Norwegian Chemical Society

Annual Meeting in Computational Chemistry

Program

Tuesday 12.06.2012

09:00	Bjørn Olav Brandsdal	Welcome
Chairman:	Per-Olof Åstrand	
09:15	Vidar Jensen	DFT-D Studies of Transition Metal-Catalyzed Reactions: Accuracy and Insight
10:00	Ulf Ekström	Wild and tame density functional theories
10:20	Ole Swang	Computational chemistry for a better society: Atom-scale modeling at SINTEF Materials and Chemistry.
10:40	Coffee break	
Chairman:	Trygve Helgaker	
11:00	Clemens Woywod	Theoretical investigation of a model system for molecular photoswitch functionality
11:20	Alexey Zatula	Proton hopping through water wires in clusters MH+(H2O)n (M = 2,2'–BiPy, 4,4'–BiPy, 2,2'–EtBiPy, 4,4'–EtBiPy)
11:40	Anna Pikulska	Optical rotatory dispersion (ORD) and circular dichroism (CD) of lactamide and 2-amino-1-propanol
12:00	Karina Kovalchuk	Molecular dynamic study of carboxylic acids at the water/oil interface
12:20	Maarten Beerepoot	Linear and non-linear absorption in fluorescent proteins
12:40	Lunch	
Chairman:	Einar Uggerud	
14:00	Hans Sverre Smalø	Stretching polymer molecules using mechanical force
14:20	Kai Lange	A paramagnetic bonding mechanism for diatomics in strong magnetic fields
14:40	Nazanin Davari	Ionization potential and excitation energy of molecules in high electric fields
15:00	Harald Møllendal	Microwave and quantum chemical investigations of cyanoacetaldehyde (CH2(CN)CHO), a potential prebiotic precursor of pyrimidines found in DNA and RNA
15:20	Artur Wodynsky	Calculations of spin-spin coupling constants and NMR shielding constants of transition metal cyanides
15:40	Coffee break	
Chairman:	Knut Børve	
16:00	Thomas Jagau	Analytic Evaluation of Electrical Anharmonicities in Møller- Plesset Perturbation Theory and Coupled-Cluster Theory
16:20	Dan Jonsson	Gauge-origin independent calculations of Jones birefringence
16:40	Heike Fliegl	Aromatic pathways in porphin type molecules
17:00	Eirik Hjertenæs	Benchmark data and DFT evaluation for sodium-graphite interactions
17:20	Trinh Thaut	Simulating CO_2 adsorption and transport on graphite surface
17:40	End of session	
17:45	Break	Annual meeting in Computational Chemistry
18:00		Outdoor jacuzzi – suits for rent!!
20:00	Dinner	

Wednesday 13.06.2012

Chairman	Kenneth Ruud	
09:15	Xin Xu	Development of New Density Functionals for Accurate Descriptions of Nonbond Interactions, Thermochemistry, and Thermochemical Kinetics
10:00	Kathrin Hopmann	Iridium-Catalyzed Enantioselective Imine Hydrogenation: Mechanism and Stereocontrol
10:20	Taye Demissie	Four-Component Relativistic Chemical Shift Calculation Combined with Atomic Force Microscopy for the Structural Elucidation of Breitfussin A and B
10:40	Coffee break	
Chairman	Ole Swang	
11:00	Bin Gao	Plasmon resonances in linear noble metallic chains
11:20	Simen Reine	Efficient and parallel Kohn-Sham DFT developments for large molecular systems
11:40	Stella Stopkowicz	Relativistic Corrections via Fourth-Order Direct Perturbation Theory
12:00	Magnus Ringholm	A general open-ended response code
12:20	Stig-Rune Jensen	Chemistry at the basis set limit using multiwavelets
12:40	Lunch	
14:00	Departure	Bus transport to Bardufoss and Tromsø