's cooperation is not smaller than the classical fidelity  $F_{cl} = 2/5$ . Therefore, in order for the controller to play a useful role  $|x_{00}|$  should be chosen less than  $1/2$  and the smaller  $|x_{00}|$  the more powerful the controller.

**Presenter: Nguyen Van Hop**

P.57 – Poster, NCTP-40

### Production and decay of radion and Higgs boson $h_0$ in Randall - Sundrum model

*Bui Thi Ha Giang (1), Dao Thi Le Thuy (1), Dang Van Soa (2)*

*(1) Hanoi University of Education (2) Hanoi Metropolitan University*

We get to analyse the production and decay of the scalar sector of the Randall - Sundrum model. The mixture of the original Higgs and radion causes the interesting physical results. Consequently, we turn to our main focus: both the production of radion and  $h_0$  in the  $\phi/h$  propagator in  $f^+f^-$  collision and the scalar particles' main decay channels.

Keywords : Radion, Higgs boson, decay channel.

**Presenter: Bui Thi Ha Giang**

P.58 – Poster, NCTP-40

### Hypercharge Y and gauge couplings in 3-3-1 models with $\beta$ arbitrary

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*Phuc; (2) Xuan Hoa high school, Xuan Hoa, Phuc Yen, Vinh Phuc.*

Recently, 3-3-1 models as the extension of the standard model were get many success. Depending on the value of  $\beta$  that we obtained the various versions of the 3-3-1 model. In this work, we research 3-3-1 model with  $\beta$  arbitrary and give conditions for spontaneous symmetry breaking which transform  $SU(3)_C \otimes SU(3)_L \otimes U(1)_X$  gauge group to  $SU(3)_C \otimes SU(2)_L \otimes U(1)_Y$  of the standard model. Also, after this stage of spontaneous symmetry breaking, hypercharge Y and gauge couplings are given. This result is generalized to the 3-3-1 models.

**Presenter: Ha Thanh Hung**

P.59 – Poster, NCTP-40

### **Sphaleron electroweak phase transition in the economical 3-3-1 Model**

*Vo Quoc Phong (1), Hoang Ngoc Long (2), Vo Thanh Van (1), Tran Thi Ai Nhi (1)*

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We calculate the electroweak sphaleron rates in the Economical 3-3-1 (E331) model. In the context of the early Universe, this model undergoes a sequence of two first-order phase transitions,  $SU(3) \rightarrow SU(2)$  at the TeV scale and  $SU(2) \rightarrow U(1)$  at the 100 GeV scale, as the Universe cools down from the hot big bang. By a thin-wall approximation, we show that for each phase transition in this sequence, the sphaleron rate is larger than the cosmological expansion rate at temperatures higher than the critical temperature, and after the phase transition, the sphaleron process is decoupled. This may provide baryon-number violation (B violation) necessary for baryogenesis in the relationship with nonequilibrium physics in the early Universe.

**Presenter: Vo Quoc Phong**

P.60 – Poster, NCTP-40

### **Hawking radiation and black hole evaporation**

*Nguyen Hoang Vu*

*Institutue of physics, Vietnam Academy of Sciences and Technology, Hanoi, Vietnam*

The Hawking radiation is one of the interesting effect of the theoretical physics. Black holes can radiate and evapor by the quantum effect. By the methods of quantum field theory in curved space time and thermodynamics, we will find temperature, entropy, life time of black holes, and the character of Hawking radiation.

**Presenter: Nguyen Hoang Vu**

P.61 – Poster, NCTP-40

### **The ab-plane complex conductivity in type-II superconductor**

*Bui Duc Tinh (1), Nguyen Quang Hoc (1), Nguyen Duc Hien (2)*

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In this paper we use the time-dependent Ginzburg-Landau to calculate ab-plane complex fluctuation conductivity in type-II superconductor in 3D model under magnetic field. We assume

that thermal fluctuations are strong enough to melt the Abrikosov vortex lattice by the magnetic field into a vibrating vortex liquid. The nonlinear interaction term in the time dependent Ginzburg-Landau is treated within self-consistent Gaussian approximation. An additional assumption often made in analytical calculations that only the lowest Landau level significantly contributes to physical quantities of interest in the high-field limit is lifted by including all the Landau levels. We obtain expression for the ab-plane complex conductivity summing all Landau levels which are applicable essentially to whole liquid phase and is compared to experimental data on high-Tc superconductor  $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$ . Keywords: Complex conductivity; Type-II superconductor

**Presenter: Nguyễn Đức Hiền**

P.62 – Poster, NCTP-40

### **The Radioelectric effect in doped superlattices under the influence of confined phonon**

*Nguyen Quang Bau(\*), Dao Thu Hang and Do Tuan Long*

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The Radioelectric effect in doped superlattice under the influence of confined phonon has been theoretically studied. The analytical expression for the Radioelectric field is obtained by using quantum kinetic equation method. The theoretical expression shows that the Radioelectric field in doped superlattice depends on the frequencies and amplitudes of the laser and the linearly polarized electromagnetic wave, the period of the superlattice and especially the quantum number  $m$  characterizing the phonon confinement. Numerical calculation is also applied for n-GaAs/p-GaAs doped superlattice. It is found that the Radioelectric field has multiple resonance peaks and increases as the increasing of quantum number  $m$ . All results are compared with those in normal bulk semiconductor as well as those in two dimensional systems when phonons are unconfined to show the differences.

**Presenter: Nguyen Quang Bau**

P.63 – Poster, NCTP-40

### **Quasi-bound states in circular graphene quantum dots**

*Nhung T. T. Nguyen (1), D. Quang To (1), and H. Chau Nguyen (2)*

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We study quasi-bound states of Dirac electrons in circular graphene quantum dots. We show that known results about the life-times of quasi-bound states in quantum dots modelled by one-step potentials can be derived in a comprehensive way. We then extend this study to investigate the effects of the slope of the confinement potential on the quasi-bound states. We found that while the energy levels stay roughly the same, the life-times of these quasi-bound states are strongly increased by the decreasing of the slope of the confinement potential. This is qualitatively in agreement with known results for one-dimensional confinement potential, which suggest that the life-time of quasi-bound states in two dimension can also be controlled by controlling the slope of the confinement potential.

**Presenter: To Duy Quang**

# Workshop Abstracts

I.1 – Invited, IWTCP-3

## Density Functional Theory and Fermi Surfaces

*Mukunda P. Das*

*Department of Theoretical Physics, RSPE, The Australian National University, Canberra, ACT 6201, Australia*

Density functional theory (DFT) is considered as the standard model for low energy physics by its great achievement in the field of condensed matter science. The theory is based on theorems by Hohenberg and Kohn that the ground state properties of an interacting many-body system can be described exactly by a functional of the one particle density. Unfortunately this functional remains unknown in the exact sense. However, a number of approximate functionals are used over the past several decades to a variety of condensed matter problems.

In this talk I shall describe ground state properties of metals by using the DFT. Particular attention will be paid to a special property of a metal, i.e. its Fermi surface. Generally it is believed by the DFT practitioners that the Fermi surface is a ground state property, therefore, DFT in its Kohn-Sham (local density version) is capable of producing a physical Fermi surface. In fact, there seems to be some controversy about this perception, where Fermi surface is not a-priori obviously a ground state property. I shall present some rigorous arguments towards the correct understanding of this predicament.

**Presenter: Mukunda P. Das**

I.2 – Invited, IWTCP-3

## Quantum field theory of interacting plasmon-photon-phonon system

*Nguyen Van Hieu*

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This work is devoted to the construction of the quantum field theory of the interacting system of plasmon, photon and phonons on the basis of general fundamental principles of electrodynamics and quantum field theory of many-body systems. Since plasmon is a quasiparticle appeared as a resonance in the collective oscillation of the interacting electron gas in solids, the starting point is the total action functional of the interacting system comprising electron gas, electromagnetic field and phonon fields. By means of the powerful functional integral technique, this original total action is transformed into that of the system of the quantum fields describing plasmons, transverse photons, acoustic as well as optic longitudinal and transverse phonons.

The collective oscillations of the electron gas is characterized by a real scalar field  $\phi(x)$  called

the collective oscillation field. This field is split into the static background field  $\phi_0(x)$  and the fluctuation field  $\zeta(x)$ . The longitudinal phonon fields  $\mathbf{Q}^{al}(x)$ ,  $\mathbf{Q}^{ol}(x)$  are also split into the background fields  $\mathbf{Q}_0^{al}(x)$ ,  $\mathbf{Q}_0^{ol}(x)$  and dynamical fields  $\mathbf{q}^{al}(x)$ ,  $\mathbf{q}^{ol}(x)$  while the transverse phonon fields  $\mathbf{Q}^{at}(x)$ ,  $\mathbf{Q}^{ot}(x)$  themselves are dynamical fields  $\mathbf{q}^{at}(x)$ ,  $\mathbf{q}^{ot}(x)$  without background fields.

After the canonical quantization procedure, the background fields  $\phi_0(x)$ ,  $\mathbf{Q}_0^{al}(x)$ ,  $\mathbf{Q}_0^{ol}(x)$  remain the classical fields, while the fluctuation fields  $\zeta(x)$  and dynamical phonon fields  $\mathbf{q}^{al}(x)$ ,  $\mathbf{q}^{ol}(x)$ ,  $\mathbf{q}^{at}(x)$ ,  $\mathbf{q}^{ot}(x)$  become quantum fields. In quantum theory, plasmon is the quantum of hermitian scalar field  $\sigma(x)$  called the plasmon field, longitudinal phonons as complex spinless quasiparticles are the quanta of the effective longitudinal phonon hermitian scalar fields  $\theta^a(x)$ ,  $\theta^0(x)$  while transverse phonons are the quanta of the original hermitian transverse phonon vector fields  $\mathbf{q}^{at}(x)$ ,  $\mathbf{q}^{ot}(x)$ . By means of the functional integral technique the original action functional of the interacting system comprising electron gas, electromagnetic field and phonon fields is transformed into the total action functional of the resultant system comprising plasmon scalar quantum field  $\sigma(x)$ , longitudinal phonon effective scalar quantum fields  $\theta^a(x)$ ,  $\theta^0(x)$  and transverse phonon vector quantum fields  $\mathbf{q}^{at}(x)$ ,  $\mathbf{q}^{ot}(x)$ .

**Presenter: Nguyen Van Hieu**

I.3 – Invited, IWTCP-3

### **A rigorous approach to the derivation of analytical potentials in physics-based coarse-grained force fields**

*Adam K. Sieradzan, Agnieszka G. Lipska and Adam Liwo\**

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Coarse-grained approaches, which implement simplified representations of molecules, are widely used in biomolecular simulations. These approaches offer a tremendous reduction of the cost of computations compared with the all-atom models. However, designing the functional forms of the coarse-grained energy terms poses a serious problem and these terms are very often imported from all-atom force fields or assigned on a heuristic basis. In such approaches at coarse-graining the multibody terms (which are necessary to generate regular structures [1]) are not considered and inadequate variables are often chosen to express the effective energy terms.

Based on statistical physics, the coarse-grained energy functions originate from the potentials of mean force (PMF), also termed restricted free-energy functions (RFE) of the systems under consideration, where the degrees of freedom that are not considered explicitly in the coarse-grained model (the so-called fine-grain degrees of freedom) are integrated out [1,2]. Expansion of the PMF into Kubo cluster-cumulant functions [3], termed factor expansion (FE) [1] or use of the force-matching (FM) method [2] enable us to split the PMF into specific terms. Additionally, approximate analytical formulas for the effective energy terms are possible to derive through generalized Kubo cumulant expansion [3] of the PMF factors.

In this work, the FE approach is pursued further to design a general method for the determination of the energy expressions in the coarse-grained force fields. The all-atom potential energy is expressed in terms of the squares of interatomic distances, which (and, thereby, also the energy) are then expanded into the Taylor series in the fine-grain degrees of freedom. By using the Kubo cumulant expansion of the factors [3] and averaging over the fine-grain degrees of freedom, the combinations of variables which the effective energy terms depend on, and approximated energy expressions can be determined. This new systematic approach to the coarse-grained force-field derivation is illustrated with the example of the local and correlation energy terms in the UNRES force field developed in our laboratory [1,4]. In particular, it is demonstrated that pure ‘torsional’

potentials are meaningless with coarse-grained force fields, because the trigonometric functions of the virtual-bond-dihedral angles are always multiplied by the sines of the adjacent virtual-bond-valence angles. The new formalism also enables us to rationalize the dependence between the backbone-virtual-bond-dihedral angles and the adjacent backbone-virtual-bond-valence angles in proteins derived from the Protein Data Bank.

Supported by grant DEC-2012/06/A/ST4/00376 from the National Science Center of Poland and grant Mistrz 7./2013 from the Foundation for Polish Science. Calculations were carried out using the computer resources at the Academic Computer Centre in Gdansk (CI TASK) and Interdisciplinary Center of Mathematical and Computer Modeling, University of Warsaw.

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**Presenter: Adam Liwo**

I.4 – Invited, IWTCP-3

### **Improved prediction of protein complex binding affinities: the role of entropy**

*Antonio Trovato*

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Protein-protein interactions play an essential role in the biological function of many proteins. We will tackle the problem of predicting the binding affinities of protein complexes, based on the knowledge of both the complex and the unbound subunits. We will rely on the BACH statistical potential, recently developed in our group, that showed excellent performances in discriminating the native states of monomeric proteins.

We will first show that the BACH scoring function is successful as well in recognizing native and close-to-native protein complexes. We will then employ our scoring function as the basis of a method to predict the binding affinities of protein complexes, which is in general a very difficult task. We will show that, in order to improve the predictive performance of our method, it is crucial to properly estimate how the change in protein fluctuations upon binding determines the entropic contribution to the binding affinity.

This is done by means of simple coarse-grained elastic network models; yet, it relies on determining the proper structure-dependent elastic constant by means of a novel self-consistent procedure based on matching the residue mobilities computed within the network model with those estimated from molecular dynamics all atom explicit solvent simulations initiated from the experimental structures.

**Presenter: Antonio Trovato**

I.5 – Invited, IWTCP-3

## Thermoelectric effects in graphene nanostructures

*V. Hung Nguyen (1,2), M. Chung Nguyen (1,2), H. Viet Nguyen (2), J. Saint-Martin (1), P. Dollfus (1)*

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The thermoelectric effect enables direct conversion of a temperature difference into an electric voltage and vice versa, and provides a viable route for electrical power generation from waste heat. The thermoelectric properties of graphene and graphene nanostructures have recently attracted significant attention from the physics and engineering communities. First, the analysis of Seebeck and Nernst effects is very useful in elucidating some details of the electronic band structure of graphene that cannot be probed by conductance measurements alone, due in particular to the ambipolar nature of this gapless material. Second, the potential of graphene in thermoelectric devices is also quite intriguing. On the one hand, to be a good thermoelectric channel, graphene has two major disadvantages to overcome. The first disadvantage is its gapless character, which leads to a small Seebeck coefficient due to the opposite contributions of electrons and holes. The second one is the high thermal conductivity of graphene that makes it an excellent thermal conductor but not a thermoelectric material. However, several nanostructuring and bandgap engineering techniques for graphene have been recently explored, which suggests various strategies to concomitantly reduce the lattice thermal conductance and enhance the Seebeck coefficient without dramatically degrading the electronic conductance. Hence, in various graphene nanostructures, the thermoelectric efficiency has been predicted to be high enough to make them attractive for energy conversion. In this talk, I will review the main studies reported recently on the thermoelectric properties of graphene and its nanostructures, and also of other graphene-like materials.

Reference: Philippe Dollfus, Viet Hung Nguyen and Jérôme Saint-Martin, *J. Phys.: Condens. Matter* 27 133204 (2015)

**Presenter: Viet-Hung Nguyen**

I.6 – Invited, IWTCP-3

## Energy transduction and dissipation in biomolecular motors and pumps

*Gerhard Hummer*

*Department of Theoretical Biophysics, Max Planck Institute of Biophysics, 60438 Frankfurt am Main, Germany (Email: Gerhard.Hummer@biophys.mpg.de)*

We have used molecular dynamics simulations and statistical mechanical theory to characterize the molecular mechanisms of biological energy transduction processes in the proton pumps cytochrome *c* oxidase and complex I, and in the coupled rotary motors of F<sub>o</sub>F<sub>1</sub>-ATP synthase. These biomolecular machines efficiently interconvert chemical, electrostatic, and mechanical energy. Simulations and reduced physical models highlight their key mechanistic elements and shed light on the function of the bioenergetic machinery.

**Presenter: Gerhard Hummer**

I.7 – Invited, IWTCP-3

## Defining behavior states of indicator animals under stressful or conflict conditions in a confined area

*Tae-Soo Chon (1,2)*

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Behavior monitoring would be feasible in on-line, early warning system for ecological risk assessment since stress affectedness could be sensitively and continuously reflected on overall motion of animals by reflecting total physiological network responses to stressors. However, behavior data are complex and difficult to analyze, especially under stressful conditions (e.g., toxic chemical treatment). In this study, recent computational approaches are overviewed in defining behavior states of indicator animals across different time scales in a confined observation arena. Parameters regarding position distribution (e.g., skewness) are used for expressing instantaneous behaviors of animals to detect affectedness by stimuli under conflict conditions. Internal behavior states and transition probability matrix are defined by Hidden Markov Model in a short time sequence (i.e., seconds – minutes) based on external observation data during the course of response to stressors. In an intermediate time scale (i.e., minutes – hours), the whole data sets were transformed including filtering by integration to address test organisms' response and adaptation to stressors (e.g., intoxicating and recovering processes). Intermittency is additionally used for analyzing overall data structure in long time sequences (i.e., hours – days) to define behavior states in specific areas in the observation arena in individuals and groups.

**Presenter: Tae-Soo Chon**

I.8 – Invited, IWTCP-3

### **Electrostatics in viruses**

*Rudolf Podgornik*

*Department of Theoretical Physics, J. Stefan Institute and Department of Physics, Faculty of Mathematics and Physics, University of Ljubljana - SI-1000 Ljubljana, Slovenia, EU*

I will present several models of the effects of electrostatic interactions on viruses. Starting from a discussion of charge distribution and the pertaining charge regulation description, I will explore in detail several examples of the role of charge-charge interactions for capsid stability as well as the interactions between the capsid proteins and the compactified genetic cargo.

**Presenter: Rudolf Podgornik**

I.9 – Invited, IWTCP-3

### **Eukaryotic chromatin folding and gene regulation**

*Naoko Tokuda, Shin Fujishiro, Masaki Sasai*

*Nagoya University*

In the last decade, we have witnessed great advances in our understanding of bacterial gene regulation. In particular, quantitative comparison between the theoretical analyses of model gene networks and the experimental single cell-level analyses has played important roles in revealing statistical features of intensely fluctuating dynamics of gene expression. For eukaryotes, however, the theoretical framework for modeling gene regulation is still at the infancy level. By calculating “epigenetic landscape” from model eukaryotic gene network, we show that histone modification and the associated chromatin structure change should modify topology of landscape and thereby significantly affect associated dynamics of gene activities. In order to further quantify the effects

of chromatin structure fluctuation on gene expression, we have started projects to simulate 3D genome architectures. The simulated results suggest that genome structure of interface budding yeast shows large liquid-like fluctuation, but spatial distributions of genes in nucleus are correlated with their expression level suggesting the intrinsic relation between gene regulation and chromatin structure. Our efforts to simulate human genome, where difficulty lies in its large size and degeneration in diploid copies, are also discussed.

[References] M. Sasai, et al., PLoS Comp. Biol. 9: e100338 (2013); S. S. Ashwin, M. Sasai, arXiv:1410.2337 [q-bio.MN] (2014); N. Tokuda, TP. Terada, M. Sasai, Biophys. J. 102: 296-304 (2012).

**Presenter: Masaki Sasai**

I.10 – Invited, IWTCP-3

### **One-dimensional diffusion models for protein folding – how good can they be?**

*Robert B. Best*

*National Institute of Diabetes and Digestive and Kidney Diseases, National Institutes of Health, Bethesda, MD 20892, USA*

Despite the vast number of degrees of freedom involved in protein folding, theoretical models have often assumed, with some success, that folding dynamics can be described as diffusion on a low-dimensional free energy surface. However, the validity of approximating dynamics as diffusion in a low-dimensional space could until recently only be indirectly assessed by comparing theory with experimental observables such as folding rates, or with highly simplified simulation models. The availability of all-atom atomistic folding simulations of ten small proteins, in explicit solvent, allows such assumptions to be directly tested. We find that for almost all of the proteins, it is possible to embed the folding dynamics rather accurately into diffusion on only a single progress variable, the fraction of native contacts ( $Q$ ). Not only do the diffusion models, parametrized by position-dependent free energies  $F(Q)$  and diffusion coefficients  $D(Q)$ , reproduce folding and unfolding rates, but also finer details of the dynamics, such as the transition-path durations, and propagators estimated directly from simulation. For the one exception, protein G, where the diffusion model for  $Q$  cannot capture the transition-path durations, we are able to find a modified coordinate,  $Q_{opt}$ , by reweighting native contacts, which greatly improves the quality of the diffusion model. We find that the position-averaged diffusion coefficients on  $Q$  decrease with chain length, as anticipated from energy landscape theory. Overall, our results suggest that one-dimensional diffusion is a remarkably faithful model for protein folding dynamics, provided a suitable folding coordinate is chosen.

**Presenter: Robert B. Best**

I.11 – Invited, IWTCP-3

### **Codon positions that strongly influence cotranslational folding are far from equilibrium: A framework for controlling nascent-protein folding**

*Edward O'Brien*

*Department of Chemistry, Pennsylvania State University, University Park, PA 16802, USA*

Synonymous codon substitutions change the translation rate at specific positions within an mRNA's coding sequence without changing the encoded protein's amino acid sequence and can alter a nascent protein's ability to cotranslationally fold and function. The physical rules



governing why synonymous mutations at some codon positions can have a much greater impact on nascent protein folding than others remain unknown. Here, we introduce a framework that allows for the control of nascent chain folding during translation through the rational design of mRNA sequences using synonymous codons. We test this framework in silico and find it provides optimal mRNA sequences to control the simulated, cotranslational folding of a protein in a user-prescribed manner. With this approach we discover the rules governing the positioning and impact of critical codons. First, the position of a critical codon depends on the cotranslational profile, which is the probability of a protein populating different conformational states as a function of the nascent chain length. As a consequence, different cotranslational profiles can have different critical codon positions, even though the encoded protein may be the same. Second, the impact of a mutation at a critical codon position is proportional to how far from equilibrium the cotranslational folding curve is at that and subsequent codon positions. Our results show that a cotranslational profile's deviation from equilibrium, its sensitivity to single-point mutations, and its mRNA-sequence degeneracy are inter-related, and that each of these factors has direct implications for nascent protein behavior, critical codon positions and mRNA sequence evolution.

**Presenter: Edward O'Brien**

I.12 – Invited, IWTCP-3

### **DNA looping in the presence of divalent counterions, a simulation study using a coarse-grained model of DNA**

*Toan The Nguyen, Duc Viet Nguyen*

*VNU University of Science, 334 Nguyen Trai street, Hanoi, Vietnam*

DNA looping is an important structure in many biological contexts such as in nucleosome structure, in viral DNA packaging, and present in all aspects of DNA metabolism, including transcription, replication, and recombination. The elastic energy of DNA is an important contribution to the total free energy of the system and there has been many works trying to understand the elastic behavior of DNA. Experimental results for looping of DNA chain with 60 or more nucleotide base pairs (bp) is consistent with the worm-like chain (WLC) model of DNA with proper persistence length. However, for shorter DNA chain, the looping behavior deviates significantly from the WLC result and suggests a possibility of formation of permanent kinks in the DNA chain to relax the elastic stress. In the presence of high valence counterions such as  $Mg^{+2}$ , the kink behavior starts at an even larger chain length (about 100bp). In this work, a simulation study of a DNA coarse-grained model is presented to understand the role of divalent counterions in the looping of DNA. It is shown that kinks are transiently formed when DNA loop. They make DNA softened but no permanent kinks are observed in simulation

**Presenter: Toan The Nguyen**

I.13 – Invited, IWTCP-3

### **Emission in Manganese-Doped Semiconductor Nanocrystals**

*Que Huong Nguyen*

*Marshall University, One John Marshall Drive, Huntington WV 25701 USA*

With recent development of nanotechnology such as colloidal synthesis and molecular beam epitaxy, magnetic ion-doped quantum dots (QDs) become a great interest and have been studied intensively. Well known as an activator for photoluminescence (PL) and electroluminescence, the

ion  $Mn^{2+}$  has been among the first magnetic ion to be doped into a semiconductor nanocrystals (NCs). Up to date, considerable interest has been attracted in the Mn-doped semiconductor NCs. The Mn-Doped QD can not only maintain nearly all the intrinsic advantages of QDs, but also bring the additional merits such as larger Stokes shifts, enhanced thermal and chemical stabilities, as well as longer excited state lifetimes.

We theoretically investigate the magneto-PL of  $Mn^{2+}$  doped semiconductor core-shell colloidal QD to explain the experiment results from a recent magneto-PL study (1,2) of strongly confined diluted magnetic semiconductor (DMS) in  $Mn^{2+}$ -doped ZnSe/CdSe core-shell colloidal NCs. Unlike the cases in bulks or in other conventional DMS materials, the yellow emission characterized for in  $Mn^{2+}$  which is associated with the d-d internal transition  $4T_1-6A_1$ , was reported not suppressed in an applied  $B//z$  magnetic field and circularly polarized as usual and instead, developed a circular polarization. More interestingly,  $Mn^{2+}$  PL has been found to have a large splitting between  $\sigma+$  and  $\sigma-$  components which depends on the applied field. This behaviour has not been found in characteristics of the  $Mn^{2+}$  PL in bulks and other conventional DMS materials and is the result of the strong confinement of the NCs.

Our theory shows that, the reason the yellow  $Mn^{2+}$  PL band in QDs, indifferent to their counterparts in bulks and other low-dimensional systems, is not suppressed under applied magnetic field originates from the dot geometry and properties. The theory of Coulomb exchange interaction of the impurity ions with the confined electrons inside the dot as well the existence of the internal electric field inside the dot show that these two effects might be the reasons of the observed behaviors. The competition and combination between these two effects give different results depending on parameters and conditions.

References:

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2. Liu, Q., Deng, R., Ji, X. & Pan, D. Alloyed Mn-Cu-In-S nanocrystals: a new type of diluted magnetic semiconductor quantum dots. *Nanotechnology* 23, 255706 (2012).

**Presenter: Que-Huong Nguyen**

I.14 – Invited, IWTCP-3

## **Protein Misfolding and Aggregation Revealed by Fluctuating Thermodynamics Analysis**

*Sihyun Ham*

*Department of Chemistry, Sookmyung Women's University, Hyochangwon-gil 52, Yongsan-gu, Seoul 140-742, Korea*

Because biomolecular processes are largely under thermodynamic control, dynamic extension of thermodynamics is necessary to uncover the mechanisms and driving factors of fluctuating processes. The fluctuating thermodynamics technology presented in this talk offers a practical means for the thermodynamic characterization of conformational dynamics in biomolecules. The use of fluctuating thermodynamics has the potential to provide a comprehensive picture of fluctuating phenomena in diverse biological processes. Through the application of fluctuating thermodynamics, we provide a thermodynamic perspective on the misfolding and aggregation of the various proteins associated with human diseases. In this talk, I will present the detailed concepts and applications of the fluctuating thermodynamics technology for elucidating biological processes.

**Presenter: Sihyun Ham**

I.15 – Invited, IWTCP-3

### **Protein aggregation: Key principles and applications**

*Mai Suan Li (1,2)*

*(1) Institute of Physics, Polish Academy of Sciences, Al. Lotnikow 32/46, Warsaw, Poland;*

*(2) Institute for Computational Science and Technology at Ho Chi Minh City, Quang Trung Software City, Tan Chanh Hiep Ward, District 12, HCM city, Vietnam*

Protein aggregation is presumably associated with a large group of major human diseases including Alzheimer's disease (AD), prion disorders, type 2 diabetes etc. Therefore, understanding the key factors that control this process is important not only for basic research but also for drug design for relevant diseases. The fibrillogenesis of polypeptide chains depends on their intrinsic properties as well as on external conditions. Using coarse grained and all-atom models we show that fibril formation times are strongly correlated with hydrophobicity, charges and population of the so called fibril-prone conformation  $N^*$  in monomer state. The higher is the  $N^*$  population the faster is the fibril elongation and this dependence may be described by a single exponential function. Our results open up a new way to understand the propensity of biomolecules to aggregation at monomer level. We will discuss the ways of blocking aggregation and destroying fibers of amyloid beta peptides the self-assembly of which is believed to be the main cause of AD. Through in silico and in vitro experiments small molecules from large data bases and short peptides have been obtained as potential candidates for treating AD due to their strong binding to amyloid beta aggregates. Picosecond dissociation of amyloid fibrils with infrared laser will be discussed. Nonequilibrium simulation studies show that the fibril is destroyed due to the strong resonance between its amide I vibrational modes and the laser field, not just the deposited infrared thermal energy.

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**Presenter: Mai Suan Li**

O.1 – Oral, IWTCP-3

### **Coarse-grained models for the formation of self-limited supraparticle assemblies**

*Trung D. Nguyen (1,2), Benjamin A. Schultz (2), Nicholas A. Kotov (2) and Sharon C. Glotzer (2)*

*(1) Vietnam Academy of Science and Technology, Vietnam; (2) University of Michigan, Ann Arbor, MI 48109, USA*

Engineering nano-assemblies with a terminal size has been of particular interest as it enables a broad array of applications in photonics, catalysis and drug delivery. Recent experiments have indicated that terminal assemblies can be synthesized in both inorganic [1] and hybrid inor-

ganic/organic [2] systems, suggesting that a generic assembly mechanism is likely at work. In this study, we developed a generic, coarse-grained model that can explain the formation of terminal assemblies by capturing the balance between van der Waals attraction and renormalized Coulombic repulsion between the assembling particles when they aggregate. Using Molecular Dynamics simulation and energy analysis, we show that the uniform-sized supraparticles are stable over a wide range of density, indicating that they are thermodynamically stable, instead of consequences of limited diffusion or kinetic arrest. The generic nature of the governing interactions suggests great versatility in the composition, size and shape of the constituent building blocks, and allows for a large family of hierarchical self-assembled structures, including colloidal crystals.

References:

- [1] Y. Xia et al., Nat. Nanotechnol. 2011, 6, 580.
- [2] J. Park et al., Nat. Commun. 2014, 5, 3593.

**Presenter: Trung D. Nguyen**

O.2 – Oral, IWTCP-3

### **Nonlinear optically detected magnetophonon resonance via two-photon process in parabolic quantum wells**

*Tran Cong Phong (1), Vo Thanh Lam (2), Nguyen Dinh Hien (3)*

*(1) Vietnam Institute of Educational Sciences, 101 Tran Hung Dao Str., District Hoan Kiem, Ha Noi, Viet Nam; (2) Department of Physics, Sai Gon University, 273 An Duong Vuong Str., District 5, Ho Chi Minh City, Viet Nam; (3) Hue University's College of Education, 34 Le Loi Str., Hue City, Viet Nam*

In this work, the combined effect of aluminum concentration, hydrostatic pressure, temperature, and confinement frequency of a parabolic quantum well (PQW) on the nonlinear optically detected magnetophonon resonance (NODMPR) via two-photon absorption process is investigated theoretically. The analytical expression of the nonlinear optical absorption power (NOAP) is obtained by using the operator projection technique in case of electron-optical phonon scattering for the absorption of both one and two photons. The numerical results are calculated for typical GaAs/GaAlAs quantum well. The obtained results show that the hydrostatic pressure, aluminum concentration, temperature, and confinement frequency have a significant effect on the NOAP as well as on the half-width. Moreover, it has been found that the optical properties of the GaAs/GaAlAs PQW can be modified by changing these parameters. This gives a new capacity for optical device applications

**Presenter: Tran Cong Phong**

O.3 – Oral, IWTCP-3

### **Entanglement and teleportation in the even and odd photon-added charge coherent states**

*Truong Minh Duc (1), Dang Huu Dinh (1), and Tran Quang Dat (2)*

*(1) Center for Theoretical and Computational Physics, College of Education, Hue University, 32 Le Loi, Hue City*

*(2) University of Transport and Communications, Campus 2, 450 Le Van Viet, 9 District, Ho Chi Minh City*

In this paper, we study the intermodal entanglement as well as the process of teleportation in the even and odd photon-added charge coherent states. We show that these states are two-mode entangled, and the entanglement between two modes becomes more pronounced with increasing the number of photons added to both modes. In addition, when using these states as an entanglement resource to teleport a state, the degree of average fidelity of teleportation process becomes bigger and bigger by increasing the number of added photons.

**Presenter: Truong Minh Duc**

O.4 – Oral, IWTCP-3

### **Theoretical evaluation of maximum electric field approximation of direct band-to-band tunneling Kane model for low bandgap semiconductors**

*Nguyen Dang Chien (1), Chun-Hsing Shih (2), Phu Chi Hoa (3), Nguyen Hong Minh (1), Duong Thi Thanh Hien (1) and Le Hong Nhung (3)*

*(1) Faculty of Physics, University of Da Lat, Lam Dong 671463, Vietnam (2) Department of Electrical Engineering, National Chi Nan University, Nantou 54561, Taiwan (3) Faculty of Postgraduate Studies, University of Da Lat, Lam Dong 671463, Vietnam*

The two-band Kane model has been popularly used to calculate the band-to-band tunneling (BTBT) current in tunnel field-effect transistor (TFET) which is currently considered as a promising candidate for low power applications. This study theoretically clarifies the maximum electric field approximation (MEFA) of direct BTBT Kane model and evaluates its appropriateness for low bandgap semiconductors. By analysing the physical origin of each electric field term in the Kane model, it has been elucidated in the MEFA that the local electric field term must be remained while the nonlocal electric field terms are assigned by maximum value of electric field at the tunnel junction. Mathematical investigations have showed that the MEFA is more appropriate for low bandgap semiconductors compared to high bandgap materials because of enhanced tunneling probability in low field regions. The appropriateness of the MEFA is very useful for practical uses in quickly estimating the direct BTBT current in low bandgap TFET devices.

**Presenter: Nguyen Dang Chien**

O.5 – Oral, IWTCP-3

### **Cellular Organization and Synchronization of Pancreatic Islets**

*Danh-Tai Hoang (1), Junghyo Jo (1,2)*

*(1) Asia Pacific Center for Theoretical Physics, Pohang, Korea; (2) Department of Physics, POSTECH, Pohang, Korea*

Structure-function relationship is one of the most fundamental problems in biology. Pancreatic islets, micro-organ for maintaining blood glucose levels constant, are mainly composed of glucagon-secreting  $\alpha$  cells, insulin-secreting  $\beta$  cells, and somatostatin-secreting  $\delta$  cells. Glucagon and insulin are the two counter-regulatory hormones for increasing and decreasing blood glucose levels, respectively, in a pulsatile manner. Interestingly, the cellular composition and organization of islets are different between species: Mouse islets have a shell-core structure with dominant populations of  $\beta$  cells in the core and non- $\beta$  cells on the periphery, while human islets have a less clear structure with intermingled cells. Since the islet cells interact to stimulate or suppress hormone secretions of neighboring cells, their spatial organization should have a functional sig-

nificance. In this study, we considered islet cells as coupled oscillators that generate hormone pulses, and examined their synchronization behaviors depending on their spatial organization. Using this model, we explored the role of  $\delta$  cells by removing them in islets, and also the islet deterioration in type 1 diabetes by deleting  $\beta$  cells. Finally, we discuss potential advantages and disadvantages of the designs of islets for controlling glucose.

**Presenter: Danh-Tai Hoang**

O.6 – Oral, IWTCP-3

### **Modeling DNA condensates with generalized elastic potential**

*Trinh X. Hoang (1), Hoa Lan Trinh (1), Achille Giacometti (2), Rudolf Podgornik (3,4), Jayanth R. Banavar (5), and Amos Maritan (6)*

*(1) Institute of Physics, Vietnam Academy of Science and Technology, Hanoi, Vietnam; (2) Dipartimento di Scienze Molecolari e Nanosistemi, Facolta di Science, Universita Ca Foscari Venezia, I-30123 Venezia, Italy; (3) J. Stefan Institute and Department of Physics, University of Ljubljana, Ljubljana, Slovenia, EU; (4) Department of Physics, University of Massachusetts, Amherst, MA 01003, USA; (5) Department of Physics, University of Maryland, College Park, Maryland 20742, USA; (6) Department of Physics and Astronomy, University of Padova, Padova, Italy*

For several decades, DNA condensates have challenged scientists with fundamental questions about their sizes and shapes. In particular, DNA toroids with varying sizes and thickness to diameter ratios have been observed. On the other hand, the non-linear elasticity of DNA at short length scales, comparable to that of DNA persistence length, is still not well understood. In this study, we demonstrate that these two issues are related in a remarkable way - the microscopic details of the non-linear elasticity has a direct impact on the geometrical features of DNA toroids at macroscopic observable scales. With a novel generalized form of the worm-like chain model, we study the effects of non-linear elasticity on the phase diagram of the ground states as well as on geometrical features of DNA condensates. The model provides a simple explanation for the results of prior experimental and computational studies and makes predictions for the specific geometries of the ground states.

**Presenter: Trinh Xuan Hoang**

O.7 – Oral, IWTCP-3

### **Studies on interactions between Ebola virus protein VP35 and its partners using molecular simulation approach**

*Chuong Nguyen (1,2)*

*(1) Theoretical Physics Research Group, Department for Management of Science and Technology Development, Ton Duc Thang University, Ho Chi Minh City, Vietnam; (2) Faculty of Applied Sciences, Ton Duc Thang University, Ho Chi Minh City, Vietnam.*

Ebola virus (EBOV) disease is a severe infection that often results in death, reflecting an inability of the host immune response to control virus replication. The viruses avoid the human immune system's response to viral infections by interfering the host interferon production. The EBOV viral protein 35 (VP35) has recently emerged as a key component in this interference. The previous studies have revealed several key basic residues which are critical for the interactions between VP35 and its partners such as double-stranded RNA (dsRNA) and inhibitors. To

explore the interactions between VP35 and its partners at molecular level, we have conducted steered molecular dynamics simulations for different complexes of VP35 bound to dsRNA or its inhibitors. Our data have shown several residues which play a crucial role in binding between VP35 and its partner. These results provide an initial data to guide development of antiviral compounds against the Ebola virus disease by targeting the VP35 protein.

**Presenter: Chuong Nguyen**

O.8 – Oral, IWTCP-3

## THE EVOLUTION OF MELTING PROCESS OF GRAPHENE NANORIBBONS

*Nguyen Thi Thuy Hang*

*Department of Applied Physics, Institute of Technology, National University of Hochiminh City, 268 Ly Thuong Kiet Str., Distr. 10, Hochiminh City, Vietnam*

Melting of graphene nanoribbons model in 2D space is studied via molecular dynamics simulation. Model containing 104 atoms interacted via long-range bond-order potential (LCBOP, J.H. Los, A. Fasolino, Phys. Rev. B 68, 024107 (2003)) is heated up from 300 K to 10000 K in order to see the evolution of various thermodynamic quantities, structural characteristics, occurrence of various structural defects upon heating to a molten state. Temperature dependence of total energy exhibits a first-order-like behavior of the transition at a melting point. Heat capacity of the system exhibits a single peak at around the melting point. Occurrence and clustering of Stone-Wales (SW) defects are the first step of melting process following by breaking of C-C bonds, occurrence/growth of various types of vacancies and multi-membered rings. Melting point of graphene nanoribbons in 2D space is rather high due to constraint of the 2D space.

**Presenter: Nguyen Thi Thuy Hang**

O.9 – Oral, IWTCP-3

## Molecular Modelling of Alcohol Dehydrogenase from *Lactobacillus Brevis* in Organic Solvent

*Quy Vo (1), Jan-Hendrik Grosch (2), Antje Spiess (2), Juergen Pleiss (1)*

*(1) Institute of Technical Biochemistry, University of Stuttgart, Stuttgart, Germany; (2) Enzyme Process Technology, RWTH Aachen, Aachen, Germany*

Alcohol dehydrogenases from *Lactobacillus brevis* (LbADH, EC 1.1.1.2) is a widely used biocatalyst due to its high catalytic activity towards a broad range of substrates and its high tolerance towards non-conventional media. To investigate the structural and functional determinants of stability and activity in organic solvents, molecular dynamics simulations of a ternary complex of LbADH, NAD/NADH, and Mg<sup>2+</sup> were performed in mixtures of an organic solvent, diisopropyl ether, and water. The simulation in organic solvent was compared to simulations in pure water. The simulation results are consistent with experimental data: LbADH is stable in pure water and in the organic solvent. The enzyme is more rigid in the organic solvent than in pure water. Interestingly, the binding of functional water molecules in the binding pocket is disturbed by diisopropyl ether. In organic solvent, water molecules that are crucial for the proton relay system are withdrawn from the binding pocket, which implies that the effect of organic solvent is a dominant factor for the enzymatic activity.

**Presenter: Quy Vo**

P.1 – Poster, IWTCP-3

### **Studies on interactions between Ebola viral protein 35 and dsRNA using steered molecular dynamics approach**

*Ngan Q. Nguyen (1), Chuong Nguyen (2,3,\*)*

*(1) Department of Theoretical Physics, Faculty of Physics and Engineering Physics, University of Science, Vietnam National University, Ho Chi Minh City, Vietnam; (2) Theoretical Physics Research Group, Department for Management of Science and Technology Development, Ton Duc Thang University, Ho Chi Minh City, Vietnam; (3) Faculty of Applied Sciences, Ton Duc Thang University, Ho Chi Minh City, Vietnam. (\*) Corresponding Author: Chuong Nguyen, nguyenhahungchuong@tdt.edu.vn.*

Ebola virus causes acute hemorrhagic fever which is often fatal if untreated. Viral protein 35 (VP35) of Ebola virus has different functions in viral replication. One of those roles is acting as an interferon (IFN) antagonism, result in attenuation of the immune system. The ability of VP35 to bind double-stranded RNA (dsRNA) has been suggested to be crucial for its function. Recent crystal structures of VP35 have shown several residues which are important for protein-RNA binding. We have conducted steered molecular dynamics (SMD) simulations for wild-type also for different mutants of VP35 binding to dsRNA crystal structures to analyse molecular VP35-dsRNA interaction. Our result shows that residues R312 and K339 contribute main factor in the interaction. These results are consistent with ITC experimental studies for VP35-dsRNA complex.

**Presenter: Nguyen Quy Ngan**

P.2 – Poster, IWTCP-3

### **Modeling the interactions between putative anticancer bacteriocins and the p53 DNA-binding domain**

*Kim-Thoa Pham (1), Quy-Truong Nguyen (1), Quy-Ngan Nguyen (1), Van-Duy Nguyen (2), Chuong Nguyen (3,4)*

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Azurin, a well characterized bacteriocin, has been well known for its capability of penetrating into human cancer cells, forming a complex with protein p53, thereby activating apoptosis and growth arrest in such cells. Recently, a bioinformatics study has proposed other bacteriocins from human gut microflora that also possessed functional properties very similar to those of Azurin. We hypothesized that these putative anticancer bacteriocins can also form complexes with protein p53. In this study, we have predicted the molecular interaction between p53 and these bacteriocins using homology modeling and molecular docking approaches. The resulting structures have been further investigated by steer molecular dynamics to reveal the bacteriocins that have highest binding affinity towards p53. Our result contributes to assess and screen out the most potential bacteriocins to target human cancer cell. This can lead us to identify the novel anticancer drugs from human microflora.

**Presenter: Pham Thoa**



P.3 – Poster, IWTCP-3

### **Estimation of partial atomic charges of calcite (CaCO<sub>3</sub>) by Electrostatic Potential Fitting method**

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Atomic charge cannot be observed experimentally because they do not correspond to any unique physical property [1]. Molecules are traditionally considered as “composed” of atoms, in a more general sense, as a collection of charged particles, positive nuclei and negative electrons [2]. Researchers have so far developed several approaches and techniques for estimating the partial atomic charges of the molecule. In this paper, we will discuss two different relevant methods widely used to estimate the partial charges: Quantum chemistry and Empirical fitting method. Quantum chemistry method based on the Electrostatic Potential Fitting technique has many advantages, in this technique all ion charges of the molecule are varied in calculation processes but constraining their sum to zero. The method has been implemented in the Maestro/Jaguar quantum chemistry package [3, 4]. Here, we utilize this package to estimate the partial atomic charges of calcite (CaCO<sub>3</sub>).

Calcite crystals and calcite slabs were built using CrystalMaker software, version 2.1.4 for Windows [5]. In this work, calcite structural parameters from American Mineralogist Crystal Structure Database (AMCSD) [6, 7] were used. Calcite slabs differing in shape and size were cleaved along the (1-0-1 overbar-4) surface of the calcite crystal. After cleaving, all the broken bonds of carbon, oxygen, and calcium were deleted. The resulting calcite slabs were exported directly from CrystalMaker to Protein Data Bank (PDB) format [8]. The PDB files were then imported into Maestro/Jaguar software package, version 7.6. The estimation of the atomic charge of different calcite slabs has been done for many times, and proven to be quite challenging. For the first try, calcite structure with 30 atoms in total was used in our first attempt, which was successful. Then the total number of atoms in the calcite slab was increased to 60, 80, 90, 100, and up to 210.

The average values of partial calcite atomic charges are quite comparable to those found in Fisler et al. [9] used the Empirical fitting method, where the calcium ion charges were kept fixed at +2, and the focus was only on the carbonate group, allowing carbon, oxygen core, and oxygen shell charges to vary but constraining their sum to -2.

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**Presenter: Phan Van Cuong**

P.4 – Poster, IWTCP-3

### **Fission Product Decay Heat Calculations for Neutron Fission of $^{232}\text{Th}$**

*Pham Ngoc Son*

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Precise information of the decay heat from fission products following times after a fission reaction is necessary for safety designs and operations of nuclear power reactors, fuel storage, transport flasks, and for spent fuel management and processing. In this report, exact timing distributions of fission product concentrations and their integrated decay heat were calculated as functions of time following a neutron fission reaction of  $^{232}\text{Th}$ .

**Presenter: Pham Ngoc Son**

P.5 – Poster, IWTCP-3

### **Binding of F-19848 A and Natural Compounds to CD44: Implications to Breast Cancer**

*Trung Tin Nguyen (1), Phuoc Duy Tran (2), Pham Dinh Quoc Huy (1,3), Hoang Zung (4), Paolo Carloni (5), Phuc Van Pham (4), Chuong Nguyen (6,7) and Mai Suan Li (3)*

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CD44, a membrane protein, is a primary cell surface receptor for hyaluronan, which is one of the major components of the tumor extracellular matrix and strongly relates to the tumorigenesis of breast cancer. It has been shown experimentally that F-19848 A is a potential inhibitor for hyaluronan binding to receptor CD44. In the paper, we investigate the CD44 and F-19848 A interaction at molecular level using molecular dynamics simulation. It reveals that the van der Waals interaction contribute dominantly to the total binding energy of the complex and the extending part of F-19848 A is the most important to its binding. Screening natural products from TCM Database@Taiwan was also performed to find candidates as inhibitors for CD44 receptor by the docking and steered molecular dynamics simulation. We have found 10 compounds that are better inhibitors than F-19848 A.

**Presenter: Nguyen Trung Tin**

P.6 – Poster, IWTCP-3

### **Thermal neutron radiative capture cross-section of $^{186}\text{W}(n,g)^{187}\text{W}$ reaction**

*Vuong Huu Tan (1), Pham Ngoc Son (2)*

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Thermal neutron radiative capture cross section for  $^{186}\text{W}(n,g)^{187}\text{W}$  reaction were measured by the activation method using the filtered thermal neutron beam at the Dalat research reactor. An

optimal composition of Si and Bi single crystals has been used as neutron filters to create the high purity filtered thermal neutron beam with Cadmium ratio of 420. The induced activities in the irradiated samples were measured by a high resolution HPGe digital gamma-ray spectrometer. The present result is obtained relative to the reference value of the standard reaction  $^{197}\text{Au}(n,\text{g})^{198}\text{Au}$ . The necessary correction factors for gamma-ray true coincidence summing, and thermal neutron self-shielding effects were taken into account in this determination.

**Presenter: Pham Ngoc Son**

P.7 – Poster, IWTCP-3

### **Effect of Taiwan mutation (D7H) on structures of amyloid beta peptides: replica exchange molecular dynamics study**

*Phan Minh Truong (1), Man Hoang Viet (2), Phuong H. Nguyen (3), Chin-Kun Hu (4), and Mai Suan Li (1,2)*

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Recent experiments have shown that the Taiwan mutation (D7H) slows down the fibril formation of amyloid peptides  $\text{A}\beta_{40}$  and  $\text{A}\beta_{42}$ . Motivated by this finding we have studied the influence of D7H mutation on structures of  $\text{A}\beta$  peptides using the replica exchange molecular dynamics simulations with OPLS force field and implicit water model. Our study reveals that the mechanism behind modulation of aggregation rates is associated with decrease of beta-content and dynamics of the salt bridge D23-K28. Estimating the bending free energy of this salt bridge we have found that, in agreement with the experiments, the fibril formation rate of both peptides  $\text{A}\beta_{40}$  and  $\text{A}\beta_{42}$  is reduced about two times by mutation.

**Presenter: Phan Minh Trường**

P.8 – Poster, IWTCP-3

### **Calculation of Etingshausen coefficient in Quantum Well in the presence of Electromagnetic Wave**

*Dao Thu Hang, Nguyen Quang Bau*

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The analytic expressions for Etingshausen coefficient in the Quantum Well with parabolic potential in the presence of Electromagnetic wave are calculated by using the quantum kinetic equation for electrons. The dependence of Etingshausen coefficient on the frequency of Electromagnetic wave, the Quantum Well parameters and especially the dependence of Etingshausen coefficient on temperature gradient are obtained. The results are numerically calculated and discussed for GaAs/AlGaAs Quantum Well

**Presenter: Dao Thu Hang**

P.9 – Poster, IWTCP-3

### **Transient super-ballistic spreading of wave packets in hybrid ordered-quasi-periodic lattices**

*Ba Phi Nguyen (1) and Duy Khuong Phung (2)*

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In this work, we numerically demonstrate that hybrid ordered-quasiperiodic lattices can support the super-ballistic spreading of an initially-localized wave packet with very large exponents for certain transient time windows. Remarkably, in the case of the sublattice with on-site potential obeys the period-doubling quasiperiodic sequence, we find that the super-ballistic exponent is beyond five. Keywords: super-ballistic spreading, wave packet dynamics, lattice dynamics, quantum transport.

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**Presenter: Nguyen Ba Phi**

P.10 – Poster, IWTCP-3

### **First Principles Study on Nickel carbonophosphate $\text{Li}_3\text{NiPO}_4\text{CO}_3$ for Cathode Materials of rechargeable Li-ion batteries.**

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Lithium ion batteries (LIBs) are believed to be the best devices among many energy storage gadgets. Recently, carbonophosphate materials  $\text{Li}_3\text{MPO}_4\text{CO}_3$  ( $\text{M} = \text{Fe}, \text{Ni}, \text{Mn}, \text{and Co}$ ) with their dominant advantages were predicted to be a new family of cathode materials replacing for the obsolete ones [1-4]. The  $\text{Li}_3\text{NiPO}_4\text{CO}_3$  system was chosen to be investigated because this material has good performance such as the highest energy density of all the carbonophosphate materials, cheap and less harmful to human and environment [1,2]. Based on first principles calculations, we determined the most stable spin configuration of the Ni system, calculated its crystal and electronic structures of that configuration. Despite requiring numerous computational resources, HSE06 functional is needed for investigation of  $\text{Li}_3\text{NiPO}_4\text{CO}_3$  properties due to the failure of the GGA+U method in the defect case. The GGA+U method cannot describe bound states appearing in the band gap of DOS in the defect case, while HSE06 succeeds. We also shown that a polaron appears simultaneously with the presence of a Li vacancy; therefore, the diffusion inside this material is considered as the diffusion of a polaron-Li vacancy complex. Employing the Nudge Elastic Band (NEB) method, we explore favourable diffusion processes with low activation barriers among the explored possible elementary processes, then combine them into the favourable diffusion pathways.

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**Presenter: Dương Thị Diễm My**

P.11 – Poster, IWTCP-3

## Alzheimer's Amyloid- $\beta$ Sequesters Caspase-3 via its C-terminal Tail

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Alzheimer's disease (AD) is the most common neurodegenerative disease in the elderly. Amyloid- $\beta$  (A $\beta$ ), the main constituent in the senile plaques found in the brain of AD patients, is considered the causative factor in AD pathogenesis. Clinical examination using AD brains have found that caspase-3 colocalizes with the senile plaques and biochemical studies have shown that A $\beta$  is able to induce neuronal apoptosis via caspase-3 activation. Here, to investigate the possible direct effect of A $\beta$  to caspase-3, we performed enzymatic studies and in silico study to understand the molecular mechanism of A $\beta$  and caspase-3. We found A $\beta$  conformers can directly sequester caspase-3 activity in which A $\beta$ 42 monomer is most potent with IC<sub>50</sub> around 1.5  $\mu$ M and has a better inhibition effect in comparison to A $\beta$ 40. The inhibition is non-competitive and the C-terminal region of A $\beta$  plays an important role in the sequestration. The binding of A $\beta$  to caspase-3 was studied by the docking and all-atom molecular dynamics simulations. It was shown that, in agreement with the experiments, A $\beta$ 42 has higher binding affinity than A $\beta$ 40 and the hydrophobic C-terminal plays a key role in the caspase-A $\beta$  interaction. Overall, our result demonstrated that A $\beta$ -induced caspase-3 activation in cells is from indirect events and A $\beta$  is able to sequester caspase-3 activity via direct interaction.

**Presenter: Nguyen Hoang Linh**

P.12 – Poster, IWTCP-3

## Preformed template fluctuations promote fibril formation: Insights from lattice and all-atom models

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Fibril formation resulting from protein misfolding and aggregation is a hallmark of several neurodegenerative diseases such as Alzheimer's and Parkinson's diseases. Despite the fact that the fibril formation process is very slow and thus poses a significant challenge for theoretical and experimental studies, a number of alternative pictures of molecular mechanisms of amyloid fibril formation have been recently proposed. What seems to be common for the majority of the proposed models is that fibril elongation involves the formation of pre-nucleus seeds prior to the creation of a critical nucleus. Once the size of the pre-nucleus seed reaches the critical nucleus size, its thermal fluctuations are expected to be small and the resulting nucleus provides a template for sequential (one-by-one) accommodation of added monomers. The effect of template fluctuations on fibril formation rates has not been explored either experimentally or theoretically so far. In this paper, we make the first attempt at solving this problem by two sets of simulations.

To mimic small template fluctuations, in one set, monomers of the preformed template are kept fixed, while in the other set they are allowed to fluctuate. The kinetics of addition of a new peptide onto the template is explored using all-atom simulations with explicit water and the GROMOS96 43a1 force field and simple lattice models. Our result demonstrates that preformed template fluctuations can modulate protein aggregation rates and pathways. The association of a nascent monomer with the template obeys the kinetics partitioning mechanism where the intermediate state occurs in a fraction of routes to the protofibril. It was shown that template immobility greatly increases the time of incorporating a new peptide into the preformed template compared to the fluctuating template case. This observation has also been confirmed by simulation using lattice models and may be invoked to understand the role of template fluctuations in slowing down fibril elongation

**Presenter: Nguyen Truong Co**

P.13 – Poster, IWTCP-3

### **Improved thermoelectric properties of graphene devices by strain and doping engineering**

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The thermoelectric effect enables direct conversion of a temperature difference into an electric voltage and vice versa, and provides a viable route for electrical power generation from waste heat. It has been shown in the literature that low dimensional and/or nanostructured materials have better thermoelectric properties than that in bulk materials [1,2]. In this regard, graphene, a mono-layer of carbon atoms, is a truly 2D material and hence could be a promising channel for thermoelectric devices. However, graphene still has a drawback due to its gapless character, which makes it difficult to separate the contribution of electrons and holes and leads to a weak Seebeck effect ( $S < 100 \mu\text{K}/\text{V}$  in pristine graphene [3]). Hence, several energy-gap nanoengineerings have been suggested to solve this issue [4].

Recently, we found that strain engineering is a promising technique to generate a finite energy-gap in graphene strain heterochannels [5]. In this work, we propose to exploit this effect to enhance the thermoelectric properties (particularly, Seebeck coefficient) of graphene devices. We demonstrate that due to the strain-induced energy-gap, the Seebeck coefficient in graphene strained heterochannels can be significantly enlarged, i.e., 17 times higher than that in pristine graphene when a strain of 10% is applied. However, to avoid the requirement of a large strain, we propose to use this type of heterochannel in graphene p-n devices. In the p-n devices, the displacement of electronic structure in two highly doped sections can further enlarge the energy-gap of transmission and hence can be helpful for further enhancing the Seebeck effect. Indeed, we demonstrated that in such graphene p-n devices with a local strain, a similarly high Seebeck coefficient can be achieved with a small strain of only 5%. The dependence of these phenomena on the lengths of strain section and transition region between highly doped parts has been also clarified. Thus, we demonstrated that besides its use in strain sensors [5], this design strategy is very promising to achieve good performance in graphene devices based on the Seebeck effect, as thermal sensors [6].

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**Presenter: Mai Chung Nguyen**

P.14 – Poster, IWTCP-3

### **Interactions between small molecules and amyloid beta peptides: Implications for Alzheimer's disease**

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Since available drugs can not cure the Alzheimer's disease (AD), the computer-aided drug design has become one of the most important tools to search for potential AD drugs recently. According to the amyloid cascade hypothesis, supported by many experiments, the self-assembly of amyloid beta ( $A\beta$ ) peptides into aggregates is the major cause for this disease. Thus  $A\beta$  oligomers and fibrils are target for our computational study. Combining the molecular docking and molecular dynamics simulations to study the binding affinity of ligands to  $A\beta$  peptides, we found that small molecules Curcumin (diferulomrthane), Naproxen, Ibuprofen, [1] Propafenone [2], Dracorubin, Taraxerol, Taraxasterol, Hinokiflavone, Diosgenin [3], Vitamin K3 analogues (VK3-6, VK3-8, VK3-9, VK3-10, and VK3-224) [4] are potential compounds that may be inhibit  $A\beta$  aggregation. The binding poses of these ligands to receptors were predicted by the docking method while the binding free energy was refined using either the molecular mechanic-Poisson Boltzmann surface area or free energy perturbation methods. The binding mechanism of potential inhibitors was discovered that the interaction between ligand and  $A\beta$  is driven by the van der Waals interaction. The change in  $A\beta$  structures upon ligand binding have been also considered to clarify the impact of inhibitors on  $A\beta$  self-assembly. The pharmacological characteristics of potential drugs including the absorption, distribution, metabolism, excretion, and toxicity were studied using in silico and in vitro experiments. Finally, anti-arrhythmic medication Propafenone [2], Dracorubin, Taraxerol [3], VK3-10, VK3-6, and VK3-9 [4] were found to be more potent than Curcumin in blocking  $A\beta$  activity. Our theoretical results have been confirmed by in vitro experiments.

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**Presenter: Ngo Son Tung**

P.15 – Poster, IWTCP-3

### **A New Model for the Collective Behavior of Animals**

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We propose a new model in order to study behaviors of self-organized system such as a group of animals. We assume that the individuals have two degrees of freedom corresponding one to their internal state and the other to their external state. The external state is characterized by its moving orientation. The rule of the interaction between the individuals is determined by the internal state which can be either in the non-excited state or in the excited state. The system is put under a source of external perturbation called “noise”. To study the behavior of the model with varying noise, we use the Monte-Carlo simulation technique. The result clearly shows two first-order transitions separating the system into three phases: with increasing noise, the system undergoes a phase transition from a frozen dilute phase to an ordered compact phase and then to the disordered dispersed phase. These phases correspond to behaviors of animals: uncollected state at low noise, flocking at medium noise and runaway at high noise, respectively.

**Presenter: Nguyễn Phước Thế**

P.16 – Poster, IWTCP-3

### **A model of optical trapping cold atoms using a metallic nano wire with surface plasmon effect**

*Nguyen Thi Phuong Lan (1), Duong Thi Ha (2), Chu Thuy Anh (3), Do Thi Nga (3), Nguyen Ai Viet (3)*

*(1) Hanoi Pedagogical University 2; (2) Thainguyen University ; (3)Institute of Physics, VAST*

In this work, we construct a new model of optical trapping cold atoms with a metallic nano wire by using surface plasmon effect generated by strong field of laser beams. Using the skin effect, we send a strong oscillated electromagnetic field through the surface of a metallic nano wire. The local field generated by evanescent effect creates an effective attractive potential near the surface of metallic nano wires. The consideration of some possible boundary and frequency conditions might lead to non-trivial bound state solution for a cold atom. We discuss also the case of the laser reflection optical trap with shell-core design, and compare our model with another recent schemes of cold atom optical traps using optical fibers and carbon nanotubes.

**Presenter: Nguyen Thi Phuong Lan**

P.17 – Poster, IWTCP-3

### **Dependence of Effective Diffusivities on Boron impurity Concentration in Simultaneous Diffusion Process in Silicon**

*Vu Ba Dung*

*Hanoi University of Mining and Geology, Vietnam*

Diffusion of impurities such as boron in silicon material is the complex process that is controlled



by intrinsic point defects (self-interstitials and vacancies). Due to the interaction between boron and the crystal lattice, the diffusion process of boron in silicon often gives rise to point defects, which diffuse simultaneously and interact with the boron. Thus, diffusion coefficient of boron and point defect is dependent on that interaction, diffusion coefficient of boron is called effective diffusion coefficient (effective diffusivity). The calculation of effective diffusivity is very difficult. However, using irreversible thermodynamic theory, the effective diffusion coefficient of boron (B), self-interstitial (I) and vacancy (V) in silicon are studied and discussed. The results showed that effective diffusivities of boron and point defect in silicon are dependent on concentration of B, I and V. The calculated results also showed that when B concentration is high, effective diffusivity of boron is increased and diffusivity of point defects are reduced strongly. Furthermore, high concentration of boron makes effective diffusivity of I and V become negative and diffusion process of point defects are backward diffusion in silicon.

**Presenter: Vu Ba Dung**

P.18 – Poster, IWTCP-3

### **THE DEPENDENCE OF MELTING RATE IN HEATING PROCESS OF BORON NITRIDE NANORIBBONS**

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Melting of hexagonal Boron Nitride (BN) model in 2D space with different melting rates is studied via molecular dynamics simulation. The melting rates 1011K/s, 1012K/s, 1013K/s are applied for BN model containing 104 atoms interacted via long-range bond-order potential (LCBOP). Model is heated up from 50 K to 7000 K in order to see the melting rate dependence of various thermodynamic quantities, structural characteristics, occurrence of various structural defects upon heating to a molten state. Some thermodynamic quantities are presented: Temperature dependence of total energy exhibits a first-order-like behavior of the transition at a melting point; heat capacity of the system exhibits a single peak at around the melting point. Melting point of hexagonal Boron Nitride (BN) in 2D space is rather high due to constraint of the 2D space.

**Presenter: Nguyen Thi Thuy Hang**

P.19 – Poster, IWTCP-3

### **Generalized Bogoliubov polariton model with distribution functions for complex systems. Application to stock exchange market**

*Chu Thuy Anh, Truong Thi Ngoc Anh, Nguyen Tri Lan, Nguyen Ai Viet*

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A generalized Bogoliubov method for investigation non-simple and complex systems was developed. We take two branch polariton Hamiltonian model in second quantization representation and replace the energies of quasi-particles by two distribution functions of research objects. Application to stock exchange market was taken as an example, where the changing the form of return distribution functions from Boltzmann-like to Gaussian-like was studied.

**Presenter: Chu Thuy Anh**

P.20 – Poster, IWTCP-3

### **Pi-plasmon model for carbon nano structures. Application to porphyrin**

*Dao Thu Ha, Chu Thuy Anh, Do Thi Nga, Anh D. Phan, Le Minh Thanh, Tran Thi Thanh Van, Nguyen Ai Viet*

*institute of physics*

In traditional concept, the optical properties of semiconductors and semimetals near their fundamental optical band gaps are attributed to single excitations (such electron-hole pairs, excitons...). In our earlier article, we proposed the collective mechanism of pi-plasmons for optical properties of low dimensional carbon nano structures. A simple way to calculate the peak positions of UV-vis absorption spectra was pointed out and gave a good agreement with experimental data. In this work we analyze different schemas to calculate the UV-vis absorption peaks. A new parameter  $k$  characterizing the specific of schema depend on geometry and number of carbon sites is defined. As an example, the case of porphyrin was investigated.

**Presenter: Chu Thuy Anh**

P.21 – Poster, IWTCP-3

### **On the time-dependent spatial dimension in six dimensional space-time**

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In this paper, the time-dependent spatial dimension is considered in six dimensional space-time. The 4-brane is assumed to be a de Sitter space. Based on the form of the brane-world energy-momentum tensor proposed by Shiromizu et al. and then it is applied to five dimensions by Peter K. F. Kuhfittic, we extended the theory to the 2-codimension embedded in higher dimensions. The inflation scenario in 6D is investigated in two case of cosmological constant  $\Lambda > 0$  and  $\Lambda < 0$ .

**Presenter: Phan Hong Lien**

P.22 – Poster, IWTCP-3

### **Prediction of inhibitors of LSD1 protein using molecular modeling and simulation methods**

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LSD1 is a protein found in cell nuclear in 2004. Its main function is demethylation that removes the methyl group of Lysine from Histone protein or p53 protein. LSD1 is also found with high expression in cancer cells such as neuroblastoma, retinoblastoma, breast, lung, and bladder cancer. Thus, blocking LSD1 activity is of great interest as a potential therapy for cancers. In this work, we aim to screen out anticancer drug candidates among natural substances as LSD1

inhibitors using Lipinski's rule and molecular docking approaches. Because the docking method is not accurate enough the results are then refined by steered molecular dynamics simulations to obtain the best candidates ranked by the rupture force. We predict a number small molecules from natural product database TCM which have strong binding affinity to LSD1 protein. They are recommended for further in vitro study as the next step to develop drugs against cancer disease.

**Presenter: Nguyen Quy Truong**

P.23 – Poster, IWTCP-3

### **Folding and escape of nascent proteins at ribosomal exit tunnel**

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We investigate the interplay between folding and escape of nascent proteins at the ribosomal exit tunnel by using Langevin dynamics with coarse-grained models. It is shown that at low temperature, folding co-occurs closely with the escape process resulting in an enhancement of the foldability of protein. The co-occurrence between the two processes, however, deteriorates as temperature increases. The escape process can be characterized as an anomalous diffusion with two different regimes for temperatures below and above the folding transition temperature. It is also shown that attractive interactions between amino acids and attractive sites on the tunnel wall lead to a free energy barrier against the escape of protein from the tunnel. It is suggested this barrier slows down the escape process in order to improve folding efficiency of the released protein.

**Presenter: Bui Phuong Thuy**

P.24 – Poster, IWTCP-3

### **Non-additive effects of crowding and confinement on folding stability of proteins**

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Folding of proteins in vivo typically occurs in a crowded solution and in confined spaces. It is generally accepted that the effects of crowding and confinement are equivalent in terms of enhancement of folding stability of proteins. In this study, by molecular dynamics simulations with simplified models, we show that these two effects are not additive to each other at high concentrations of crowders. It is suggested that at sufficiently high concentrations, the crowders may screen the confinement effects on folding of proteins.

**Presenter: Bui Phuong Thuy**

P.25 – Poster, IWTCP-3

### **Identification of Potential Drugs for Alzheimer's Disease by in Silico and in**

## Vitro Experiments

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Alzheimer's disease (AD) is a disease of the brain that causes problems with memory, thinking and behavior and affects about 18 million people worldwide in the elderly. Currently, there is no efficient treatment for AD as its origin remains unknown. There exist several hypotheses for AD but the amyloid cascade hypothesis, which posits that AD is caused by oligomerization of A $\beta$  peptides, is widely accepted. Thus the target for our drug design problem is A $\beta$  fibrils (PDB ID: 2LMN). The Lipinski rule and docking method were used as a virtual screening tool to find out top hits from the large data base CHEMSPIDER which contains more than 300000 compounds. Thirty-six top-leads that can easily cross the blood-brain barrier as well as be well absorbed by human body were selected for further study by the more precise steered molecular dynamics (SMD) method. The main idea of this method is that instead of the binding free energy the rupture force needed to unbind a ligand from a receptor is used as a measure of binding affinity, i.e. the higher is rupture force, the stronger is binding. Note that the rupture force is defined as a maximum in the force-time/displacement profile. Using SMD method we have found ten top hits that are recommended for further in vitro experiments. We succeeded to purchase two compounds Hoechst 34580 (C27H29N7) and Hoechst 33342 (C27H28N6O) which are commercially available cell-permeable fluorescent dye for staining DNA and nuclei. Using the AFM and ThT fluorescence we have demonstrated that these two compounds can block A $\beta$  aggregation with the inhibition constant IC<sub>50</sub> of about 0.6 and 0.8  $\mu$ M for Hoechst 34580 and Hoechst 33342, respectively. This experimental result is in qualitative agreement with our estimation of the binding free energy ( $\Delta G_{\text{bind}} \approx -10$  kcal/mol) using the MM-PBSA method.

**Presenter: Nguyen Quoc Thai**

P.26 – Poster, IWTCP-3

## First-principles Study on Controlling Energy Gap of Graphene using Hybrid Armchair-Zigzag Structures

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The electronic and transport properties of hybrid armchair-zigzag nanostructures including U-shaped graphene nanoribbons (GRNs) and patterned nanopores structured graphene were studied using combination of density functional theory and non-equilibrium Green's function method. The density of state, electron transmission spectra, and molecular orbitals were analyzed. The obtained results show that GNRs junctions tend to open a energy gap when U-shaped structures were formed due to the formation of quasi-bound states at zigzag edges. The size of U-shaped structures has enormous influences on the electron transport of the system. We also considered the effect of corner form of the U-shaped GNRs junctions on energy gap opening. It was found that as some carbon atoms are add to the inner corner, the energy gap in U-shaped GNRs significantly changed. For patterned nanopores structured graphene, the calculated results show that patterned nanopores enormous influence on electronic and the transport properties though the GNRs junctions, depending on the shape, size, and the number of nanopores. The study suggests

that designed tailored graphene systems based on hybrid armchair-zigzag nanostructures can be used to control the energy gap of graphene.

**Presenter: Nguyen Tien Cuong**

P.27 – Poster, IWTCP-3

## PROTEIN REFOLDING UNDER AN EXTERNAL MECHANICAL FORCE

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With recent advances in single molecule manipulation techniques, it has become possible to control folding behavior of biological molecules and to obtain unprecedented information about physical basis of the refolding process [1]. The intrinsic parameters of free energy landscape, such as the distance between transition state and native state,  $x_F$ , and the folding time in the absence of force,  $\tau_F^0$ , can be reconstructed from force-dependent quantities using Bell's theory,  $\tau_F = \tau_F^0 \exp(-fx_F/k_B T)$ . Using off-lattice Go model and the Langevin dynamics, we have confirmed the exponential dependence of refolding time on external force for 20 different proteins. We discuss the  $x_F$  correlations with (1) mechanical unfolding parameters, such as mechanical stability,  $f_U$ , and the distance between unfolded and transition states,  $x_U$ , as well as (2) topological descriptors such as contact order and fraction of secondary structure content. With the help of discovered empirical relationships we propose predictive tools which would allow one to characterize unstudied experimentally proteins and to detect the proteins with desired properties.

[1] S. Kumar and M. S. Li, Biomolecules under mechanical force, Phys. Reports 486, 1-74 (2010)

**Presenter: Pham Dang Lan**

P.28 – Poster, IWTCP-3

## A New Method for Determination of Optimal Pulling Direction for ligand from Binding Pocket: Application to Ranking Binding Affinity by Steered Molecular Dynamics

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In this contribution we present a new method for finding the optimal path to pull ligand from the binding pocket using steered molecular dynamics (SMD). Scoring function is defined as the steric hindrance caused by receptor to ligand movement. Then the optimal path corresponds to minimum of the scoring function. We call the new method SMDA (SMD assisted) because SMD simulation is applied to navigate optimal direction. Contrary to existing navigation methods, our approach takes into account geometry of ligand while other methods including CAVER consider ligand as sphere with a given radius. Using three different target+receptor sets, we have shown that the rupture force  $F_{\max}$  and non-equilibrium work  $W_{\text{pull}}$  obtained by SMDA method show much higher correlation with experimental data on inhibition constants compared to CAVER. Furthermore,  $W_{\text{pull}}$  was found to be a better indicator for binding affinity than  $F_{\max}$ . Thus, new SMDA method is a reliable tool for obtaining the best direction for ligand exiting from the

binding site. Its combination with the standard SMD technique can provide reasonable results for ranking binding affinities using  $W_{pull}$  as a scoring function.

**Presenter: Vuong Van Quan**

P.29 – Poster, IWTCP-3

### **Analysis of Binding Affinity of Derivatives of Vitamin K3 to Fibrils of A $\beta$ peptides**

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Aggregation of amyloid-beta (A $\beta$ ) has been proposed as the main cause of Alzheimer's disease (AD). Vitamin K deficiency has been linked to the pathogenesis of AD. Therefore, 4 vitamin K3 (VK3) analogues were proposed and studied for their anti-amyloidogenic activity. Chemical formulas for VK3-1, VK3-2, VK3-3 and VK3-4 are C<sub>14</sub>H<sub>14</sub>O<sub>6</sub>S, C<sub>14</sub>H<sub>12</sub>O<sub>7</sub>S, C<sub>17</sub>H<sub>12</sub>O<sub>6</sub>S, and C<sub>17</sub>H<sub>12</sub>O<sub>7</sub>S, respectively. Using docking method and all-atom (Gromos 96 43a1 force field) molecular dynamics simulations in explicit water, we studied their binding affinity to A $\beta$  peptides and fibrils. The binding free energy was analyzed by the molecular mechanic-Poisson-Boltzmann surface area method (MM/PBSA). The results show that the electrostatic interaction correlates to the binding free energy better than the van der Waals interaction does. According to our estimations of the binding free energy the rank-ordering of binding affinity to A $\beta$  is VK3-1 > VK3-3 > VK3-4 > VK3-2 implying that VK3-1 is the most prominent in preventing aggregation. However, we recommend VK3-3 for further in vitro and in vivo study as it can cross the blood brain barrier better than other compounds.

**Presenter: Vu Thi Mui**

P.30 – Poster, IWTCP-3

### **pH-dependence of UV-visible Spectra of human-Neuroglobin, a sign of structural and dynamical properties based on Two-Level Model**

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Neuroglobin (Ngb), a novel member of the Globin Group, was recently discovered by Burmester et al. (2000). Its uncertain physiological function makes lots of interest. The existing of a six-coordination heme geometry with proximal and distal histidines directly creates an axis within the heme iron, while the sixth ligand coordination binds to small ligand reversibly. In this report, the dissociation form of five-coordination and six-coordinated states of human-Ngb under pH condition have been interpreted by Two-level model.

**Presenter: Nguyễn Minh Hoa**

P.31 – Poster, IWTCP-3

### **Study of amyloid fibrillation in a simple model**

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In amyloids, polypeptides self-assemble into hierarchically organized fibrils. A fibril often consists of 2-6 filaments made up from  $\beta$ -sheets running parallel to each other. We study the fibrillation process using an XY spin model, in which the spins can rotate freely in the  $xy$  plane, whereas elongation of filaments proceeds only in  $z$  direction. To model the packing of filaments, each lattice site is allowed accommodate several spins belonging to different sublattices of the same spatial coordination. At intermediate temperatures, it is shown that fibrillation happens only when the total concentration of peptides exceeds some threshold value. When the latter is satisfied, the concentration of free peptides decreases as the total concentration of peptides increases.

**Presenter: Nguyen Ba Hung**

P.32 – Poster, IWTCP-3

### **Simple model for gold nano particles GNPs concentration dependence of Resonance Energy Transfer intensity**

*Nguyen Minh Hoa (2), Chu Viet Ha (3), Do Thi Nga (1), Nguyen Tri Lan (1), Tran Hong Nhung (1), Nguyen Ai Viet (1)*

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Gold nano particles GNPs concentration dependence of the energy transfer occurs between the fluorophores and GNPs is investigated. In the case of these pairs, the gold nanoparticles can enhance or quench the fluorescence of fluorophores depending upon the relative magnitudes of two energy transfer mechanisms: i) the plasmonic field enhancement at the fluorophores emission frequencies (plasmon coupled fluorescence enhancement) and ii) the localized plasmon coupled Förster energy transfer from fluorescent particles to gold particles, which quenches the fluorescence. The competition of these mechanisms is depending on the spectral overlap of fluorophores and GNPs, their relative concentration, excitation wavelength. Simple two branches surface plasmon polariton model for gold nano particles GNPs concentration dependence of the energy transfer is proposed. We obtain quite good agreement of the theoretical results with experimental data.

**Presenter: Nguyễn Minh Hoa**

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