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

Tuesday Nov. 7 Room: A		
Session: DFTⅡ 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	**Pilmé Julien** Université Pierre et Marie Curie, France
14:25 -14:50PM	A10: Practical Applications of Computational Chemistry to Functional Material Systems	**Michihisa Koyama** Kyushu University, Japan
14:50 -15:15PM	A11: Exchange-Correlation Potentials and Energy Densities in Spherically Confined Atoms	**Sergei Vyboishchikov** Universitat de Girona, Spain
15:15 -15:40PM	A12: Spin-orbit torques in noncollinear magnets from first-principles density-functional theory	**Frank Freimuth** Peter Grünberg Institute (PGI-1) and Institute for Advanced Simulation (IAS-1), Germany
15:40 -16:00PM	Session Break	
Session: Molecular Dynamics and its Applications Ⅰ Chair: Frank Freimuth		
16:00-16:25PM	A13: Molecular Dynamics Simulations for Aggregation and Disaggregation of Amyloid-β Peptides	**Hisashi Okumura** Institute for Molecular Science, NINS, Japan
16:25P-16:50PM	A14: Design of Novel Therapeutics via Molecular Dynamics Simulations	**Chang-Guo Zhan** University of Kentucky, USA
16:50-17:15PM	A15: Replica-permutation method to obtain efficient sampling for biomolecules	**Satoru Itoh** Institute for Molecular Science, Japan
17:15-17:40PM	A16: Dynamics and thermodynamics of the dipole-type Hamiltonian mean field model	**Sergio Curilef** 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.	**Laurent Pizzagalli** Université de Poitiers, France
9:25-9:50AM	A18: A Density Functional Approach for the Superconductor	**Masahiko Higuchi** Shinshu University, Japan
9:50-10:15AM	A19: A route to permanent valley polarization in monolayer MoS2	**Nirpendra Singh** King Abdullah University of Science and Technology (KAUST), Saudi Arabia
10:15-10:40AM	A20: Design of functional materials with efficient photovoltaic parameters by DFT approach	**Javed Iqbal** University of Agriculture, Pakistan
10:40-11:00AM	Session Break	
Session: DFTⅣ　Chair: Donghwa Lee		
11:00 -11:25AM	A21: Tailoring the morphology of FeCO3 for corrosion control: insights from Density Functional Theory	**Ehsan A Ahmad** 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	**Dario Rocca** Université de Lorraine and CNRS, France
11:50-12:15AM	A23: Magnetic fields, convexity and gauge invariance in density functional theory	**Erik Tellgren** University of Oslo, Norway
12:15-12:40AM	A24: The differential virial theorem with gradient- and Laplacian-dependent operator formulas	**James Finley** 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?	**Robert Zalesny** 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	**Takao Tsuneda** University of Yamanashi, Japan
14:50 -15:15PM	A27: Theoretical spectroscopy for molecules and solids from the current density	**Arjan Berger** Université Paul Sabatier, France
15:15 -15:40PM	A28: Kohn-Sham energy decomposition of Magnetic-field DFT (BDFT)	**Alex Borgoo** University of Oslo, Norway
15:40 -16:00PM **Poster** & Session Break	P01: Study of adiabatic connection in density functional theory	**Rabeet Singh Chauhan** Indian Institute of Technology Kanpur, India
	P02: First Principles Computational Study on Hydrolysis of Hazardous Chemicals Phosphorus Trichloride and Oxychloride (PCl3 and POCl3) Catalyzed by Molecular Water Clusters	**Hyunwook Jung** Yonsei University, Korea
Session: DFTⅥ Chair: Jordi Poater		
16:00-16:25PM	A29: Application of Density Functional Theory in designing accident tolerant nuclear fuels	**Barbara Szpunar** University of Saskatchewan, Canada
16:25P-16:50PM	A30: Theoretical design of functional molecular crystals; a case of organic semiconductors	**Hitoshi Goto** Toyohashi University of Technology, Japan
16:50-17:15PM	A31: Theory-guided optimization and novel materials design from First-Principles	**Donghwa Lee** Pohang University of Science and Technology (POSTECH), Korea
17:15-17:40PM	A32: New Insights into the mechanism of oxidative coupling	**Feliu Maseras** 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	**Vangelis Daskalakis** Cyprus University of Technology, Cyprus
9:25-9:50AM	B02: Simulating Microwave Effects on Model Aqueous Solutions and Biological Macromolecules	**Urban Bren** Univerza v Mariboru, Slovenia
9:50-10:15AM	B03: Modeling and Simulation for Chromosome Condensation and Segregation	**Yuji Sakai** The University of Tokyo, Japan
10:15-10:40AM	B04: Global Sensitivity Analysis and Parameter Inference in Molecular Dynamics	**Omar M. Knio** King Abdullah University of Science and Technology, Kingdom of Saudi Arabia
10:40-11:00AM	Session Break	
Session: Molecular Dynamics and its ApplicationsⅢ Chair: Omar M. Knio		
11:00 -11:25AM	B05: Molecular Dynamics of Liquid Racemic Acid	**Hironori Shimakura** Niigata University of Pharmacy and Applied Life Sciences, Japan
11:25-11:50AM	B06: Anion polarization effects on intermediate-range ordering in molten CuBr	**Shuta Tahara** University of the Ryukyus, Japan
11:50-12:15AM	B07: The two faces of self-assembly for peptides and proteins	**Seokmin Shin** Seoul National University, Korea
12:15-12:40AM	B08: The stabilization of polar CuInSe2 (001) surface and its critical effect on the high efficiency of the thin-film solar-cell	**Lixin Zhang** 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	**Yutaka Oya** Thohoku Universyty, Japan
14:25 -14:50PM	B10: Molecular Dynamics Simulations for Rational Enzyme Redesign	**Fang Zheng** University of Kentucky, USA
14:50 -15:15PM	B11: Charge transport in mesoscale heterogeneous organic semiconductors	**Hajime Kobayashi** Advanced Materials Laboratories, Sony Corporation, Japan
15:15 -15:40PM	B12: Bending induced compressive strain recovering behavior in black phosphorus monolayer	**Douxing Pan** Hefei Institute of Physical Science, CAS, China
15:40 -16:00PM **Poster** & Session Break	P01: Study of adiabatic connection in density functional theory	**Rabeet Singh Chauhan** Indian Institute of Technology Kanpur, India
	P02: First Principles Computational Study on Hydrolysis of Hazardous Chemicals Phosphorus Trichloride and Oxychloride (PCl3 and POCl3) Catalyzed by Molecular Water Clusters	**Hyunwook Jung** Yonsei University, Korea
Session: Moller–Plesset perturbation theory and Coupled-Cluster Theory & Quantum Structure Chair: Fang Zheng		
16:00-16:25PM	B13: Computational methods for strong and weak correlation: Bridging the gap between DFT and Coupled Cluster Theory	**Odile Franck** Nicolaus Copernicus University, Poland
16:25P-16:50PM	B14: Quantum information measures of the one-dimensional Robin quantum well	**Oleg Olendski** University of Sharjah, United Arab Emirates
16:50-17:15PM	B15: Optimization of ab initio electronic structures of monohydrates of HCl●H2SO4●HNO3 aggregates: hydrogen bonds, IR spectra and dipole moments	**Marian Verdes** Universidad Autónoma de Madrid, Spain
17:15-17:40PM	B16: Analytic Energy Gradients for Coupled-Cluster Methods with the Density-Fitting Approximation	**Ugur Bozkaya** Hacettepe University, Turkey
17:40-18:05PM	B17: Computational methods of quantum chemistry for the description of the dissociation of a single bond	**Monika Musial** 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	**Masahiko Hada** Tokyo Metropolitan University, Japan
9:00-9:25AM	A34: Atomistic Modeling and NMR Characterization of the Sodium Diffusion in Black Phosphorus Anode	**Koichi Yamashita** 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	**Cheol-Hwan Park** Seoul National University, Korea
9:50-10:15AM	A6: Investigation of Weak CH/π Interaction in the Structure of Dibromo-9,9'-dialkylfluorenes	**Suzuki Nozomu** Rikkyo University, Japan
10:15-10:40AM	A37: Energy-band calculations of materials immersed in the magnetic field: Revisit of magnetic oscillations of metals	**Katsuhiko Higuchi** Hiroshima university, Japan
10:40-11:00AM	Session Break	
Session: DFTⅦ　Chair: Rika Kobayashi		
11:00 -11:25AM	A38: Prediction of Chemical Properties of heavy and super-heavy Elements by Relativistic Density Functional Theory	**Josef Anton** Karlsruhe Institute of Technology&University of Ulm, Germany
11:25-11:50AM	A39: DFT calculations applied to radiation damage modelling	**Charlotte Becquart** Université Lille1-UMET, France
11:50-12:15AM	A40: Dynamic DFT simulations of defect formation in metals	**Pär Olsson** KTH Royal Institute of Technology, Sweden
12:15-12:40AM	A41: DFT insight into new solid state ionic conductors	**Zbigniew Lodziana** 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?	**Pietro Cortona** Ecole Centrale Paris, France
14:25 -14:50PM	A43: First-Principles Molecular Dynamics Study on Ammonia Formation/Decomposition on Supported Ru Catalysts	**Manabu Sugimoto** 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	**Ol'ha O. Brovarets'** 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	**Yuwei Fu** State Key Laboratory of Electrical Insulation and Power Equipment, Xi'an Jiaotong University, China
15:40-16:00AM	Session Break	