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

**Organizers: Bogumil Jeziorski, Berta Fernández Rodríguez, and Krzysztof Szalewicz**

##### TSRC Hosts: Mark Kozak (970) 708 4426, ****Cindy Fusting (970) 708 5069, Sara Friedberg (970) 709 0622****

**Meeting Location: Ah Haa School for the Arts, 300 S Townsend Street, Telluride, CO 81435**

**All talks are 40 minutes long and are followed by 10 minutes discussions**

**All breakfasts are in the Ah Haa School for the Arts and are provided, for participants only, by TSRC**

**Sunday, March 17**

* 6:00pm-8:00pm Informal get together at the Phoenix Bean, 221 W Colorado Ave
 (this is a café with food and drinks for purchase)

**Monday, March 18**

* 7:15am-8:00am: Breakfast at TSRC meeting site
* 8:00am-8:05am Welcome by the organizers
* 8:05am-9:45am: **Session I: New developments in theory of intermolecular
 interactions** (chair: David Sherrill)
	+ 8:05am-8:55am: *Bogumil Jeziorski*: *Symmetry-adapted perturbation theory for the
	 interaction energies of degenerate states*
	+ 8:55am-9:45am: Konrad Patkowski: *Spin-flip SAPT and SAPT-F12*
* 9:45am-4:15pm: Informal scientific discussions
* 4:15pm-6:45pm: **Session II: Spectroscopy and scattering – Part I** (chair: Peter
 Schwerdtweger)
	+ 4:15pm-5:05pm: Millard Alexander: *Spin-orbit nonadiabaticity in the predissociation of
	 OH and SH: Theory and comparison with experiment*
	+ 5:05pm-5:55pm: Piotr Wcislo: *Collisional effects in the shapes of molecular spectra*
	+ 5:55pm-6:45pm: Kathy Hunt: *New ab initio results for collision-induced dipoles and
	 polarizabilities and new analytical results for transition probabilities*
* 7:00pm Dinner at La Cocina de Luz, 123 E Colorado Ave

**Tuesday, March 19**

* 7:15am-8:00am: Breakfast at the TSRC meeting site
* 8:00am-9:40am: **Session III: Intermolecular potentials** (chair Gerrit Groenenboom)
	+ 8:00am-8:50am: Richard Dawes: *Interpolated potentials for the study of spectroscopy
	 and dynamics in vdWs systems*
	+ 8:50am-9:40am: Berta Fernández Rodríguez: *Improving the accuracy of intermolecular
	 potentials and spectra of weakly-bonded complexes*
* 9:45am-4:15pm: Informal scientific discussions
* 4:15pm-6:45pm: **Session IV: Spectroscopy and scattering – Part II** (chair: Kathy Hunt)
	+ 4:15pm-5:05pm: Edit Matyus: *Rovibrational states of molecular systems with several
	 large-amplitude motions: recent developments and applications of a
	 general variational approach*
	+ 5:05pm-5:55pm: Gerrit Groenenboom: *Quantum scattering beyond the gold standard*
	+ 5:55pm-6:45pm: Piotr Zuchowski: *Resonances in (ultra)cold collisions: lessons for ab-
	 initio and the wishlist*
* 7:00pm Dinner at High Pie, 100 West Colorado

**Wednesday, March 20**

* 7:15am-8:00am: Breakfast at TSRC meeting site
* 8:00am-9:40pm: **Session V: Intermolecular interactions in outer space** (chair: Edit
 Matyus)
	+ 8:00am-8:50am: Jacek Klos: *Carbon and Fluorine Chemistry in the Interstella
	 Media: Ab initio Studies versus Experiment*
	+ 8:50am-9:40am: Robert Hinde: *Collision-induced absorption in planetary atmospheres
	 Molecules, models, and measurements*
* 9:45am-4:15pm: Informal scientific discussions
* 4:15pm-6:45pm: **Session VI: Going beyond few-atomic systems - Part I** (chair: Millard
 Alexander)
	+ 4:15pm-5:05pm: Robert DiStasio: *Attracting Opposites: Promiscuous Ion-pi Binding in
	 the Nucleobases*
	+ 5:05pm-5:55pm: Krzysztof Szalewicz: *Dispersion energy in density-functional theory*
	+ 5:55pm-6:45pm: *Alexander Tkatchenko*: *Non-Covalent Interactions in Large
	 Molecules: Can We Trust Quantum-Chemical Benchmarks?*
* 7:30pm: Workshop banquet: Village Table in Mountain Village, 618 Mountain
 Village Blvd, Mountain Village (TSRC subsidizes $20; charge to
 participants, NOT included in the workshop fee, is $35 payable to
 Cindy. This can be settled during a workshop break.)

**Thursday, March 21**

* 7:15am-8:00am: Breakfast at TSRC meeting site
* 8:00am-12:30pm: **Session VII: Going beyond few-atomic systems - Part II** (chair:
 Robert Hinde)
	+ 8:00am-8:50am: Lyudmila Slipchenko: *The effective fragments for electronic excitations
	 and ligand-protein binding atmospheres*
	+ 8:50am-9:40am: Tatiana Korona: *Partitioning of Intermolecular Interactions -- New
	 Ideas and Their Applications*
* 9:45am-4:15pm: Informal scientific discussions
* 4:15pm-6:45pm: **Session VIII: Going beyond few-atomic systems – Part III** (chair:
 Richard Dawes)
	+ 4:15pm-5:05pm: Rafal Podeszwa: *A quest for the missing quadrupole moment*
	+ 5:05pm-5:55pm: Peter Schwerdtweger: *From Sticky Hard Spheres to Lennard-Jones
	 potentials, Epstein zeta functions and many-body expansions for rare
	 gas solids*
	+ 5:55pm-6:45pm: David Sherrill: *Non-covalent interactions in solution and crystals*
* 7:30pm Dinner at Smugglers Union, 225 South Pine Street

**Friday, March 22**

* 7:15am-8:00am: Breakfast at TSRC meeting site
* 8:00am-9:30am: **Session IX: Summary of the workshop and general discussion of
 intermolecular interactions** (Bogumil Jeziorski)
* 9:30am-9:35am Closing of the workshop