Poster Session I
Friday, January 13

1	Nandini	Ananth	Cal Tech	Reactive flow in quantum systems: A study of proton-coupled electron tranfer reactions
2	Sergio	Bacallardo	Stanford Univ.	Bayesian nonparametric analyses of Markov models of molecular dynamics
3	Andy	Ballard	Univ. of Maryland	Calculating solvation free energies from replica exchange with nonequilibrium switches
4	Ayelet	Benjamini	UC Berkeley	Lipid mediated packing of transmembrane Helices
5	Gregory	Bowman	UC Berkeley	A Bayesian agglomerative clustering engine (BACE) for coarse-graining Markov state models
6	Scott	Carmichael	UC Santa Barbara	A new multiscale algorithm and its application to coarse-grained peptide models for self-assembly
7	Raghunath	Chelakkot	Brandeis Univ.	A particle based computational model for eukaryotic cilia and flagella
8	Bin	Li	UC Berkeley	Semiclassical treatment of Fermionic systems
9	Brian	Jo	UC Berkeley	Optimizing solute-water van der Waals interactions to reproduce solvation free energies
10	Lester	Hedges	Lawrence Berkeley Lab	Homogeneous and heterogeneous nucleation in the Ising model
11	Bruno	Barbosa Rodriguez	Univ. Federal de Minas Gerais	Influence of water force fields on the structure of DNA under denaturation
12	Todd	Gingrich	UC Berkeley	Extended ensemble path sampling for identifying optimal out-of-equilibrium protocols
13	Jason	Goodpaster	Cal Tech	Wavefunction exact embedding theory for transition metal complexes
14	Kevin	Haas	UC Berkeley	Path integral statistical learning theory for protein dynamics
15	Shekhar	Garde	Rensselaer	Water mediated interactions at extended hydrophobic surfaces
16	Suri	Vaikuntanathan	UC Berkeley	Investigating the adsorption of ions to liquid vapor interfaces: insights from lattice gas models
17	Jakub	Kaminski	Cal Tech	Dynamics of electron solvation at molecule/metal interfaces
18	Pablo	Debenedetti	Princeton Univ.	Evaporation rate of water in hydrophobic confinement
19	Yoji	Kubota	Kyushu Univ.	Fine structure in dielectric behaviors of water around a solute molecule
20	Aviel	Chaimovich	UC Santa Barbara	Multiscale studies of hydrophobic association

Poster Session I
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21	Artur R.	Menzeleev	Cal Tech	Direct simulation of nonadiabatic systems with ring polymer molecular dynamics
22	David	Limmer	UC Berkeley	Phase and kinetic behavior of water confined to hydrophillic nanopores
23	Christopher	Ryan	UC Berkeley	Membrane remodeling driven by steric effects of adhered proteins.
24	Aaron	Keys	Lawrence Berkeley Lab & UC Berkeley	Manifestations of Dynamical Facilitation in Supercooled Liquids and Related Materials
25	Erik	Lascaris	Boston Univ.	Nanoscale dynamics of phas flipping in ST2 water near its (hypothesized) liquid-liquid critical point
26	Erik	Steed	Griffith Univ.	Proposal for unfolding single biomolecules in an ion trap
27	Rupert	Tscheliessnig	UC Berkeley	Form and structure predition of proteins by a fractal concept
28	Patrick	Varilly	Univ. of Cambridge	Predicting interaction potentials for DNA-coated colloids
29	Evan	Wang	UC Berkeley	Actin filament curvature and its implications for filopodial structure
30	Michael	Hagen	Brandeis Univ.	Water behavior during the association of HIV capsid proteins
31	Jianzhong	Wu	UC Riverside	A new Fermi-liquid theory for electron correlations
32	Yoshiteru	Yonetani	Japan Atomic Energy Commission	What determines water residence times at the surface of biomolecules?
33	Ken	Tokunaga	Kogakuin Univ.	Conversion process of chemical reaction into directed motion through a solvation motor
34	Laura	Armstrong	UC Berkeley	Modeling the self-assembly of caroxysome shells
35	K. Aurelia	Ball	UC Berkeley	Amyloid-beta heterogeneous conformational ensembles; differences between the 40- and 42- residue peptides and implications for dimer polymorphism.
36	Taylor	Barnes	Cal Tech	Exactly embedded DFT treatment of large systems
37	Nicholes	Boekelheide	Cal Tech	Dynamics and dissipation in enzyme-catalyzed charge transfer

Poster Session II
Saturday, January 14

37	Joohyun	Jeon	UC Santa Barbara	Charge effects on the fibril-forming peptide KTVIIE: a two-dimensional replica exchange simulation study
38	Guohua	Tao	UC Berkeley	Efficient Semiclassical methods for chemical reaction rate calculations
39	Shuangliang	Zhao	UC Riverside	Direct correlation in molecular fluids and application to solvation
41	Nathan	Duff	UC Santa Barbara	Polymorph specific order parameters: An analysis of surface melted layer thickness for glycine nuclei
42	Rene	Corrales	The Univ. of Arizona	Statistical mechanics of lower critical solution temperatures in ionic liquid - water mixtures
43	skip			
44	Katerie	DuBay	Columbia Univ.	Modeling the morphology of conjugated polymers
45	Shervin	Fatehi	Univ. of Pennsylvania	Derivative couplings with built-in electron-translation factors for translational invariance.
46	David	Limmer	UC Berkeley	Nonequilibrium phase transitions in supercooled water
47	Bryan	Goldsmith	UC Santa Barbara	A systematic ab initio strategy for predicting structure-activity relationships in amorphous catalysts and supports
48	Michael	Gruenwald	UC Berkeley	Metastability in structural transformations of CdSe/ZnS core/shell nanocrystals
49	Itay	Hen	UC Santa Cruz	Complexity of the quantum algorithm
50	Tom	Haxton	Lawrence Berkeley Lab	Design rules for the self-assembly of a protein crystal
51	Pengfei	Huo	Cal Tech	Partial linearized density matrix propagation for modeling coherent excitation energy transfer in light harvesting systems
52	Margaret	Johnson	NIH	How nonspecific binding between proteins shapes their interaction networks and expression levels
53	Aaron	Keys	UC Berkeley	Self-assembly of soft matter quasicrystals and their approximants.
54	Patrick	Shaffer	UC Berkeley	Ion solvation at interfaces
55	Frank	Lin	UC Berkeley	Computer simulation of Ising model and model with local favorable structure
56	Samuel	McCandish	Brandeis Univ.	Spontaneous segregation of self-propelled particles with different motilities

Poster Session II
Saturday, January 14

57	Baron	Peters	UC Santa Barbara	Coupling between slow diffusion transport and barrier crossing in nucleation: a new origin for the two step mechanism
58	Carl	Rogers	UC Berkeley	The impact of constraints on a Gaussian field theory.
59	Anna	Schneider	UC Berkeley	Phase diagram of self-assembling photosynthetic membrane proteins.
60	David	Sivak	Lawrence Berkeley Lab	Driven Langevin dynamics: heat, work and pseudo-work
61	Ali	Tabei	Univ. of Chicago	Entrainment of a driven oscillator as a dynamical phase transition
62	Joshua	Kretchmer	Cal Tech	Direct simulation of proton coupled electron transfer dynamics
63	Evan	Hohlfeld	UC Berkeley	Amplification of weak correlations by a molecule-thick depleted boundary layer in a many-body Brownian ratchet
64	Suri	Vaikuntanathan	UC Berkeley	Modeling Maxwell's demon with a microcanonical Szilard engine
65	Connie	Wang	Cal Tech	Molecular simulation of SRP binding in co-translational protein targeting
66	Julian	Weichsel	UC Berkeley	The limit of autocatalytic branching in growing actin networks.
67	Adam	Willard	Univ. of Texas	Ultrafast charge transfer at the organic donor-acceptor interface
68	Jianhua	Xing	Virginia Tech	Coupling between switching regulation and torque generation in bacterial flagellar motor
69	Bin	Zhang	Cal Tech	Dynamics of sec-facilitated protein translocation and integral membrane protein topogenesis
70	Steve	Whitelam	Lawrence Berkeley Lab	Random and ordered phases of off-lattice rhombus tiles
71	Rene	Corrales	The Univ. of Arizona	Molexular dynamics simulations of interfacial structuring in alkane - water mixtures (displayed on poster easel 43)
72	Jeff	Weber	Stanford University	Mechanism in Markov state models of protein folding dynamics
73	Il-Hyung	Lee	UC Berkeley	Temperature dependent FCS shows mammalian cell membrane is not poised near miscibility transition temperature.

Poster Session II
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75	Swapna	Lekkala	Cornell University	Dielectric flucuations over polymer films detected using an atomic force microscopy
76	Jordi	Silvestre-Ryan	Inst. For Research in Biomed.	Critical assessment of ensemble structure calculation of disordered proteins from paramagnetic relaxation enhancement.