Berkeley Statistical Mechanics Meeting – Poster Session I

Friday, January 10, 2020

#	Name	Institution	Title of poster
1	Agrawal, Nikhil	UC Berkeley	Electrostatic wetting transition: Charge renormalization and charge inversion
2	Atsango, Austin	Stanford University	An *ab initio* molecular dynamics study of the proton transport mechanism in liquid imidazole
3	Cox, Stephen	University of Cambridge	Electromechanical coupling at the air/water interface: A local molecular field theory approach
4	Jia, Qizhang	University of Virginia	Modeling the surface diffusion of dopamine and its derivatives on carbon electrode surfaces
5	Limaye, Aditya	Massachusetts Institute of Technology	Modeling interfacial electron transfer in the double layer: Electrode coupling vs. electrostatic driving
6	Perez, Tynan	UC Berkeley	Addressing finite size effects in ion adsorption to the air/water interface
7	Self, Julian	UC Berkeley	Ion speciation diagrams for low permittivity electrolytes
8	Sousa Castellanos, Sebastian	University of Colorado Boulder	Biomimetic nanoporous graphene: Solute permeation and free energy reconstructions
9	Takeda, Michika	Kyushu University	Condensation of patchy macroanions mediated by cations: Analysis based on the effective second virial coefficient
10	Gomez, Yessica	UC San Francisco	Probing transmembrane stability using integral membrane model mutants
11	Patel, Amish	University of Pennsylvania	Identifying hydrophobic protein patches to inform protein interaction interfaces
12	Rogers, Julia	UC Berkeley	Molecular insights into the dynamics of phospholipid exchange between membranes
13	Duan, Chao	UC Berkeley	Conformation of a single polyelectrolyte chain in poor solvents: Globule, pearl-necklace and vesicle
14	Frechette, Layne	UC Berkeley	Mean-field behavior of an elastic Ising model
15	Liu, Lucie	UC Berkeley	Charged Ising models can be used to study dynamics of surfactant self-assembly at interfaces
16	Zhang, Zhongmin	University of Virginia	Studying the effect of chain stiffness on sequence in step-growth copolymerization
17	Carpenter, John	University of Utah	Using kinetics to predict crystal structures
18	Denk, Jonas	UC Berkeley	Self-organization and criticality in spatially coupled ecosystems

19	Fu, Ray	Northwestern University	Effective equilibrium in a system of active Janus colloids
20	Remsing, Rick	Rutgers University	Plastic crystals: Electronic and organic
21	Albaugh, Alex	Northwestern University	Estimating reciprocal partition functions to enable design space sampling
22	Das, Avishek	UC Berkeley	Variational control forces for enhanced sampling of nonequilibrium molecular dynamics simulations
23	Epstein, Jeffrey	UC Berkeley	Active matter, time reversal symmetry breaking, and Onsager reciprocal relations
24	Hargus, Cory	UC Berkeley	Active matter, time reversal symmetry breaking, and Green-Kubo calculations
25	Louwerse, Miranda	Simon Fraser University	Minimum work control of small-N 2D Ising models
26	Rose, Dominic	University of Nottingham	A reinforcement learning approach to rare trajectory sampling
27	Sahu, Amaresh	UC Berkeley	Active contact forces drive non-equilibrium fluctuations in membrane vesicles
28	Saxena, Saloni	Brown University	Stochastic dynamics and wavenumber selection in a model of pattern formation
29	Strand, Nils	Northwestern University	Current inversion in a periodically driven two-dimensional Brownian ratchet
30	Chen, Ming	UC Berkeley	Reducing noise in stochastic density functional theory
31	Cline, Peyton	University of Colorado Boulder	The quantum impurity problem: How coupling to the environment affects local operators
32	Mao, Yuezhi	Stanford University	Generating diabatic states for electron and hole transfer from electronic structure calculations
33	Park, Yoonjae	UC Berkeley	Simulations on the dynamics of charge carriers in crystalline lattice using path integral framework
34	Philbin, John	UC Berkeley	Exciton dynamics in nanocrystal monomers and dimers
35	Ranya, Srinath	Cornell University	Multi-state ring polymer instantons and nonadiabatic reaction rates
36	Wrona, Paul	UC Berkeley	Exciton-exciton interactions in coupled quantum wells

Berkeley Statistical Mechanics Meeting – Poster Session II

Saturday, January 11, 2020

#	Name	Institution	Title of poster
1	Chen, Michael	Stanford University	Exploiting machine learning to efficiently predict optical spectra in solution
2	Menzl, Georg	Lawrence Berkeley National Lab	Coarse-graining polarization fluctuations in water
3	Niblett, Sam	UC Berkeley	Efficient machine learning schemes to simulate the structure and dynamics of water
4	Hocky, Glen	New York University	Infinite switch simulated tempering in force
5	Khot, Aditi	Purdue University	Evidence of information limitations in bottom-up coarse-graining models
6	Pahng, Seong Ho	Harvard University	Predicting ground state configuration of energy landscape using graph neural network
7	Johnson, Margaret	Johns Hopkins University	Quantifying kinetics of multi-protein self-assembly, remodeling, and disassembly
8	Li, Yongle	California Institute of Technology	Bioferroelectric properties of glycine crystals
9	Martis, Stephen	UC Berkeley	Epistasis can drive diversification in the competition for many resources
10	Stephens, Christina	UC San Francisco	Computational methods to determine the mechanism of TMEM16 lipid scramblases
11	Zhang, Bin	Massachusetts Institute of Technology	Multi-scale modeling of genome organization
12	Zimmer, Matthew	California Institute of Technology	Cotranslational forces can influence a protein's sequence
13	Hasyim, Muhammad	UC Berkeley	On a relation between theory of elasticity and dynamical facilitation theory of glass formers
14	Karnes, John	Lawrence Livermore National Lab	Network topology of crosslinked acrylate polymers
15	Merz, Steven	University of Virginia	Using simulation to probe the sequence determinants within ATRP copolymerizations in bulk and on nanoparticle surfaces
16	Jacobson, Daniel	California Institute of Technology	Universal dynamical phase transition in dendritic growth
17	Niblo, Jessica	University of Virginia	Self-assembly of viral capsid-like structures in an oscillatory energy landscape
18	Olsen, Nicholas	University of Utah	Simple molecular models for chiral crystallization

19	Swartley, Jacob	University of Virginia	Modeling the self-assembly of mixed ligand monolayers on Ag nanoparticles
20	Galib, Mirza	UC Berkeley	Understanding reactive uptake of N_2O_5 in atmospheric aerosol using machine learning and *ab-initio* MD
21	Gao, Chloe	UC Berkeley	What do rare fluctuations tell us about nonequilibrium systems?
22	GrandPre, Trevor	UC Berkeley	General features of entropy production and dynamical phases in active matter systems
23	Helms, Phillip	California Institute of Technology	Large deviations in a 2D nonequilibrium system via tensor networks
24	Kim, Jeongmin	California Institute of Technology	Energy conversion via metal nanofilms
25	Kuznets-Speck, Ben	UC Berkeley	Taking transition-state theory for a drive: Rate estimation far from equilibrium
26	Lawniczak, James	California Institute of Technology	Embedded mean-field theory for solution-phase polyolefin catalysis
27	Sheth, Janaki	UC Los Angeles	Noisy driven oscillators: Adaptive drives break the fluctuation-dissipation theorem
28	Vroylandt, Hadrien	Northwestern University	Isometric uncertainty relations
29	Bocquet, Marie-Laure	École Normale Supérieure & CNRS	Two dimensional materials get electrified in water: *Ab initio* simulations of the surface reactivity of graphene, h-BN, their heterostructures and graphene oxide in water
30	Cheng, Lixue Sherry	California Institute of Technology	Machine learning for electronic structure via the molecular orbital basis
31	Korol, Roman	California Institute of Technology	Dimension-free path-integral molecular dynamics
32	Mullen, Ryan	Lawrence Livermore National Lab	Quantum accurate prediction of plutonium–plutonium dihydride phase equilibrium using a spin-lattice model
33	Ng, Nathan	UC Berkeley	Localization dynamics in a centrally coupled system
34	Qiao, Zhuoran	California Institute of Technology	Accelerating GFN-xTB SCF convergence with machine learning initial guess
35	Rosa, Jorge	California Institute of Technology	Dimension-free path integral simulations of water
36	Schile, Addison	UC Berkeley	Hybrid trajectory methods for treating conical intersection dynamics in condensed phases
37	Tao, Xuecheng	California Institute of Technology	Nuclear quantum effects in scattering of H-atom from graphene