Many-Body Interactions: From Quantum Mechanics to Force Fields (Virtual)

Monday, June 8 – Friday, June 12

Join Many Bodies Zoom Meeting

https://zoom.us/j/93767253912?pwd=d2J5eFVEc2UxZGp4ZlZpckRwc3JjUT09

Meeting ID: 937 6725 3912

Password: TSRCMB-20

One tap mobile

+12532158782,,93767253912#,,1#,552458# US (Tacoma)

+13462487799,,93767253912#,,1#,552458# US (Houston)

Tips on how to use Zoom:
Joining a Meeting: https://www.youtube.com/watch?list=RDCMUC2SxmE4C-KAQuHaEfHVymgQ&v=hIkCmbvAHQQ&feature=emb_rel_end

Meeting Controls: https://www.youtube.com/watch?v=ygZ96J_z4AY&feature=emb_rel_end

Please find below an updated draft of the schedule for our TSRC workshop. The meeting will start 9:45 AM, EDT, USA on Monday and at 10:00 AM the other days. Times listed are East Coast, US. These times were chosen to be convenient for participants in both the USA and Europe. If there is any problem with the day/time we have listed below, please let us know as soon as possible.

Note, indented time entries indicate time for questions/discussion following each talk or pair of coupled talks.

Best wishes,

Ken, Clemence, Jean-Philip

Monday, June 8 (All times EDT)

9:45 – 10:00	Introductory remarks	
10:00 – 10:30	J. R. Schmidt	"Ab initio force fields for modeling metal-organic framework structures, defects, and reactivity"
10:30 – 10:40		
10:40 – 11:00	Jean-Philip Piquemal	"Accelerating polarizable molecular dynamics in Tinker-HP using GPUs"
11:00 – 11:10		
11:10 – 11:20	general discussion/break	
11:20 – 11:40	Chen Qu	"Fragmented permutationlly invariant polynomial potential energy surfaces"

11:40 – 11:50		
11:50 – 12:10	Frédéric Celerse	"How to efficiently evaluate the polarization effects in Classical Molecular Dynamics"
12:10-12:20		

Tuesday, June 9 (All times EDT)

10:00 – 10:30	Mary Van Vleet	
10:20 – 10:30		
10:30 – 10:50	Judy Herzfeld	"Animating Lewis Dots: Features of Reactive Force Fields Based on Semi-Classical Electrons"
10:50 – 11:00		
11:00 – 11:20	Michele Nottolli	"Adiabatic excited state molecular dynamics in a QM/MM polarizable embedding"
11:20 – 11:30		
11:30 – 11:40	general discussion/break	
11:40 – 12:00	Feng Wang	"Development of force field for CO2, surprising large contribution from basis set superposition error"
12:00 – 12:10		
12:10 – 12:30	Sehr Naseem-Khan	"Status and current development of the GEM water model"
12:30 – 12:40		

Wednesday, June 10 (All times EDT)

10:00 – 10:30	Francesco Paesani	"Data-driven many-body models for predictive simulations: Where we are and where we are going".
10:30 – 10:40		
10:40 – 11:00	Pier Paolo Poier	"Polarizable charges in a generalized Born reaction potential"
11:00 – 11:10		
11:10 – 11:20	general discussion/break	
11:20 – 11:40	David Sherrill	"Machine Learning Models of Intermolecular Interactions"
11:40 – 11:50		
		"Multitask prediction of chemical properties with an atoms-in-molecules neural network (AIMnet)"

11:50 – 12:10	Olexandr Isayev	
12:10-12:20		
12:20 – 12:35	Ken Jordan	"Analysis of the Molecular Virial Theorem using Dalgarno-Lewis Perturbation Theory"
12:35-12:40		

Thursday, June 11 (All times EDT)

10:00 – 10:30	Krzysztof Szalewicz	"Symmetry-adapted perturbation theory calculations at complete basis set limit for systems with hundreds of atoms".
10:30 – 10:40		
10:40 – 11:10	Chiara Capelli	"Fully Polarizable Embedding Approach for the Computational Spectroscopy of Complex Systems: Status and Perspectives"
11:10 – 11:20		
11:20 – 11:30	general discussion/break	
11:30 – 11:50	Toon Verstraelen	"Accurate transferable polarization model derived from the monomer electron density"
11:50 – 12:20		
12:00 – 12:20	Henry Chan	"Bridging the electronic, atomistic, and mesoscopic scales using machine learning"
12:20-12:30		

Friday, June 12 (All times EDT)

10:00 – 10:30	Greg Beran	"Overcoming the limits of widely used density functionals in crystal structure prediction with dispersion-corrected MP2 methods"
10:30 – 10:40		
10:40 – 11:10	Alston Misquitta	
11:10 – 11:20		
11:20 – 11:30	general discussion/break	
11:30 – 11:50	Gabor Csanyi	"From empirical force fields to machine learned potentials and back"
11:50 – 12:10	Cas van der Oord	

12:10-12:20

12:20-12:30 Wrap-up comments