**INTERMOLECULAR INTERACTIONS**: ***New Challenges for ab initio Theory***

**Organizers: Grzegorz Chalasinski, Malgorzata Szczesniak, and Krzysztof Szalewicz**

**TSRC Hosts: Director Nana Naisbitt (970-708-0004) and Asst. Director Rory Sullivan (970-708-4542)**

**Meeting Location: Telluride Intermediate School, 725 W. Colorado**

**All invited talks are 40 minutes long and are followed by 10 minutes discussions (except when shorter talks requested by speakers).**

**Contributed talks are 10 minutes long and are followed by discussions at the respective posters.**

**All breakfasts are in the Telluride Intermediate School and are provided, for participants only, by TSRC.**

**Monday, July 15**

* 7:30am-8:00am: Breakfast at TSRC meeting site
* 8:00am-8:05pm Welcome by organizers
* 8:05am-12:30pm: **Session I: New developments in theory of intermolecular
 interactions**
	+ 8:05am-8:55am: Georg Jansen: *Single-determinant-based symmetry-adapted
	 perturbation theory without single-exchange approximation:
	 derivation and applications*
	+ 8:55am-9:45am: David Sherrill: *Density Fitting and Natural Orbitals in Coupled-
	 Cluster Theory and Symmetry-Adapted Perturbation Theory*
	+ 9:45am-10:35am Alston Misquitta: *Charge-transfer from regularized
	 symmetry-adapted perturbation theory*
	+ 10:35am-10:50am: Break
	+ 10:50am-11:40am: John Herbert: *Efficient monomer-based approaches for
	 computing intermolecular interactions in many-body systems*
	+ 11:40am-12:30pm: Rafal Podeszwa: *Efficient calculations of accurate
	 interaction energies for nano-scale systems*
* 12:30pm-2:00pm: Lunch time in town
* 2:00pm-4:00pm: **Session II: Benchmark interaction energies**
	+ 2:00pm-2:50pm: Pavel Hobza: *How accurate are “gold standard" CCSD(T)/CBS
	 interactions energies?*
	+ 2:50pm-3:40pm: Ken Jordan: *Use of the quantum Monte Carlo method in calculations
	 of weak interactions*
	+ 3:40pm-4:00pm: Break
* 4:00pm-5:00pm: **Session III: Contributed talks**
	+ 4:00pm-4:10pm: Trent Parker: *Systematic studies of various truncations of symmetry
	 adapted perturbation theory*
	+ 4:10pm-4:20pm: Robert Parrish: *Spatial partitioning of the SAPT0 decomposition: a
	 direct visualization heuristic for noncovalent interactions*
	+ 4:20pm-4:30pm: Michal Hapka: *Unusual Van der Waals complexes with SAPT: RG +
	 BeO, excited He and Ne atoms + H2, RG*
	+ 4:30pm-4:40pm: Evangelos Miliordos: *Variation of the atomic states of metal ions with
	 the degree of solvation: the case of Mg, Ca, Al, and Fe*
	+ 4:40pm-4:50pm: Oleksandr Loboda: *Electronic contributions to linear and nonlinear
	 optical properties in fullerene-based molecular systems*
	+ 4:50pm-5:00pm: Koushik Chatterjee: *Excitation energy from extended random phase
	 approximation employed with approximate one- and two-electron
	 reduced density matrices*
* 6:00pm-Dark: **TSRC Picnic Ah Haa School @ 300 S. Townsend. Families and
 guests welcome free of charge**

**Tuesday, July 16**

* 7:30am-8:00am: Breakfast at the TSRC meeting site
* 8:00am-12:10am: **Session IV: Development and applications of potential energy
 surfaces**
	+ 8:00am-8:50am: Piotr Jankowski: *High resolution spectra of van der Waals complexes
	 from first principles*
	+ 8:50am-9:40am: Berta Fernández Rodríguez: *Interaction potentials and
	 (hyper)polarizabilities in weakly-bonded complexes*
	+ 9:40am-10:30am: Claude Millot: *Modeling of water distributed multipoles and
	 polarizabilities*
	+ 10:30am-10:50am: Break
	+ 10:50am-11:40am: Millard Alexander: *Nonadiabaticity in the F+HF and F+HCl reaction*
	+ 11:40am-12:10pm: Richard Wheatley: *Theoretical and experimental studies of nitric oxide
	 interactions*
* 12:10pm-1:10pm: Lunch time in town
* 1:10pm-5:30pm: **Group Hike**
* 6:00pm-7:15pm: **Town Talk at the Historic Sheridan Opera House, 110 N. Oak**
* 8:00pm: **Group Dinner**

**Wednesday, July 17**

* 7:30am-8:00am: Breakfast at TSRC meeting site
* 8:00am-12:30pm: **Session V: Clusters and condensed phases**
	+ 8:00am-8:50am: Claude Leforestier: *Calculation of IR shifts in water clusters*
	+ 8:50am-9:40am: Francesco Paesani: *Potential problems with water simulations: From
	 the dimer to the liquid at the fully quantum-mechanical level*
	+ 9:40am-10:30am: Greg Schenter: *Assessment of the role of broken symmetry on
	 solvation structure using MD-EXAFS techniques*
	+ 10:30am-10:50am: Break
	+ 10:50am-11:40am Joachim Sauer: *Towards Chemical Accuracy for Molecule-Surface
	 Interactions*
	+ 11:40am-12:30pm: Maria Pilar de Lara-Castells: *Helium-mediated deposition on the
	 TiO2(110) surface: Insights from DFT/TDDFT*
* 12:30pm-2:00pm: Lunch time in town
* 2:00pm-6:30pm: **Session VI: Post-DFT methods applicable to intermolecular
 interactions**
	+ 2:00pm-2:50pm: Katarzyna Pernal: *Extended random phase approximation: excitation
	 energies and prospects of describing molecular interactions*
	+ 2:50pm-3:40pm: Andreas Hesselmann: *Nonlocal correction approach to conventional
	 density functional theory methods*
	+ 3:40pm-4:30pm: Krzysztof Szalewicz: *Density functional plus dispersion methods with
	 dispersion energies computed from first principles*
	+ 4:30pm-4:50pm: Break
	+ 4:50pm-5:40pm: Janos Angyan: *Recent progress and perspectives in rangehybrid RPA
	 method*
	+ 5:40pm-6:30pm Lukasz Rajchel: *Range-Separated Flavours of Pauli Blockade and
	 Symmetry-Adapted Perturbation Theory Methods*
* 6:30pm: Dinner Time

**Thursday, July 18**

* No breakfast
* Until 1:00pm: Free time for hiking and lunch
* 1:00pm-5:30pm: **Session VII: Collisions**
	+ 1:00pm-1:50pm: Jacek Klos: *Potentials and dynamics of complexes of NO and OH
	 radicals in their excited electronic states with noble gas atoms*
	+ 1:50pm-2:40pm: Ad van der Avoird: *Intermolecular potentials probed by controlled
	 collisions; challenges for open-shell systems*
	+ 2:40pm-3:30pm: Laurent Wiesenfeld: *Interaction of simple molecules with H2 and He:
	 from potentials to experiments and astrophysical observations*
	+ 3:30pm-3:50pm: Break, snacks provided by TSRC
	+ 3:50pm-4:40pm: Balakrishnan Naduvalath: *Collisions and Reactions in Ultracold Gases*
	+ 4:40pm-5:30pm: Robert Moszynski: *Efficient scheme for the optical production of
	 deeply bound ultracold Sr2 molecules from state-of-the-art ab initio
	 calculations*
* 5:30 Dinner time

**Friday, July 19**

* 7:30am-8:00am: Breakfast at TSRC meeting site
* 8:00am-10:00am: **Session VIII: Post-DFT methods applicable to intermolecular
 interactions (part 2)**
	+ 8:00am-8:50am: Grzegorz Chalasinski: *New range separation ideas in DFT for
	 intermolecular interactions*
	+ 8:50am-9:40am: Malgorzata Szczesniak: *Interaction energies from range-separated
	 functionals*
	+ 9:40am-10:00am: Break
* 10:00am-12:00am **Session IX: Clusters and condensed phases (part 2)**
	+ 10:00am-10:50am: Robert Hinde: *Interaction-induced spectroscopy in molecular quantum
	 solids*
	+ 10:50pm-11:40pm: Ramon Hernández: *Molecular oxygen clusters and the epsilon solid
	 phase*
	+ 11:40pm-12:00pm: Closing of the meeting