INTERMOLECULAR INTERACTIONS: New Challenges for *ab initio* Theory

Organizers: Bogumil Jeziorski, Malgorzata Szczesniak, and Krzysztof Szalewicz
TSRC Host: Mark Kozak

Meeting Location: Telluride Elementary School, 447 West Columbia Avenue

- All invited talks are 40 minutes long and are followed by 10 minutes discussions.
- Contributed talks are 10 minutes long and are followed by discussions at the respective posters throughout the week.
- All breakfasts are in the Telluride Elementary School and are provided, for participants only, by TSRC.
- Lunches and dinners (except for picnic in Wednesday) are on your own, but we will have a designated restaurant for dinner each day.
- Note two hike times: we plan to go with the whole group. Hike leaders are needed.

Tuesday, July 7

8:00	8:29	Breakfast at TSRC	
8:29	8:30	Opening remarks	

Session I: New developments in theory of intermolecular interactions (Chair: Kathy Hunt)

8:30	9:20	Mark Gordon	Intermolecular interactions with fragmentation methods
9:20	10:10	Malgorzata Szczesniak	New developments in DFT for intermolecular interactions
10:10	11:00	Georg Jansen	Enhancing intermolecular perturbation theory
11:00	11:20	Coffee break	
11:20	12:10	John Herbert	Recent developments in the XSAPT methodology
12:10	13:00	David Sherrill	Atomic and fragment partitioning of symmetry adapted perturbation theory
13:00	14:30	Lunch	

Session II: Contributed talks (Chair: David Sherrill)

14:30	14:40	Wiktor Beker	Analysis of catalytic activity of PT3 theozyme mutants through the lenses of intermolecular interaction theory
14:40	14:50	Mary van Veleet	Deriving accurate, transferable intermolecular potentials from SAPT and an iterated stockholder atoms procedure
14:50	15:00	Emilie Guidez	A first-principles dispersion correction for density functional theory and Hartree-Fock theory based on the effective fragment potential method
15:00	15:10	Chen Qu	Permutationally invariant fitting of non-covalent interactions and application to clathrate hydrates
15:00	15:10	Colleen Bertoni	Analytic gradients for the effective fragment molecular orbital method
15:10	15:30	Coffee break	
15:30	15:40	Michal Hapka	Untypical conformation of aurophilic complexes with 2-Mercapto-4-methyl-5-thiazoleacetic acid ligands determined by noncovalent interactions
15:40	15:50	Daniel Smith	Refitting damping parameters for DFT-D3
15:50	16:00	Muhammad Shahbaz	Dispersion energy, response functions, and non-local correlation functionals

16:00	16:10	Mike Metz	Automatic generation of intermolecular potentials
16:10	17:10	Poster session	
18:00	19:00	Town talk in Mountain Village Conference Center	

Wednesday, July 8

8:00	8:30	Breakfast at TSRC	

Session III: Dispersion energy (Chair: Dan Chipman)

8:30	9:20	Ken Jordan	Use of Drude oscillators and polarization potentials in modeling long-range correlation effects
9:20	10:10	Lyudmila Slipchenko	Dispersion interactions in the effective fragment potential method
10:10	10:30	Coffee break	
10:30	11:20	Alexander Tkatchenko	Quantum Fluctuations and Non-Covalent Interactions in Large Molecular Complexes
11:20	12:10	John Dobson	Spooky correlations and unusual van der Waals forces between gapless and near-gapless molecules
12:10	18:00	Free time for hiking and lunch	
18:00	21:00	Picnic at Telluride Elementary School	

Thursday, July 9

8:00	8:30	Breakfast at TSRC	

Session IV: Development and applications of potential energy surfaces (Chair: Mark Gordon)

8:30	9:20	Piotr Jankowski	Are full-dimensional interaction-energy surfaces of spectroscopic accuracy feasible?
9:20	10:10	Alston Misquitta	Experiments with the iterated stockholder atoms procedure in intermolecular interaction models
10:10	11:00	Berta Fernandez	Interaction potentials and further developments
11:00	11:20	Coffee break	
11:20	12:10	Krzysztof Szalewicz	Strategies for development of potentials in investigations of crystal structures and in molecular simulations
12:10	13:00	Richard Wheatley	Calculating atomic properties and potential energy surfaces
13:00	14:30	Lunch	

Session V: Collisions (Chair: Ken Jordan)

14:30	15:20	Robert Moszynski	Asymptotic physics with subradiant and superradiant states of diatomic molecules
15:20	16:10	Kathy Hunt	Collision-induced infrared absorption and light scattering by interacting hydrogen molecules
16:10	17:00	Gerit Groenenboom	Nonadiabatic effects in atomic and molecular collisions
17:00	17:20	Coffee break	

Session VI: Clathrates (Chair: Robert Hinde)

17:20	18:10	Zlatko Bacic	Molecular hydrogen in nanoscale confinement: From intermolecular potentials to quantum dynamics, neutron scattering spectroscopy, and unexpected selection rules
18:10	19:00	Ramon Hernandez	Local correlation studies of dihalogens inside clathrate cages
19:00		Time for dinner	

Friday, July 10

8:00	15:30	Time for hike (no breakfast at TSRC)

Session VII: Clusters (Chair: Lyudmila Slipchenko)

15:30	16:20	Greg Tschumper	Getting down to the fundamentals of hydrogen bonding: benchmark harmonic and anharmonic vibrational frequencies for small water clusters and other prototypes
16:20	17:10	Konrad Patkowski	Accurate modeling of the CH_4 and CO_2 adsorption on carbon nanotubes
17:10	18:00	Rafal Podeszwa	Successes and challenges in calculations of intermolecular interaction energies
18:00		Workshop dinner (not included in workshop fee)	

Saturday, July 11

8:00	8:30	Breakfast at TSRC

Session VIII: Condensed phases (Chair: Georg Jansen)

8:30	9:20	Dan Chipman	Implicit solvation models for dispersion, exchange, and hydrogen bonding interactions
9:20	10:10	Margarita Bernal	Halogen bonds -vs- hydrogen bond: Hydration of Br_2 in liquid water
10:10	11:00	Robert Hinde	Three-body interactions in low-temperature quantum solids
11:00	11:10	Closing remarks	