

## Schedule for the Telluride Workshop on Many-Body Interactions from Quantum Mechanics to Force Fields

### Monday Morning

- 7:30-8:00 Breakfast at the meeting site
- 8:00-8:10 Opening Remarks
- 8:10-8:50 Ken Jordan "Incorporating Electron Correlation Effects in Electron-Water Interactions via Model Potentials"
- 8:50-9:30 Teresa Head-Gordon "iAMOEBA: a direct polarization model"
- 9:30-9:50 Lori Burns "Assessing the Performance of Density Functional and Wavefunction Methods for Noncovalent Interactions"
- 9:50-10:10 Break
- 10:10-10:50 Alston Misquitta "The role of Explicit Polarization on the Energy Landscape of Pyridine Clusters"
- 10:50-11:30 Greg Schenter "EXAFS Analysis of Molecular Interaction"
- 11:30-11:50 Jan Steckel "Electronic Structure Calculations of the Acetate-CO<sub>2</sub> Interaction: Implications for Force Field Development"
- 11:50-12:10 Open Discussion

### Monday Evening

- 7:00-7:40 Susan Sinnott "Charge Optimized Many-Body (COMB) Potentials: Development and Applications"
- 7:40-8:20 Carsten Mueller "Electron Correlation Effects in Extended Systems"

### Tuesday Morning

- 7:30-8:00 Breakfast at the meeting site

8:00-8:40	Jay Ponder	"The AMOEBA Force Field: Current Problems and Possible Solutions"
8:40-9:20	Andreas Cisneros	"Use of Gaussian Electrostatic Model Distributed Multipoles in AMOEBA"
9:20-9:40	Fangfang Wang	"DPP2 and DPP3 Water Models"
9:40-10:00	Break	
10:00-10:40	David Sherrill	"The Importance of Charge Penetration of Pi-Interactions"
10:40-11:20	Gary Kedziora	"DFT molecular dynamics: from validation to simulation"
11:20-11:40	Aude Marjolin	"Modeling of Lanthanide and Actinide Cations: From QM to MM"
11:40-12:00	Open Discussion	

## **Tuesday Evening**

### **6:00 - 7:15 p.m., Town Talks at the Palm Theatre**

"Learning from Nature's 3-Billion-Year Solar Energy Program," Gregory Scholes, University of Toronto

"Plastic Solar Cells: Learning how molecule think," Peter Rossky, Departments of Chemistry and Chemical Engineering, University of Texas at Austin

7:30-8:10	Carine Clavaguera	"IR Spectroscopy of Gas Phase and Micro-Hydrated Biomolecules with New Generation Force Fields"
8:10-8:30	A. Donchev/John Klepeis	"Polarizable Force Field Development at D. E. Shaw"

## **Wednesday Morning**

7:30-8:00	Breakfast at the meeting site	
8:00-8:40	Liem Dang	"Understanding Ion-Ion Interactions in Bulk and Aqueous Interfaces Using Molecular

## Simulations"

- 8:40-9:20 Jiali Gao "Variational Many-body Expansion in the Framework of Block-Localization"
- 9:20-9:40 Karl Diebec "Atomistic Simulations of a Two-Domain Protein on the Microsecond Time-Scale"
- 9:40-10:00 Break
- 10:00-10:40 Gabor Csanyi "A Systematic Bayesian Approach to Potentials"
- 10:40-11:20 Jean-Philip Piquemal "Improving polarizable force fields: from small energy differences to free energies."
- 11:20-11:40 Mike Schnieders "Accelerating Polarizable Multipole AMOEBA Free Energy Calculations Using Orthogonal Space Methods"
- 11:40-12:00 Open Discussion

## Wednesday Evening

5:00-7:00 Workshop dinner at Floradora

- 7:20-8:00 Nohad Gresh "Development, Validation, Applications, and Perspectives of Polarizable, Anisotropic Molecular Mechanics Potentials"
- 8:00-8:40 Laura Gagliardi "Bridging the Gap between Quantum Chemistry and Classical Simulations for CO<sub>2</sub>"

## Thursday Morning

- 7:30-8:00 Breakfast at the meeting site
- 8:00-8:40 Feng Wang "Investigating the Free Energy of Ice and Water on a Coupled Cluster Quality Potential Energy Surface through a Force Field"
- 8:40-9:20 Pengyu Ren "Development of Polarizable Multipole Force Field and its Applications"

9:20-9:40 Break

9:40-10:20 Alexander Tkatchenko "Accurate and Efficient First-Principles Calculation of van der Waals Energy"

10:20-11:00 Robert DiStasio "Many-Body van der Waals Interactions: Theory and Applications"

11:00-11:40 Jean-Pierre Dognon "f-Elements Theoretical Chemistry: From Structure to Thermodynamics"

11:40-12:00 Open Discussion

### **Thursday Evening**

6:00-9:00 Picnic

### **Friday Morning**

Departure