Program for EMN Meeting on Computation and Theory		
Monday November 9 **Room B**		
Session: Moller–Plesset perturbation theory and Coupled-Cluster Theory I Chair: Takayoshi Ishimoto		
9:00-9:25 AM	B01: Robust Validation of Approximate 1-matrix Functionals with Few-Electron Harmonium Atoms	**Jerzy Cioslowski** University of Szczecin, Poland
9:25-9:50 AM	B02: Reaching sub-kJ/mol accuracy for periodic systems using local correlation methods	**Denis Usvyat** University of Regensburg, Germany
9:50-10:15 AM	B03: Analytic Energy Gradients for the Coupled-Cluster Singles and Doubles method with the Density-Fitting Approximation	**Ugur Bozkaya** Ataturk University, Turkey
10:15-10:35 AM	Session Break	
Session: Density Functional Theory and its applications I Chair: Jerzy Cioslowski		
10:35-11:00 AM	B04: Biomimetic catalysts for water oxidation	**Sandra Luber** University of Zurich, Switzerland
11:00-11:25 AM	B05: Applications of Electronic Structure Analysis at Nanomaterial Interface	**Takayoshi Ishimoto** Kyushu University, Japan
11:25-11:50 AM	B06: TELEMAN: a versatile real time TDDFT package for irradiation dynamics	**Eric Suraud** Université Paul Sabatier, France
12:00 PM	Lunch Break	

Monday November 9 Room B		
Session: Molecular Electronics Chair: Elena Orlenko		
14:00-14:25 PM	B07: Theoretical Design of Quantum-dot Cellular Automata based on Mixed-Valence Metal Complexes	**Ken Tokunaga** Kogakuin University, Japan
14:25 -14:50 PM	B08: Exploiting orbital resonances in single molecules	**Mickael Perrin** Delft University of Technology, The Netherlands
14:50 -15:15 PM	B09: Insights into molecular transmission through chemical concepts	**Thijs Stuyver** Vrije Universiteit Brussel, Belgium
15:15-15:40 PM	B10: A Spin-Orbit Interaction and Magnetic Properties of Fullerens	**Elena Orlenko** Peter the Great St.Petersburg Polytechnic University, Russia
15:40-16:00 PM	Session Break	
Session: General Chair: Ken Tokunaga		
16:00-16:25 PM	B11: Electron-transfer characteristics of layer dependence and metal contacts in 2-dimensional materials	**Seong Chan Jun** Yonsei University, Korea
16:25-16:50 PM	B12: U-doped CeO2 for H2 production from water	**Jessica Scaranto** SABIC CRD Center, KAUST, Saudi Arabia
18:00 PM	Dinner Social	

Tuesday November 10 Room B		
Session: Moller–Plesset perturbation theory and Coupled-Cluster Theory II Chair: Alexander Yefremov		
9:00-9:25 AM	B13: Fast and reliable black-box electron-correlation methods	**Daniel Kats** Universität Stuttgart, Germany
9:25-9:50 AM	B14: Chemistry of Caesium - CASPT2 and Coupled-Cluster Studies	**Ivan Cernusak** Comenius University in Bratislava, Slovakia
9:50-10:15 AM	B15: Unrestricted MP2 forces for condensed systems within Gaussian and Plane-Waves Approach	**Vladimir Rybkin** ETH Zürich, Switzerland
10:15-10:35 AM	Session Break	
Session: Quantum Structure Chair: Ivan Cernusak		
10:35-11:00 AM	B16: Fractal Nature of Quantum Mechanics and Bohr-type Solution of Schrodinger Equation	**Alexander P. Yefremov** Russian Academy of Natural Sciences, Russia
11:00-11:25 AM	B17: Nonadiabatic transitions at the singlet lowest states of NiH2	**Juan Horacio Pacheco-Sánchez** Instituto Tecnológico de Toluca, México
12:00 PM	Lunch Break	

Tuesday November 10 Room B		
Session: NMR Calculation Chair: Alexander Pergament		
14:00-14:25 PM	B18: Lattice simulations and NMR in energy storage materials: including dynamic processes in NMR spectra prediction	**Céline Merlet** University of Cambridge, United Kingdom
14:25 -14:50 PM	B19: Simulating NMR relaxation with stochastic methods	**Magnus Ögren** Örebro University, Sweden
14:50 -15:15 PM	B20: NMR & DFT in iron oxides	**Vojtech Chlan** Charles University in Prague, Czech Republic
15:15-15:40 PM	B21: Towards ab initio NMR calculations for large systems	**Rika Kobayashi** ANU Supercomputer Facility, Australia
15:40-16:00 PM	Session Break	
Poster Session		
16:00-16:30 PM	P1: The transport properties study of slow electrons beam in solids and the first transport cross section correlation by using Monte Carlo method	**Abdelouahab Bentabet** Université de Bordj Bou-Arreridj, Algeria
	P2: The antioxidative properties of kynurenines: DFT level calculations	**Aleksandr V. Zhuravlev** Pavlov Institute of Physiology RAS, Russia
	P3: Theoretical Study of Hydrogen Adsorption and Diffusion in Spillover Process on Microporous Carbon	**Masanori Tachikawa** Yokohama City University, Japan
Session: Oxide Electronics Chair: Magnus Ögren		
16:30-16:55 PM	B22: Vanadium Dioxide: Metal-Insulator Transition, Electrical Switching and Oscillations. A Review of State of the Art and Recent Progress	**Alexander Pergament** Petrozavodsk State University, Russia
16:55-17:20 PM	B23: Electric-field-induced Spontaneous Magnetization and Phase Transitions in d0 Semiconductor Nanostructures	**Gang Xiang** Sichuan University, China
18:00 PM	Dinner Social	

Wednesday November 11 Room B		
Session: Density Functional Theory and its applications II		**Chair: Takayoshi Ishimoto**
9:00-9:25 AM	B24: Design of functional Hückel and Möbius expanded porphyrins using computational chemistry	**Mercedes Alonso** Free University of Brussels (VUB), Belgium
9:25-9:50 AM	B25: Band gap engineering in skutterudites: the role of X4 rings geometry in CoSb3-RhSb3 system	**Andrzej Kolezynski** AGH University of Science and Technology, Poland
9:50-10:15 AM	B26: Advanced Electron density properties by ab initio calculations: a parellel implementation in the CRYSTAL code	**Silvia Casassa** Università degli Studi di Torino, Italy
10:15-10:35 AM	Session Break	
10:35-11:00 AM	B27: Structure-function correlations in metal oxides -- Insights from density functional and many body theory	**Eva Rauls** Universität Paderborn, Germany
11:00-11:25 AM	B28: Interpreting the Linear Response Kernel	**Zino Boisdenghien** Vrije Universiteit Brussel, Belgium
11:25-11:50 AM	B29: A Novel Approach for Highly Stable Doping of Semiconducting Graphene Nanomeshes	**Ahmed Maarouf** Zewail City of Science and Technology, Egypt
12:00 PM	Lunch Break	