SCHEDULE

TSRC Many-Body Interactions Workshop: From Quantum Mechanics to Force Fields
June 15 – 19, 2024

Note that there is a reception from 5:00-6:30 PM Friday the 14th at Alibi– 157 S. Fir Street

Saturday, June 15

9:00 – 9:35	Greg Beran	*Modern challenges in organic crystal structure prediction: Results from the 7th Blind Test and beyond*
9:30 – 10:10	Thomas Plé	*FeNNol: an efficient and flexible library for building force-field-enhanced neural networks.*
10:10 – 10:30	Feng Wang	*Dispersion from a minor to a major component in intermolecular forces is key for accurate material properties.*
10:30 – 10:45		**coffee break**
10:45 – 11:20	David Sherrill	*Faster Computation of Interaction Energy Components in Symmetry-Adapted Perturbation Theory*
11:20 – 11:55	Michael Schnieders	*Constant-pH Molecular Dynamics with the Polarizable AMOEBA Protein Force Field*

Sunday, June 16

1:00 – 1:35	Kersti Hermansons	*From Quantum Mechanics (to Force Fields) to Properties*
1:35 – 2:10	Hai Lin	*Let QM and MM join hands*
2:10 – 2:30	Ken Jordan	*Convergence of the polarization potential of large PAHs to the image potential of graphene*
2:30 –2:45		**coffee break**
2:45 –3:20	Markus Meuwly	*Advanced Models for Electrostatic Interactions: Multipoles, Distributed Charges and Machine-Learning-Based Models*
3:20 –3:55	Krzysztof Szalewicz	*Quantum mechanical intramolecular force fields*
3:55 –4:30	Piotr Zuchowski	*New avenues in Many-Body SAPT: interaction induced properties, and density changes*

Monday, June 17

9:00 – 9:35	Frank Jensen	*Charge-flow polarization*
9:35 – 10:10	Teresa Head-Gordon	*Wat makes a force field accurate?*
10:10 – 10:30	Jorge Nochebuena	*Implementation of GEM, a density-based force field for QM/MM calculations.*
10:30 – 10:45		**coffee break**
10:45 – 11:20	Martin Head-Gordon	*Quantifying and characterizing charge transfer in intermolecular interactions.*
11:20 – 11:55:	John Herbert	*Enabling High-Order Many-Body Expansions with Energy-Based Screening*
5:30-7:30		**Picnic**

Tuesday, June 18

9:00 – 9:20	Bruno von Bruening	*Distributed Multipoles from Stockholder Density Partitioning: New Developments, Benchmarking, and Machine Learning*
9:20 – 9:40	Mary van Vleet	*TBA*
9:40 – 10:00	Jean-Philip-Piquemal	*What can we learn from large scale simulations with polarizable force fields*
10:00 – 10:20	Emile Guidez	*Development of multilayer adaptive partitioning methods to model ion transport*
10:15 – 10:35		**coffee break**
10:35 – 11:10	Josh Rackers	*Can AI algorithms learn many-body interactions? Lessons from a journey in drug discovery.*
11:10 – 11:30	Saswata Dasgupta	*Elevating the Accuracy of DFT for Condensed Phase Simulations Using Machine Learning and Many-Body Techniques*
11:30 – 11:50	Louis Lagardere	*Free energy simulations using many-body force fields with Tinker-HP*
6:30-7:30		**Town talk**