deMon 2006, Kananaskis

Date	Start	Length	End	Speaker	Status	Title
Fri, Apr 21						
	10:00					Check-in begins
	13:00	4:00	17:00			Hike to mount Baldy/lookout (weather permitting)?
	18:30	1:30	20:00			Supper and get-together
Sat, Apr 22						
	8:30	0:30	9:00			Breakfast
	9:00	0:30	9:30	Dennis Salahub	C	Introduction
	9:30	0:45	10:15	Andreas Koester	C	Response theory in deMon
	10:15	0:35	10:50	Tom Ziegler	C, A	The application of TDDFT to systems with a spin or space degenerate ground state
	10:50	0:15	11:05			Coffee break
	11:05	0:45	11:50	Alberto Vela	C	The Lieb-Oxford bound and the large gradient limit in the exchange-correlation energy
	11:50	0:25	12:15	Mark E. CASIDA	C	Progress on TDDFT in deMon2k
	12:15	0:25	12:40	Mike Seth	C, A	The Calculation of MCD Spectra with TDDFT
	13:00	1:00	14:00			Lunch
	14:00	2:30	16:30			Free time (?)
	16:30	0:35	17:05	Florian Janetzko	C, A	Ab initio CCM: Inclusion of long-range interactions
	17:05	0:25	17:30	Hongjuan Zhu	C, A	A Theoretical Study of the Original Shilov Reaction Involving Methane Activation by Platinum Tetrachloride (PtCl42-) in an Acidic Aqueous Solution
	17:30	0:25	17:55	Jorge Martín del Campo Ramírez	C,A	Structure Optimization with Levenberg-Marquardt Methods
	17:55	0:25	18:20	Alicija Haras	C,A	DFT Study on the Copolymerization of Ethylene with Polar Monomers Catalyzed by Transition Metal Complexes
	18:30	1:30	20:00			Supper and get-together
	20:00	0:25	20:25			Family matters - warm-up discussion
Sun, Apr 23						
	8:00	0:30	8:30			Breakfast
	9:00	0:35	9:35	Tomasz A. Wesolowski	C, A	Subsystem formulation of DFT:
	9:35	0:35	10:10	Annick Goursot	C	hydrophobic interactions, evaluation and understanding
	10:10	0:35	10:45	Nino Russo	C,A	Mechanism of nitrate reduction by desulfovibrio desulfuricans nitrate reductase. A theoretical investigation.
	10:45	0:15	11:00			Coffee break
	11:00	0:35	11:35	Thomas Heine	C, A	Multi-scale simulations with deMon
	11:35	0:25	12:00	Patrizia Calaminici	C, A	Applications on Large Systems with deMon2k
	12:00	0:25	12:25	Tzonka Mineva	C, A	On the applicability of numerical algorithms based on Slater sum rule to atomic multiplets within DFT
	12:25	0:35	13:00	Sourav Pal	C	Density functional response approach: deMON implentation of approximate CPKS scheme
	13:00	1:00	14:00			Lunch
	14:00	2:30	16:30			Free time (?)
	16:30	0:25	16:55	Max Dion	C, A	A Density Functional for Dispersion Forces

In good weather, mid-day sections may be rescheduled after supper.

C: Confirmed speaker; A: Abstract available

16:55	0:35	17:30	Sandro Chiodo	C, A	Solvent Effect by a quasilinear RISM approach
17:30	0:25	17:55	Simone Tomasi	C, A	Methyl Acrylate Group Transfer Polymerizations with Early d-Block and f-Block Metallocenes
17:55	0:25	18:20	Marcin Dulak	C, A	Accuracy of Coulomb based density fitting approaches for the calculation of intermolecular electrostatic energies
18:30	1:30	20:00			Supper and get-together
20:00	0:45	20:45			Evening session?
20:45	0:25	21:10			
21:10	0:25	21:35			
21:35	0:25	22:00			

Mon, Apr 24

8:00	0:30	8:30			Breakfast
9:00	0:35	9:35	Lars G.M. Pettersson	C	X-ray spectroscopy calculations in StoBe
9:35	0:35	10:10	Klaus Hermann	C, A	Recent developments of StoBe and application to systems of catalytic interest
10:10	0:25	10:35	Bernardo Zuniga	C, A	Implementation of an NMR Module in deMon2k
10:35	0:20	10:55	Gerald Geudtner	C, A	Technical notes on the parallel deMon code
10:55	0:15	11:10			Cofee break
11:10	0:25	11:35	Rui Zhu	C, A	Water clusters by QM/MM using deMon+Tinker
11:35	0:25	12:00	Yue Zhang	C, A	Implementation of meta-GGA in deMon code
12:00	0:25	12:25	Jan Andzelm	C, A	Multiscale modeling of sulfonated copolymers
12:25	0:25	12:50	Anastassiia Moussatova	C, A	Theoretical study of the mechanism of catalysis by adenosine deaminase
13:00	1:00	14:00			Lunch
14:00	0:45	14:45			Licence discussion and other family matters
14:45	0:45	15:30	Dennis Salahub		Early wrap-up
16:00	3:00	19:00			Departing to Banff/free time
19:00	2:00	21:00			Conference Dinner (Coyote's Deli and Grill, Banff)

Tue, Apr 25

8:00	0:30	8:30			Breakfast
9:00	0:25	9:25	Petr Jurecka	C, A	Density Functional Theory Augmented with an Empirical Dispersion Term
9:25	0:25	9:50	K. B. Sophy	C, A	Implementation of the numerical-analytic CPKS procedure in the deMon 2k
9:50	0:25	10:15	Serguei Patchkovskii	C, A	Calculation of heat conductivities with non-equilibrium MD
10:15	0:15	10:30			Cofee break
10:30	0:35	11:05	Alexei Arbuznikov	C, A	Local hybrid functionals: recent progress in their development, and thermochemical tests
11:05	0:25	11:30	Victor Dominguez	C, A	An Iterative Solver for the Coulomb Fitting
11:30	0:15	11:45			closing remarks
13:00	1:00	14:00			Lunch

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C: Confirmed speaker; A: Abstract available