PROGRAM TIME TABLE

Day 1 (21/11/2022)	**Arrivals at the Conference Venue**
13:00 - 17:00	▪ Registration ▪ Meeting of the International Advisory Board and the Key Scientific Program Committee
18:00 - 20:00	Welcome party for Invited speakers and International Advisory Board
Day 2 (22/11/2022)	**Conference** (1/2)
8:00 - 8:30	**Registration**
8:30 - 9:00	**Opening ceremony** **Chairmen: Wu-Ching Chou, Michael Lang** ▪ Sponsors remarks: 8.30-8.40: Nguyen Dang Khoa, Energy and Environment – LiB applications with PSA and XGT, Horiba Viet Nam ▪ Organizers remarks ▪ Keynote speeches by Chairmen
	Opening Plenary Session **Chairmen: Masato Yoshiya, Nguyen Nang Dinh**
9:00 - 9:30	Plenary talk **PL1** ***Akihide Kuwabara*** *Japan Fine Ceramics Center* First-principles calculations of defect formation behavior and ion dynamics in solid state ionics materials
9:30 - 10:00	Plenary talk **PL2** ***Yoon-Hwae Hwang, Hyung-Kook Kim and Dong-Myeong Shin*** *Pusan National University* Nanogenerators: self-powered energy for technology innovation
10:00 - 10:30	Plenary talk **PL3** ***Nguyen The Toan*** *VNU-University of Science* Molecular understanding of protein structure and interaction related to Covid-19 and gout diseases by using computational biophysics
10:30 - 11:00	Coffee break (1/3) Group photographs/photography of participants

11:00 - 12:30	**Parallel sessions 1** (15)		
Time	**Section MM** Multiferroics and magnetic materials (1/3) **Chairmen: Nguyen Huu Duc, Jehn Yih Juang**	**Section EE** Materials for energy and environment (1/2) **Chairmen: Yoon-Hwae Hwang, Masato Yoshiya**	**Section PH** Photonics and Hybrid Materials (1/2) **Chairmen: Mikhail Brik, Way-Faung Pong**
11:00 -11:20	**MM-I01** (Invited) ***Michael Lang, Christian Thurn, Paul Eibisch, et al.*** $PbCuTe_2O_6$ – a quantum spin liquid candidate showing ferroelectric order close to a quantum critical point	**EE-I01** (Invited) ***Nguyen Hoang Nam, Do Quang Loc, Phi Thi Huong et al.*** $CD4^+$ T cell counting using anti-CD4 antibody conjugated magnetic nanoparticles and microfluidic counter	**PH-I01** (Invited) ***Tomoyuki Yamamoto*** Local environment of emission center ions in phosphor materials
11:20-11:40	**MM-I02** (Invited) ***Yoshifuru Mitsui and Keiichi Koyama*** Application of magnetic field for selective reaction in magnetic alloys	**EE-I02** (Invited) ***Kei Nakayama, Ryo Ishikawa and Yuichi Ikuhara*** Structural analysis of battery materials by atomic-resolution scanning transmission electron microscopy	**PH-I02** (Invited) ***Michal Piasecki, Galyna Muronchuk, Andrzej Suchocki et al.*** Luminescence and non-linear optical properties at mid-infrared spectral range
11:40-12:00	**MM-I03** (Invited) ***Hajime Yamamoto*** Crystal structures and electronic properties of vanadium oxides	**EE-I03** (Invited) ***Ho Won Jang*** Si-based photoelectrodes for water splitting	**PH-I03** (Invited) ***Huu-Quang Nguyen, My-Chi Nguyen and Jaebeom Lee*** Magnetoplasmonic core-shell nanowires: synthesis and self-assembly for structural colors and chiral metasurfaces
12:00-12:15	**MM-O01** (Oral) ***Jiunn-Yuan Lin*** An emergent quasi-2D metallic state derived from the Mott insulator framework	**EE-O01** (Oral) ***Thi Thao Vu, Xuan Tung Nguyen, Dinh Tu Bui, et al.*** Review of Langmuir-Blodgett films of octadecylamine: Fabrication, properties, and application	**PH-O01** (Oral) **(Cancelled)** ~~***Minh Triet Dang, Pham Vu Nhat and Van An Dinh***~~ ~~Optoelectronic and vibrational properties of nitrogen-doped hexagonal graphene quantum dots~~
12:15-12.30	**MM-O02** (Oral/Online) ***Yoyo Hinuma*** Deriving maximally orthogonalized supercells with given size	**EE-O02** (Oral) ***My-Chi Nguyen, Huu-Quang Nguyen and Jaebeom Lee*** Lanthanide-based magnetoplasmonic probes for highly sensitive aqueous copper(II) sensing	**PH-O02** (Oral) ***Chia-Chun Wei, Tung-Han Wu and Wen-Bin Jian*** Preparation of nanoparticulate WO_3/MoO_3 films for making electrochromic devices
12:30 - 13:30	Lunch		
13:30 - 14:30	**Poster sesstions** Note: (i) All posters are requested to be in the A1 format; (ii) to be put on each panel from afternoon of Nov 21st and (iii) removed from the panel before lunch time of Nov 23rd		

- Best posters: 02 - Silver: 03 - Bronze: 05	**Section EE** Materials for energy and environment ***Chairmen:*** **Nguyen Dinh Lam** **Codes: EE-P01 - EE-P30** **Location: Ballroom 1**	**Section MM** Multiferroics and magnetic materials ***Chairmen:*** **Phan Bach Thang** **Codes: MM-P01 - MM-P29** **Online: MM-P01, P03, P08, P09, P13, P15** **Location: Ballroom 2**	**Section SD** Spintronic materials and devices ***Chairman:*** **Do Thi Huong Giang** **Codes: SD-P01 - SD-P10** **Location: Ballroom 3**	**Section PH** Photonics and Hybrid Materials ***Chairman:*** **Nguyen Kien Cuong** **Codes: PH-P01 - PH-P08** **Location: Ballroom 3**	**Section TC** Theory and computation ***Chairman:*** **Nguyen Quang Bau** **Codes: TC-P01 - TC-P07** **Location: Ballroom 3**
	Best poster Awards Committee **- Chairman: Prof. Yoon-Hwae Hwang** **- Members:** Do Thi Huong Giang, Nguyen Dinh Lam, Phan Bach Thang, Chun-Liang Lin, Ray-Hua Horng, Chung-Li Dong, Susumu Fujii, Kei Nakayama, Tetsuya Yokoi, Jin Young Kim, Ho Won Jang, Bernd Wolf, Matthijs Jansen				

14:30 - 16:30	**Parallel sessions 2** (18)		
Time	**Section MM** Multiferroics and magnetic materials (2/3) **Chairmen: Kazunori Sato, Ray-Hua Horng**	**Section TC** Theory and computation (1/2) **Chairmen: Vu Ngoc Tuoc, Susumu Fujii**	**Section SD** Spintronic materials and devices (1/3) **Chairmen: Takashi Kimura, Sungkyun Park**
14:30-14:50	**MM-I04** (Invited) **(Free)** ~~***Dong-Hyun Kim***~~ ~~Spin Dynamics in Ferromagnetic Thin Films~~	**TC-I01** (Invited) ***Andreas Honecker*** Thermodynamic properties of the Shastry-Sutherland model for $SrCu_2(BO_3)_2$	**SD-I01** (Invited) ***Wataru Norimatsu*** Observation of flat band in millimeter-scale magic-angle twisted bilayer graphene
14:50-15:10	**MM-I05** (Invited) ***Bernd Wolf, Felix Spathelf, Jan Zimmermann et al.*** Tuning the ground state of strongly correlated $EuPd_2(Si_{1-x}Ge_x)_2$ using He-gas pressure	**TC-I02** (Invited) ***Koun Shirai*** The Activation Energy of Glass Transition	**SD-I02** (Invited) ***Chanyong Hwang*** Towards Magnetic Skyrmionics
15:10-15:30	**MM-I06** (Invited) ***Ivan Skorvanek, Branislav Kunca, Jozef Marcin et al.*** Soft magnetic Fe(Co)-based high Bs nanocrystalline alloys for applications at elevated temperatures	**TC-I03** (Invited) ***Masato Yoshiya, Tomofumi Hara, Wataru Sekimoto et al.*** Selective control of propagation-conduction of two different quantum waves by lattice imperfections: electrons and phonons	**SD-I03** (Invited) ***Bae Ho Park*** Neuromorphic devices based on electrochemical metallization and charge trapping
15:30-15:50	**MM-I07** (Invited) ***Way-Faung Pong*** X-ray spectro- and microscopic-techniques on novel materials	**TC-I04** (Invited / Online) ***Manh-Thuong Nguyen*** Computational approaches to study heavy element materials	**SD-I04** (Invited) ***Teruo Ono*** Superconducting diode effect in Rashba superlattice
15:50-16:10	**MM-I08** (Invited) ***Tahta Amrillah, My Ngoc Duong and Jenh-Yih Juang*** Substrate polarity, phase stability, electronic structure and magnetic properties of multiferroic $YMnO_3$ thin films	**TC-I05** (Invited) ***Tatsuya Yokoi, Yu Oshima and Katsuyuki Matsunaga*** Artificial-neural-network descriptor and interatomic potential for molecular simulations of lattice defects	**SD-I05** (Invited / Online) ***Takeshi Seki*** Enhanced anomalous Nernst effect in metallic superlattices
16:10-16:30	**MM-I09** (Invited) ***Masanobu Shiga, Takurou Harada, Tsubasa Teramoto et al.*** Point contact Andreev reflection spectroscopy on topological Kondo insulator SmB_6	**TC-O01** (Oral) ***Katsuhiro Suzuki, Takao Kotani and Kazunori Sato*** The first-principles analysis of Multiplet excitations using QSGW	**SD-I06** (Invited) ***Hieu Ho, Hai Hoang, Minh-Hanh Pham and Hai Tran*** Extended x-ray absorption spectroscopy and Debye–Waller factor under pressure
16:30 - 16:45	Coffee break (2/3)		
16:50 - 18:30	**Parallel sessions 3** (21)		
Time	**Section MM** Multiferroics and magnetic materials (3/3) **Chairmen: Kei Nakayama, Thi Ngoc Anh Nguyen**	**Section TC** Theory and computation (2/2) **Chairmen: Tatsuya Yokoi, Vu Thanh Tra**	**Section SD** Spintronic materials and devices (2/3) **Chairmen: Nguyen Trong Tinh, Bae Ho Park**
16:50-17:10	**MM-I10** (Invited) ***Sungkyun Park and Sehwan Song*** Searching for the origin of magnetic inhomogeneity of FeRh film	**TC-I06** (Invited) ***Tien Quang Nguyen, Yusuke Nanba, Michihisa Koyama et al.*** Accelerating materials discovery using universal neural network potential and *ab-initio* calculations	**SD-I07** (Invited) ***Ray Hua Horng*** Material properties and growth mechanism of β-Ga_2O_3 epilayers grown on sapphire by metal organic chemical vapor deposition
17:10-17:30	**MM-I11** (Invited) ***Yoshishige Suzuki, Soma Miki, Ryo Ishikawa et al.*** Magnetic skyrmion for the Brownian computing	**TC-I07** (Invited) ***Susumu Fujii, Yuta Shimizu, Junji Hyodo et al.*** Exploration for non-perovskite proton-conducting oxides using high-throughput computation and machine learning	**SD-I08** (Invited/Online) ***Masashi Akabori*** Fabrication of quantum devices by fine sputtering using a focused ion beam with nitrogen gas field ion source

17:30-17:45	**MM-O03** (Oral) ***Yuichi Okazaki, Yushi Fujita, Hidenobu Murata et al.*** Bayesian optimization design of high entropy oxide for oxygen evolution catalysis	**TC-I08** (Invited) (*17:30-17:50*) ***Kazunori Sato, Genta Hayashi, Kazuma Ogushi et al.*** Computational materials design of high-entropy alloys based on FPKKR-CPA calculations and machine learning techniques	**SD-O01** (Oral) ***Ngoc Nam Ho, Katsuhiro Suzuki, Akira Masago et al.*** Solid-liquid structure of Cu2S: theoretical acanthite-like model for electronic and transport properties investigations
17:45-18:00	**MM-O04** (Oral) ***Ba Hung Tran and Yu-ichiro Matsushita*** Magnetocaloric effect from first-principles calculations and Monte Carlo simulations	**TC-I09** (Invited) (*17:50-18:10*) ***Huan Tran*** Accelerating materials science with artificial intelligence	**SD-O02** (Oral) ***Shiuanhuei Lin, Stefan Petrov and Vera Marinova*** Graphene supported liquid crystal phase retarders on rigid glass and flexible polydimethylsiloxane substrates
18:00-18:15	**MM-O05** (Oral) ***Phi Thi Huong, Bui Duc Tri, Nguyen Thi Thanh Van et. al*** Synthesis of bifunctional magnetic-plasmonic Fe3O4@SiO2-Au nanoparticles by an ultrasound assisted chemical method		**SD-O03** (Oral) ***Chung Li Dong*** Advantages, Challenges and Opportunities of X-ray Absorption spectroscopy for advanced investigation of energy materials
18:15-18:30	**MM-O06** (Oral) ***Nguyen Duy Thien, Nguyen Quang Hoa, Vuong Van Hiep et al.*** Thermal evaporation synthesis and some properties of WO3/ITO electrochromic thin films	**TC-I10** (Invited) (*18:10-18:30*) ***Hirofumi Tanaka*** Material intelligence: in-materio reservoir computing devices composed by random network of nanoparticles	**SD-O04** (Oral) ***Canh Tuan Nguyen, Nam Nguyen Phuong Hoai, Cuong Nguyen Duc et al.*** Fabricate electrospun nanofiber for rechargeable batteries
18:30-18:45	**MM-O07** (Oral) ***Thi Van Anh Nguyen and Duong Vu*** Fabrication of RuO_2 thin film for spin orbit torque – induced magnetization switching	**TC-O02** (Oral) ***Sena Hoshino, Yu Oshima, Tatsuya Yokoi et al.*** Carrier-trapping induced transformation of dislocation core structures in Zn compounds	**SD-O05** (Oral) ***Minh Nhat Dang, Surinder Singh, Thomas G. Pattison, et al.*** Is it possible to electropolish tungsten carbides?
19:30-21.30	Banquet		
Day 3 (23/11/2022):	**Conference** (2/2)		
08:00 - 09:45	**Parallel sessions 4** (18)		
Time	**Section EE** Materials for energy and environment (2/2) **Chairmen: Yoon-Hwae Hwang, Akihide Kuwabara**	**Section SD** Spintronic materials and devices (3/3) **Chairmen: Bui Dinh Tu, Huan Tran**	**Section PH** Photonics and Hybrid Materials (2/2) **Chairmen: Michal Piasecki, Ngac An Bang**
08:00-08:20	**EE-I04** (Invited) ***Jessiel Siaron Gueriba, Nur Ellina Annisa Salehuddin, Wilson Agerico Diño et al.*** Defluorination and adsorption of tetrafluoroethylene (TFE) on TiO_2(110) and Cr_3O_3(0001)	**SD-I09** (Invited/Online) ***Takashi Kimura*** Study of nano-scale heat transports using magneto-thermoelectric effects	**PH-I04** (Invited) ***Jin Young Kim*** High-performance colorful semitransparent organic solar cells with etalon electrodes
08:20-08:40	**EE-I05** (Invited) ***Moongyu Jang*** Single cell capacitance measurement of NIH 3T3 cell using impedance biosensor	**SD-I10** (Invited/Online) ***Tho Duc Nguyen*** Sub-second and ppm-level optical sensing of hydrogen using templated control of nano-hydride geometry and magnetic composition	**PH-I05** (Invited) ***Matthijs Jansen*** Probing the exciton wavefunction in low-dimensional materials by photoemission momentum microscopy
08:40-08:55	**EE-O03** (Oral) ***Cong Doanh Sai, Van-Phu Vu, Viet Tuyen Nguyen et al.*** Fast synthesis of ZnO/Ag heterostructure nanoparticles for enhanced photocatalytic	**SD-O06** (Oral) ***Tan Le Hoang Doan*** Tandem cyclooxidative reaction of anthranilamide and alcohols over Fe(III)-based MOFs: effect of structure on catalytic efficiency	**PH-O03** (Oral) ***Chun-Liang Lin*** Studying Defects in TMD Materials and Devices by STM

08:55-09:10	**EE-O04** (Oral) **Pham Ngoc Thanh, Yuji Hamamoto, Kouji Inagaki et al.** Van der Waals density functional study of NO-H$_2$O coadsorption on Cu(111)	**SD-I11** (Invited) ***Thi Ngoc Anh Nguyen, Quang Ngan Pham, Van Thanh Chu et al.*** Detection of weak, low-frequency magnetic field using single nanoscale MgO magnetic tunnel junctions	**PH-O04** (Oral) ***Heongkyu Ju, Saikiran Kosame, Than Thi Nguyen and Jun-Ho Lee*** Abnormal spectral shift of surface plasmon resonance
09:10-09:30	**EE-I06** (Invited) ***Ngoc Dinh Nguyen, Vinh Thang Tran, Van Thanh Pham et. al*** Development of a 3D bio-printing system for tubular tissue creation using umbilical cord-derived stem cell spheroids as bio-ink	**SD-I12** (Invited) ***Dang Ngoc Toan*** Neutron diffraction study of state-of-the-art 2D materials	**PH-I06** (Invited) *Nguyen Thanh Tung* Metamaterials: plasmonic properties, ultrafast dynamics, heat transfer, and tuneability
09:30-09:45	**EE-O05** (Oral) ***Ngo Tran, Ruey-Bin Yang and B. W. Lee*** Development of high-efficient multi-layer microwave absorbers using Co-doped $BaMnFe_{11}O_{19}$ nanoparticles	**SD-O07** (Oral) ***Thi Thuy Nguyen, Tatsuaki Hirata and Shin-Ichiro Kuroki*** Nanowire single crystal grain field effect transistors and their applications	**PH-O05** (Oral) ***Der Hsien Lien*** Electronics and optoelectronics of atomically thin semiconductors
09:45 - 10:15	Coffee break (3/3)		
	Closing Plenary Session **Chairmen: Tomoyuki Yamamoto, Hyung Kook Kim**		
10:15 - 10:45	Plenary talk **PL4** ***Ssu Kuan Wu, Nhu Quynh Diep, Hua Chiang Wen, Wu-Ching Chou and Thanh Tra Vu*** *National Yang Ming Chiao Tung University* Growth dynamics and physical properties of III-VI two dimensional semiconductors grown by molecular beam epitaxy		
10:45 - 11:15	Plenary talk **PL5** ***Ekkes Bruck*** *Delft University of Technology* Fe2P type alloys: an intriguing magnetic playground		
11:15 - 11:45	Plenary talk **PL6** ***Mikhail Brik*** *Jan Dlugosz University, Poland* Optical and electronic properties of crystalline solids from the first-principles and semiempirical methods		
11:45 - 12:00	**Final remarks** **Chairmen: Wu-Ching Chou, Michael Lang** - Introduction of the next FMS - Publication notes: available journals, manuscript submission deadlines		
Conference closes			

HORIBA Scientific

Particle Size Analysis& X-ray fluorescence Analysis in Li-Battery Materials

Abstract

This topic focusesmainly on particle size analysis & EDXRF analysis in battery. Battery technology is improving, keeping up with the demand for more portable devices and the desire for better power storage for longer periods between chargingand changing batteries.Batteries production also requires fast, easy, and accurate QC monitoring, which provides fast detection of faults in safety and performances issues, along with fast decision making when fault is suspected. This will save time and money, while providing perfect traceability. Particle size analyzer from Horiba was used to perform particle size distribution measurements on various materials used in the creation of lithium-ion batteries. Additionally, non-destructive analytical technique which can inspect defects, evennon-visibleones, inside a sample because of the high penetration of X-rays by using XGT-9000. HORIBA analytical instruments provide unprecedented levels of reliability, reproducibility and sensitivity, combined with advanced data sciences, to contribute in the development of renewable source of energy, and making energy production and consumption more efficient.

Introduction

The particle size distribution (PSD) of the materials used to make these batteries is tested in both R&D environments and in QC for product acceptance since a PSD specification typically exists for the material. Particle size influences both capacity and coulombic efficiency. Reducing the PSD will increase the specific surface area, increasing reaction rates, and changing the size of the voids between electrode particles, which can reduce battery capacity. Thus, tracking PSD during battery development and manufacture is important to optimizing performance. A few examples for using laser scattering (LA series & SZ-100V2) and centrifuge (CN-300)are presented in this introduction. On the other hand, some applications for the use of XGT-9000 in materials battery testing and fabrication will be included in this topic.

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CN-300

LA-960V2

SZ-100V2

XGT-9000

PL1

First-principles calculations of defect formation behavior and ion dynamics in solid state ionics materials

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Solid state ionics devices are widely utilized as battery, fuel cell, gas sensor, and so on. Functional properties of these devices are originated from ionic conduction in ionic crystals. Therefore, we need to control optimally the formation and diffusion of the point defects in order to improve the performance of the solid state ionics devices. First principles calculation is powerful method for analysis of the defect structures because it can theoretically optimize atomic positions around defects and can evaluate quantitatively energy states of defective systems without empirical information. In this presentation, we report formation behavior and dynamics of point defects in solid state ionics devices such as Li ion batteries (LIB) and proton-conductive ceramics fuel cells (PCFC).

Li_2MnO_3-$LiTMO_2$ (TM = Ni, Co, Mn) solid solution systems is promising materials for use cathodes of LIBs with higher energy density and capacity. However, the Li_2MnO_3-$LiTMO_2$ system has a problem regarding lower mobility of charge carriers. We investigated Li ion migration behavior in $Li_{1.2}Mn_{0.567}Ni_{0.167}Co_{0.067}O_2$ by combination of first-principles calculations and scanning transmission electron microscopy. Our calculations reveal that the energy barrier against Li-ion diffusion across the domain boundary is 0.2~0.3 eV higher compared to that in the crystal bulk. In addition, Ni segregation suppresses Li-ion migration.

PCFC is regarded as one of clean energy resources in the next generation because PCFC can convert chemical energies of water generation from H_2 and O_2 gases to electric power. It is necessary to find oxides having high protonic conductivity used for a solid electrolyte of the PCFC. Several kinds of acceptor-doped $BaZrO_3$ systems were systematically studied using first principles calculations. Hydration and association energies are least negative for Er and Y, whose ionic radii are around 0.89−0.9 Å, whereas the oxygen affinity of the strongest proton trapping site is most negative for Lu, with an ionic radius of 0.86 Å. The results reveal that the compound with the highest proton conductivity has the most negative hydration energy and the least negative association energy, in other words, the most negative oxygen affinity.

Keywords: first-principles calculation, solid state ionics, point defect, diffusion, interface

References

[1] H. Yu, Y. -G. So, A. Kuwabara, E. Tochigi, N. Shibata, T. Kudo, H. Zhou, and Y. Ikuhara, Nano Lett. 2016, 16, 2907−2915.
[2] Y. Yamazaki, A. Kuwabara, J. Hyodo, Y. Okuyama, C. A. J. Fisher, and S. M. Haile, Chem. Mater. 2020, 32, 7292−730

PL2

Nano generators : Self Powered Energy for Technology Innovation

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Recently, self powered electric devices attract much attentions due to the future technology trend of IoT based mobile, portable, patchable and even implantable nanodevices in the 4th industrial revolution. The energy harvesting is the process by which an electric energy is delivered from external sources such as solar power, thermal energy, wind energy, mechanical energy, and etc. The energy harvesting, also called energy scavenging, is the promising sustainable, safe, and environmentally friendly technology for the next generation because it harvests electric power directly from the nature without any pollution problems. Nanogenerators are the one of the representative self powered energy harvesting devices which can be used for various nanoelectronic devices. In this talk, I would like to deliver the importance of the nanogenerators in future technology innovation and the underlying interesting physics such as flexoelectgricity, contact electrification and etc. which can enhance the output power of nanogenerators

Keywords: Nanogenerators, Self Powered, Flexoelectricity, Triboelectricity, Piezoelectricity

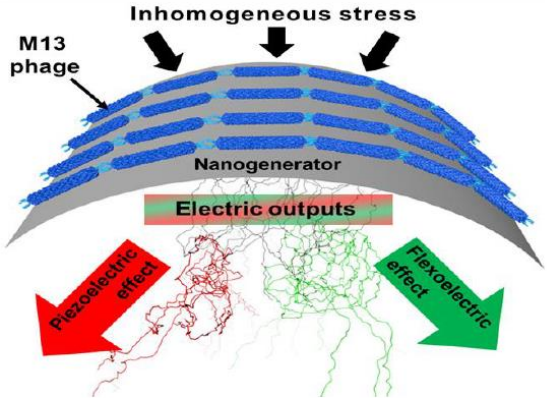

FIG. 1. Schematic explanation of flexoelectric effect in flexible devices

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[2] Hai Phan et al., Nano Energy. 33 (2017) 476.
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PL3

Molecular understanding of protein structure and interaction related to Covid-19 and Gout diseases by using computational biophysics

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In this talk, I will give an overview of Multidisciplinary computational biomolecules research at the Key Laboratory for Multiscale Simulation of Complex Systems. By using and integrating an extensive array of bioinformatics, computational quantum and classical modelling and simulation methods, we can have comprehensive understanding of biomolecules, their structure and functions. Particular focus in this talk will be new research about Gout and Covid-19 being done at the KeyLAB. Unlike biochemical studies, we focus significantly more on understanding the physic picture of viral molecules' structure and interaction. For covid-19 disease, it is found that

(i) the SARS-CoV-2 Spike is more structural stable and has higher binding energy to the human ACE2 receptor than SARS-CoV Spike;

(ii) SARS-CoV-2 RBD-ACE2 binding interface is more stable, has higher binding area, and has more interactions than in SARS-CoV;

(iii) the mutation -PPA469-471/GVEG482-485 in Spike structure has most important and favorable impact for SARS-CoV-2 Spike binding to the ACE2 receptor;

(iv) the SARS-CoV-2 Mpro has hot-spots in the binding pocket of both covalent and non-covalent compounds: His41, Cys145, His163, Glu166 and GLN189.

The results assist in in-silico screening of phytocompounds found in Vietnam plants for finding potential natural compounds against SARS-CoV-2 virus. For Gout disease, the protein NLRP3 is targeted with some potential phytocompounds are found and in-vitro and in-vivo testing being conducted by our experimental colleagues.SCAR reaction to the allopurinol Gout drug due to HLA protein polymorphism in Vietnamese patients are studied. Other active researches are also briefly presented such as those involving biased and unbiased painkiller targeting mu-opioid, brain inflammation, ...

Keywords: bioinformatics, covid-19, Multiscale, Gout, disease

PL4

Growth dynamics and physical properties of III-VI two dimensional semiconductors grown by molecular beam epitaxy

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III-VI two dimensional (2D) semiconductors were grown by molecular beam epitaxy (MBE) on GaN, GaAs, mica or glass substrates. The in-situ reflective high energy electron diffraction (RHEED) was used to monitor the surface epitaxy dynamics. High crystal quality of 2D III-VI semiconductors, InSe [1], GaSe [2-4], or GaTe [5] was revealed by the photoluminescence (PL), X-ray diffraction, Raman scattering, and transmission electron micrographs (TEM).

Raman scattering spectra, X-ray diffraction, and high-resolution transmission electron microscopy reveal that 2D InSe phase can be fabricated under both indium-rich and -poor conditions [1]. Strong red-shifts in the energy of in-plane E_{2g}^{2} vibration modes and bound exciton emissions observed from Raman scattering and PL spectra in GaSe samples are attributed to the unintentionally biaxial in-plane tensile strains, induced by the dissimilarity of symmetrical surface structure between the 2D-GaSe layers and the substrates during the epitaxial growth [3]. The temporal in-situ RHEED patterns illustrate the transition from 2D hexagonal GaTe to one dimensional (1D) monoclinic GaTe growth mode at different growth temperatures [5]. Current investigation on the growth dynamics and physical properties of III-VI 2D semiconductors pave the way for future fabrication and device application of the hetero-structures made of these III-VI 2D semiconductors.

Keywords: two dimensional semiconductors, molecular beam epitaxy, InSe, GaSe, GaTe

References

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PL5

Fe2P type alloys: an intriguing magnetic playground

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The Fe2P intermetallic compound, is a prototypical example of a first order ferromagnetic phase transition, known since the 1980s to exhibit a sharp, but weak, FOMT at 216 K (-57°C)[1]. In this hexagonal system, the Fe atoms occupy two inequivalent atomic positions, referred to as 3f (in a tetrahedral environment of non-metallic atoms) and 3g (in a pyramidal environment). Also, for P we find two distinct lattice sites 1a and 2b. One intriguing aspect is the large uniaxial magnetic anisotropy leading to an anisotropy field of about 7T at 5K [2]. This anisotropy is quite unique for a mainly itinerant electron system as evidenced by the reduction (partial quenching) in the magnetic moments of the iron atoms on the 3f sites when TC is crossed from the ferromagnetic to the paramagnetic state, whereas there is only a limited decrease on the 3g site. This observation has led to a cooperative description of the FOMT, linking the loss of long-range magnetic order at TC with the loss of local moments on the 3f site [3]. Replacing Fe and or P by other elements leads to a rich variety of phenomena. Magnetic ordering temperature and first order character of the phase transition can be either enhanced or reduced. The anisotropy is strongly reduced on reduction of the c lattice parameter and a wide range of compositions display easy-plane anisotropy rather than easy axis, which is favourable for magnetocaloric applications. We will discuss both theoretical and experimental results for a wide range of elements substituting either Fe or P and combined substitutions on both Fe and P sites, while maintaining the hexagonal Fe2P type of structure. Most prominent results are achieved when partially replacing Fe with Mn or Co, and simultaneously Si substituting P. This leads for Mn to soft magnetic materials with excellent magnetocaloric properties [4]. Conversely, hard magnetic properties and Curie temperatures up to 640 K are found for Co substitutions [5].

Keywords: Magneto-caloric materials, gap magnets, transition-metal magnets

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Optical and Electronic Properties of Crystalline Solids from the First-Principles and Semiempirical Methods

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Smart design and efficient search for new effective optical materials implies understanding of their physical parameters, such as structural, electronic, optical etc properties. Various first-principles and semiempirical models have been developed so far to elucidate relations between structure and properties of crystalline materials and between their various properties. In this presentation several examples of consistent application of the first-principles calculations to the large families of isostructural compounds, pure [1, 2] and doped [3, 4] will be discussed in detail with an emphasis of relations between the chemical composition, structure and properties. In addition, a semiempirical model that allows to make predictions of positions of emission maxima in the Eu^{2+}-doped ternary sulfides will be presented (Fig. 1) [5].

Keywords: First-principles calculations; Mn^{4+}-based phosphors; Eu^{2+}-based phosphors

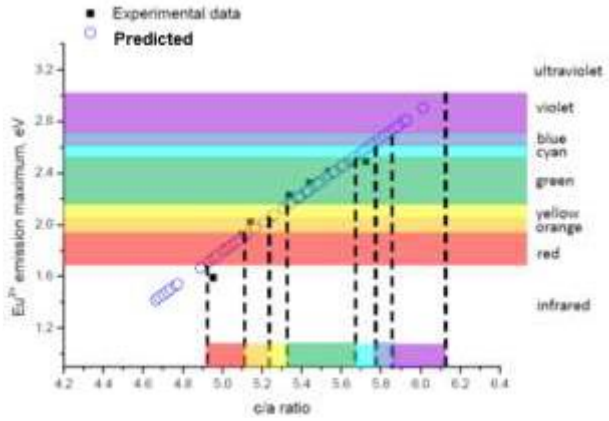

FIG. 1. Experimental and predicted Eu^{2+} emission maxima in the ternary sulfides with indication of emission color.

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