

<b>Monday Nov. 6</b> (14:00-17:00PM) On Site Registration		
<b>Tuesday Nov. 7</b> <b>Room: A</b>		
8:55-9:00AM	Opening	
<b>Session: DFT I Chair: Hoon Ryu</b>		
9:00-9:25AM	A01: DFT Modeling of Co-C Bond Activation and Cleavage in Vitamin B12-Dependent Systems	<b>Pawel M. Kozlowski</b> University of Louisville, USA
9:25-9:50AM	A02: Hydration of Nitriles at the Water/Metal-Oxide Interface: First-Principles Molecular Dynamics Simulations	<b>Akira Nakayama</b> Hokkaido University, Japan
9:50-10:15AM	A03: Solitonic Natural Orbitals	<b>Jerzy Cioslowski</b> University of Szczecin, Poland
10:15-10:40AM	A04: Bridge between the aromaticity of polycyclic aromatic hydrocarbons and closo borohydrides	<b>Jordi Poater</b> Universitat de Barcelona, Spain
10:40-11:00AM	Session Break	
<b>Session: General I Chair: Pawel M. Kozlowski</b>		
11:00 -11:25AM	A05: HPC trends in chemistry computation	<b>Rika Kobayashi</b> Australian National University, Australia
11:25-11:50AM	A06: Large-scale Electronic Structure Simulations with GPU Computing	<b>Hoon Ryu</b> National Institute of Supercomputing and Networking, KISTI, Korea
11:50-12:15AM	A07: Numerical Simulation of Noise and Nonlinearities in Fibre-optic Transmission Systems	<b>Werner Rosenkranz</b> University of Kiel, Germany
12:15-12:40AM	A08: New insights into molecular interactions using concepts of quantum information theory	<b>Pawel Tecmer</b> Nicolaus Copernicus University in Toruń, Poland
12:40-14:00 PM	Lunch Break	

**Tuesday Nov. 7**

**Room: A**

**Session: DFT II Chair: Werner Rosenkranz**

14:00 -14:25PM	A09: Nature and stability of carbon-astatine bonds: a combined density functional theory and quantum chemical topology study	<b>Pilmé Julien</b> Université Pierre et Marie Curie, France
14:25 -14:50PM	A10: Practical Applications of Computational Chemistry to Functional Material Systems	<b>Michihisa Koyama</b> Kyushu University, Japan
14:50 -15:15PM	A11: Exchange-Correlation Potentials and Energy Densities in Spherically Confined Atoms	<b>Sergei Vyboishchikov</b> Universitat de Girona, Spain
15:15 -15:40PM	A12: Spin-orbit torques in noncollinear magnets from first-principles density-functional theory	<b>Frank Freimuth</b> Peter Grünberg Institute (PGI-1) and Institute for Advanced Simulation (IAS-1), Germany
15:40 -16:00PM	Session Break	
<b>Session: Molecular Dynamics and its Applications I Chair: Frank Freimuth</b>		
16:00-16:25PM	A13: Molecular Dynamics Simulations for Aggregation and Disaggregation of Amyloid- $\beta$ Peptides	<b>Hisashi Okumura</b> Institute for Molecular Science, NINS, Japan
16:25P-16:50PM	A14: Design of Novel Therapeutics via Molecular Dynamics Simulations	<b>Chang-Guo Zhan</b> University of Kentucky, USA
16:50-17:15PM	A15: Replica-permutation method to obtain efficient sampling for biomolecules	<b>Satoru Itoh</b> Institute for Molecular Science, Japan
17:15-17:40PM	A16: Dynamics and thermodynamics of the dipole-type Hamiltonian mean field model	<b>Sergio Curilef</b> Universidad Católica del Norte, Chile

**Wednesday Nov. 8**

**Room: A**

**Session: DFTIII Chair: Donghwa Lee**

9:00-9:25AM	A17: Dislocations properties in semiconductor nano-objects and in nitride thin films, investigated by DFT calculations.	<b>Laurent Pizzagalli</b> Université de Poitiers, France
9:25-9:50AM	A18: TDDFT Study of Subcycle Electron Dynamics, Transient Spectroscopy, and Coherent Control of Ultrafast Attosecond Pulse Generation	<b>Shih-I Chu</b> University of Kansas, USA
9:50-10:15AM	A19: A Density Functional Approach for the Superconductor	<b>Masahiko Higuchi</b> Shinshu University, Japan
10:15-10:40AM	A20: A route to permanent valley polarization in monolayer MoS <sub>2</sub>	<b>Nirpendra Singh</b> King Abdullah University of Science and Technology (KAUST), Saudi Arabia
10:40-11:00AM	Session Break	
<b>Session: DFTIV Chair: Donghwa Lee</b>		
11:00 -11:25AM	A21: Tailoring the morphology of FeCO <sub>3</sub> for corrosion control: insights from Density Functional Theory	<b>Ehsan A Ahmad</b> Imperial College London, UK
11:25-11:50AM	A22: Accurate ground-state correlation energies within the RPA and beyond: Theory and applications to molecules and solids	<b>Dario Rocca</b> Université de Lorraine and CNRS, France
11:50-12:15AM	A23: Magnetic fields, convexity and gauge invariance in density functional theory	<b>Erik Tellgren</b> University of Oslo, Norway
12:15-12:40AM	A24: The differential virial theorem with gradient- and Laplacian-dependent operator formulas	<b>James Finley</b> Eastern New Mexico University, Mexico
12:40-14:00 PM	Lunch Break	

**Wednesday Nov. 8**

**Room: A**

**Session: DFTV Chair: Jordi Poater**

14:00 -14:25PM	A25: (Non)Linear Optical Properties of Molecules and Their Aggregates: Should We Trust DFT?	<b>Robert Zalesny</b> Wroclaw University of Science and Technology, Poland
14:25 -14:50PM	A26: Reactive orbital energy theory based on the quantitative orbital energies of long-range corrected DFT	<b>Takao Tsuneda</b> University of Yamanashi, Japan
14:50 -15:15PM	A27: Theoretical spectroscopy for molecules and solids from the current density	<b>Arjan Berger</b> Université Paul Sabatier, France
15:15 -15:40PM	A28: Kohn-Sham energy decomposition of Magnetic-field DFT (BDFT)	<b>Alex Borgoo</b> University of Oslo, Norway
15:40 -16:00PM <b>Poster &amp; Session Break</b>	P1: TBD	<b>Rabeet Singh Chauhan</b> Indian Institute of Technology Kanpur, India

**Session: DFTVI Chair: Jordi Poater**

16:00-16:25PM	A29: Application of Density Functional Theory in designing accident tolerant nuclear fuels	<b>Barbara Szpunar</b> University of Saskatchewan, Canada
16:25P-16:50PM	A30: Theoretical design of functional molecular crystals; a case of organic semiconductors	<b>Hitoshi Goto</b> Toyohashi University of Technology, Japan
16:50-17:15PM	A31: Theory-guided optimization and novel materials design from First-Principles	<b>Donghwa Lee</b> Pohang University of Science and Technology (POSTECH), Korea
17:15-17:40PM	A32: New Insights into the mechanism of oxidative coupling	<b>Feliu Maseras</b> ICIQ, The Barcelona Institute of Science and Technology, Spain

**Wednesday Nov. 8**

**Room: B**

**Session: Molecular Dynamics and its Applications II Chair: Seokmin Shin**

9:00-9:25AM	B01: The effect of proton and potential gradients on integral membrane proteins: Insights from Molecular Dynamics simulations	<b>Vangelis Daskalakis</b> Cyprus University of Technology, Cyprus
9:25-9:50AM	B02: Simulating Microwave Effects on Model Aqueous Solutions and Biological Macromolecules	<b>Urban Bren</b> Univerza v Mariboru, Slovenia
9:50-10:15AM	B03: Modeling and Simulation for Chromosome Condensation and Segregation	<b>Yuji Sakai</b> The University of Tokyo, Japan
10:15-10:40AM	B04: Global Sensitivity Analysis and Parameter Inference in Molecular Dynamics	<b>Omar M. Knio</b> King Abdullah University of Science and Technology, Kingdom of Saudi Arabia
10:40-11:00AM	Session Break	
<b>Session: Molecular Dynamics and its Applications III Chair: Omar M. Knio</b>		
11:00 -11:25AM	B05: Molecular Dynamics of Liquid Racemic Acid	<b>Hironori Shimakura</b> Niigata University of Pharmacy and Applied Life Sciences, Japan
11:25-11:50AM	B06: Anion polarization effects on intermediate-range ordering in molten CuBr	<b>Shuta Tahara</b> University of the Ryukyus, Japan
11:50-12:15AM	B07: The two faces of self-assembly for peptides and proteins	<b>Seokmin Shin</b> Seoul National University, Korea
12:15-12:40AM	B08: The stabilization of polar CuInSe <sub>2</sub> (001) surface and its critical effect on the high efficiency of the thin-film solar-cell	<b>Lixin Zhang</b> Nankai University, China
12:40-14:00 PM	Lunch Break	

**Wednesday Nov. 8**

**Room: A**

**Session: Molecular Dynamics and its ApplicationsIV & Molecular Electronics Chair: Seokmin Shin**

14:00 -14:25PM	B09: Molecular dynamics simulation for cross-linked polymer system	<b>Yutaka Oya</b> Tohoku University, Japan
14:25 -14:50PM	B10: Molecular Dynamics Simulations for Rational Enzyme Redesign	<b>Fang Zheng</b> University of Kentucky, USA
14:50 -15:15PM	B11: Charge transport in mesoscale heterogeneous organic semiconductors	<b>Hajime Kobayashi</b> Advanced Materials Laboratories, Sony Corporation, Japan
15:15 -15:40PM	B12: TBD	<b>Douxing Pan</b> The state key laboratory of nonlinear mechanics, Institute of Mechanics, CAS, China
15:40 -16:00PM <b>Poster &amp; Session Break</b>	P1: TBD	<b>Rabeet Singh Chauhan</b> Indian Institute of Technology Kanpur, India
<b>Session: Moller–Plesset perturbation theory and Coupled-Cluster Theory &amp; Quantum Structure Chair: Fang Zheng</b>		
16:00-16:25PM	B13: Computational methods for strong and weak correlation: Bridging the gap between DFT and Coupled Cluster Theory	<b>Odile Franck</b> Nicolaus Copernicus University, Poland
16:25P-16:50PM	B14: Quantum information measures of the one-dimensional Robin quantum well	<b>Oleg Olendski</b> University of Sharjah, United Arab Emirates
16:50-17:15PM	B15: Optimization of ab initio electronic structures of monohydrates of HCl●H <sub>2</sub> SO <sub>4</sub> ●HNO <sub>3</sub> aggregates: hydrogen bonds, IR spectra and dipole moments	<b>Marian Verdes</b> Universidad Autónoma de Madrid, Spain
17:15-17:40PM	B16: Analytic Energy Gradients for Coupled-Cluster Methods with the Density-Fitting Approximation	<b>Ugur Bozkaya</b> Hacettepe University, Turkey
17:40-18:05PM	B17: Computational methods of quantum chemistry for the description of the dissociation of a single bond	<b>Monika Musial</b> University of Silesia, Poland

**Thursday Nov. 9**

**Room: A**

**Session: General II Chair: Charlotte Becquart**

8:35-9:00AM	A33: Relativistic Quantum-Chemical Calculations of NMR Chemical Shifts in Molecules Containing Heavy Metals	<b>Masahiko Hada</b> Tokyo Metropolitan University, Japan
9:00-9:25AM	A34: TBD	<b>Koichi Yamashita</b> The University of Tokyo, Japan
9:25-9:50AM	A35: Hidden orbital polarization in centrosymmetric materials and the electronic structure of Weyl semimetals from first-principles calculations	<b>Cheol-Hwan Park</b> Seoul National University, Korea
9:50-10:15AM	A36: Investigation of Weak CH/ $\pi$ Interaction in the Structure of Dibromo-9,9'-dialkylfluorenes	<b>Suzuki Nozomu</b> Rikkyo University, Japan
10:15-10:40AM	A37: Energy-band calculations of materials immersed in the magnetic field: Revisit of magnetic oscillations of metals	<b>Katsuhiko Higuchi</b> Hiroshima university, Japan
10:40-11:00AM	Session Break	
<b>Session: DFTVII Chair: Rika Kobayashi</b>		
11:00 -11:25AM	A38: Prediction of Chemical Properties of heavy and super-heavy Elements by Relativistic Density Functional Theory	<b>Josef Anton</b> Karlsruhe Institute of Technology&University of Ulm, Germany
11:25-11:50AM	A39: DFT calculations applied to radiation damage modelling	<b>Charlotte Becquart</b> Université Lille1-UMET, France
11:50-12:15AM	A40: Dynamic DFT simulations of defect formation in metals	<b>Pär Olsson</b> KTH Royal Institute of Technology, Sweden
12:15-12:40AM	A41: DFT insight into new solid state ionic conductors	<b>Zbigniew Lodziana</b> Instytut Fizyki Jądrowej PAN, Poland
12:40-14:00 PM	Lunch Break	

**Thursday Nov. 9**

**Room: A**

**Session: DFTVIII Chair: Zbigniew Lodziana**

14:00 -14:25PM	A42: Can standard DFT calculations correctly describe the physical properties of AlOOH under pressure?	<b>Pietro Cortona</b> Ecole Centrale Paris, France
14:25 -14:50PM	A43: First-Principles Molecular Dynamics Study on Ammonia Formation/Decomposition on Supported Ru Catalysts	<b>Manabu Sugimoto</b> Kumamoto University, Japan
14:50 -15:15PM	A44: New QM/QTAIM horizons of the microstructural mechanisms of the spontaneous and induced transitions and transversions in DNA	<b>Ol'ha O. Brovarets'</b> Institute of Molecular Biology and Genetics, National Academy of Sciences of Ukraine, Ukraine
15:15 -15:40PM	A45: The Application of Density Functional Theory in Electrical Engineering Field: Theoretical Study of the Decomposition Mechanism of Insulating/Arc Quenching Gas in Electrical Equipment	<b>Yuwei Fu</b> State Key Laboratory of Electrical Insulation and Power Equipment, Xi'an Jiaotong University, China
15:40-16:00AM	Session Break	