**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 (with one exception)**

**All breakfasts are in the Baked in Telluride and TSRC will provide a $10 coupon for each breakfast. On Monday, stop in Ah Haa on your way to Baked in Telluride (opens 7 AM).**

**Sunday, March 19**

* 6:00pm-8:00pm Informal get together at the **Liberty Bar** 121S Fir St (this is a café with
 food and drinks for purchase)

**Monday, March 20**

* 8:00am-8:05am Welcome by the organizers
* 8:05am-9:45am: **Session I: New developments in theory of intermolecular
 interactions – Part I** (chair: Rafał Podeszwa)
	+ 8:05am-8:55am: Georg Jansen: *The interplay of dispersion and other contributions to
	 intermolecular interactions*
	+ 8:55am-9:45am: Konrad Patkowski: *Making symmetry-adapted perturbation theory
	 more accurate and more robust*
* 9:45am-4:15pm: Informal scientific discussions
* 4:15pm-6:45pm: **Session II: Spectroscopy and scattering** (chair: Piotr Żuchowski)
	+ 4:15pm-5:05pm: Piotr Jankowski: *New information from old data with the help of
	 theory: orthoH2-CO and orthoD2-CO revisited*
	+ 5:05pm-5:55pm: Piotr Wcisło: *Accurate laser spectroscopy for studying molecular*
	  *structure and interactions*
	+ 5:55pm-6:45pm: Edit Matyus: *Exact quantum dynamics developments for floppy
	 molecular system*
* 7:00pm Dinner at La Cocina de Luz, 123 E Colorado Ave

**Tuesday, March 21**

* 8:00am-9:40am: **Session III: Intermolecular potentials** (chair: Piotr Jankowski)
	+ 8:00am-8:50am: Seymour Wang: *It is all about polarization, polarization cooperativity
	 and polarization frustration*
	+ 8:50am-9:40am: Andrzej Sokalski: *Hierarchies of non-empirical intermolecular
	 interaction models*
* 9:40am-4:15pm: Informal scientific discussions
* 4:15pm-6:45pm: **Session IV: Interpretations of intermolecular forces** (chair: Edit
 Matyus)
	+ 4:15pm-5:05pm: Julia Contreras García: *New developments in NCI: coupling to
	 extremely localized molecular orbitals*
	+ 5:05pm-5:55pm: John Herbert: *Studies of Pi-Stacking Interactions with XSAPT+MBD*
	+ 5:55pm-6:45pm: Margarita Bernal: *The Exchange Picture of Non-Covalent Interactions.
	 A Study of Two Halogen Bonds*
* 7:00pm Dinner at High Pie, 100 West Colorado

**Wednesday, March 22**

* 8:00am-9:40pm: **Session V: New developments in theory of intermolecular
 interactions – Part II** (chair: Alexandre Tkatchenko)
	+ 8:00am-8:50am: Rafał Podeszwa: *Three-body interaction energies with low-cost
	 methods*
	+ 8:50am-9:40am: Daniel Boese: *In Pursuit of Accuracy: QM:QM Methods*
* 9:40am-4:15pm: Informal scientific discussions
* 4:15pm-6:45pm: **Session VI: Going beyond few-atomic systems** (chair: John Herbert)
	+ 4:15pm-5:05pm: Gerrit Groenenboom: *Interactions involving open-shell molecules:
	 NO+NH3 and TiH on a MgO crystal surface*
	+ 5:05pm-5:55pm: Berta Fernández: *The FGC approach for correcting noncovalent
	 interactions in SQM methods*
	+ 5:55pm-6:45pm: Tatiana Korona: *Reproducing the intermolecular interaction energy by
	 molecular fragmentation methods*
* 7:15pm: Workshop banquet: Talay in Mountain Village, 119 Lost Creek Lane,
 Mountain Village (TSRC subsidizes $25; charge to participants, NOT
 included in the workshop fee, is $10 payable to Cindy. This can be
 settled during a workshop break.)

**Thursday, March 23**

* 8:00am-9:40pm: **Session VII: Molecular properties** (chair: Tatiana Korona)
	+ 8:00am-8:50am: Kathy Hunt: *Interaction-induced properties of H, He, and H2*
	+ 8:50am-9:40am: Ken Jordan: *Polarizabilty and Polarization Potentials of Hexagonal
	 Polyaromatic Hydrocarbons*
* 9:40am-4:15pm: Informal scientific discussions
* 4:15pm-6:45pm: **Session VIII: Condensed phases** (chair: Daniel Boese)
	+ 4:15pm-5:05pm: Krzysztof Szalewicz: *Crystal structure predictions*
	+ 5:05pm-5:55pm: JR Schmidt: *Intermolecular interactions and atomic anisotropy from
	 molecular liquids to metal-organic frameworks*
	+ 5:55pm-6:45pm: Alexandre Tkatchenko: *Benchmarking the Benchmarks and
	 Embedding the Benchmarks for Non-Covalent Interactions*
* 7:00pm Dinner at Butcher & Baker, 201 E. Colorado

**Friday, March 24**

* 8:00am-9:40pm: **Session IX: Other important developments in intermolecular
 interactions** (chair: Konrad Patkowski)
	+ 8:00am-8:50am: Piotr Żuchowski: *Advances of many-electron SAPT based on second
	 quantisation approach*
	+ 8:50am-9:40am Mary van Vleet: *Ab initio, atomically-anisotropic force fields: a
	 benzene case study*
	+ 9:40am-10:00am Adil Kabylda: *Understanding interatomic interactions in large
	 molecules from machine-learned force fields*
* 10:00am-10:20am **Session X: Summary of the workshop and general discussion of
 intermolecular interactions** (Berta Fernandez and Krzysztof
 Szalewicz)
* 10:20am-10:25am Closing of the workshop