THURSDAY AFTERNOON
Chung F. Wong, Presiding

1:30 (629), Exploring photo-induced electron transfer leading to "oxidative redding" in fluorescent proteins. A. Acharya, A. Kolomeisky, A. Krylov
1:45 (630), Molecular dynamics studies of the effects of drug-resistant mutations of EGFR on inhibitor binding affinities and the drug target selectivity profiles. J. Park, J. McDonald, R. Petter, K.N. Houk
2:00 (631), Sequence-level prediction and control of the production of a membrane protein. M. Niesen, S.S. Marshal, W.M. Clemons, T.F. Miller
2:15 (632), Molecular simulation of concentration-dependent interactions of hydrophobic drugs with cellular membrane. M. Kang, S. Loverde
2:30 INTERMISSION
2:45 (633), Quantum-classical path integral simulations of ferrocene-ferrocenium charge transfer in solution. P.L. Walters, N. Makri
3:00 (634), Molecular dynamics simulations of stacked DNA base surrogates. A. Mazareripour, C. Markegard, J. Jocson, A.M. Burke, M.N. Dickson, A.A. Gorodetsky, H. Nguyen
3:15 INTERMISSION
3:30 (635), Sampling rare events in molecular simulations: Heterogeneous ice nucleation – a case study. R. DeFever, W. Judge, B. Glatz, S. Sarupria
3:45 (636), Computational study on the catalytic role of the magnesium ions in the active site of the DNA polymerase B. R.A. Matute, A. Warshel
4:00 (637), Nucleation of NaCl from aqueous solution: critical sizes, ion-attachment kinetics, and rates. N.E. Zimmermann, B. Vorselaars, D. Quijley, B. Peters
4:30 (639), Multiscale modeling of the chromatin fiber. T. Schlick

THURSDAY MORNING
Dimitri E. Makarov, Presiding

8:00 (572), Dynamics of dopamine transporters: Insights from simulations at multiple scales. M.H. Cheng, C. Kaya, A. Sorkin, J.R. Faeder, I. Bahar
8:30 (573), Free energy calculations and reaction coordinates from transition path sampling of enzymatic reactions. S.D. Schwartz
9:00 INTERMISSION
9:15 (574), Solvation thermodynamics of biosolutes in mixed protecting-denaturing osmolytes. P. Garguly, N. van der Vegt, J.E. Shea
9:30 (575), Development of a multi-scale sampling methodology to examine the favored ligand binding pathways of influenza neuraminidase. A.W. Van Wynsberghe
9:45 (576), Damage recognition and base extrusion strategies of DNA repair glycosylase enzyme. B. Kossmann, I.N. Ivanov
10:00 (577), Bending and base step flexibilities of normal, methylated, and damaged DNA. A. Van Der Vaart
10:15 (578), Molecular stripping in the NFκB/nκB/DNA genetic regulatory network. D. Potovan, P.C. Wolynes
10:30 INTERMISSION
10:45 (579), Replica exchange multiscale CFD-MD integrator. A.V. Popov, R. Hernandez
11:00 (580), Generalized maming model captures the RNA ion atmosphere. U. Mohanty
11:15 (581), Wigner phase space distribution via classical adiabatic switching. A. Bose, N. Makri
11:30 (582), Conformationally gated charge transfer in DNA three-way junctions. Y. Zhang, C. Liu, D.N. Beratan

WEDNESDAY AFTERNOON
Daniel M. Zuckerman, Presiding

1:30 (319), Umbrella sampling folding of intrinsically disordered proteins. A. Dinner
2:00 (320), Exploring channel permeation with enhanced sampling. M. Grabe
2:30 (321), Complex role of solvation in micelle and reverse micelle environments. J.E. Straub, R. Urano
3:00 INTERMISSION
3:45 (323), Enhanced sampling and its applications in high-accuracy refinement of protein low-resolution models. T. Zang, J. Ma
4:15 INTERMISSION
4:30 (324), Dependence of internal friction on local and global barrier height. W. Zheng, D. De Sancho, R.B. Best
5:00 (325), Molecular origins of friction in unfolded proteins. D.E. Makarov, S. Avdoshenko, A. Das

THU SDAY MORNING
Dmitri E. Makarov, Presiding

8:00 (572), Dynamics of dopamine transporters: Insights from simulations at multiple scales. M.H. Cheng, C. Kaya, A. Sorkin, J.R. Faeder, I. Bahar
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SUNDAY MORNING
Lillian T. Chong, Presiding

8:00 (1). Recent techniques for acceleration and interpretation of molecular dynamics simulations
E. Vanden-Eijnden
8:30 (2). Markov models at multiple thermodynamic states with applications to protein-ligand complexes. F. Nave
9:00 (3). Markovian milestoning MD simulations for computing on- and off-rates. T. Yu, A. Bucci, E. Vanden-Eijnden, C.F. Abrams
9:30 INTERMISSION
9:45 (4). Advancements in milestone: Computational speedup by re-weighting artificially accelerated trajectories and venturing into the non-equilibrium with coarse-grained random walks in milestone space.
G. Graziani, I. Andricioaei
E. Suarez, D.M. Zuckerman
10:45 INTERMISSION
11:00 (6). Multiscale estimation of binding kinetics using molecular dynamics, Brownian dynamics, and milestone.
R.E. Amaro, L. Votapka
11:30 (7). Exact milestone.
J.M. Bello-Rivas, R. Elber

SUNDAY AFTERNOON
Ron Elber, Presiding

1:30 (48). Increasing the power of accelerated molecular dynamics methods. A.F. Voter
2:00 (49). Exploring rare events in proteins with adaptive molecular dynamics.
C. Clementi
P.J. Rossky
3:00 INTERMISSION
3:15 (51). WESTPA: An interoperable, highly scalable software package for weighted ensemble simulation and analysis.
L.T. Chong
3:45 (52). Insight into folding, binding, and peptideconformer design from molecular simulations and kinetic network models.
V.A. Voelz, A. Razavi, S. Mukherjee, G.A. Pantelopoulo, G. Zhou
4:15 INTERMISSION
4:30 (53). Modeling density fluctuations and thermodynamics of membranes with milestone.
A.E. Cardenas, R. Elber
5:00 (54). Large scale studies of molecular binding processes on computational grids and heterogeneous hardware resources.

MONDAY MORNING
Rob D. Coalson, Presiding

8:00 (96). Long-time and large-scale conformational kinetics in biomolecular systems.
I. Andricioaei
8:30 (97). Replica exchange transition interface sampling: The latest method developments and applications using ab initio molecular dynamics. T. van Erp
9:00 (98). Describe protein dynamics using diffusion maps with an improved Gaussian kernel.
S. Hou
9:30 INTERMISSION
9:45 (99). Large-scale conformational transitions in the transport cycle of the ATP-driven calcium pump.
B. Roux, A. Das
10:15 (100). Temperature-accelerated and multi-scale simulation algorithms for exploration and generation of free energy landscapes of molecular crystals and oligopeptides.
M.E. Tuckerman
10:45 INTERMISSION
11:00 (101). Quantitative comparison of macromolecular pathways.
O. Beckstein, S. Seyler, A. Kumar, M.F. Thorpe
11:30 (102). Time-dependent effects of DNA replication on mRNA noise.
J.R. Peterson, J. Cole, J. Fei, T. Ha, Z. Luthey-Schulten

MONDAY AFTERNOON
Cameron F. Abrams, Presiding

G.A. Voth
2:00 (147). How structure-directing agents control nanocrystal shape: Simulation of the PVP-mediated growth of Ag nanocubes from first principles.
K.A. Fichthorn, X. Qi, T. Balanaka
2:30 (148). Protein allostery and conformation dynamics.
H. Zhou
3:00 INTERMISSION
R.D. Coalson
M. Feig
4:15 INTERMISSION
4:30 (151). Over a decade of folding@home: How citizen science has led to key new advances in biophysics and fighting disease.
V.S. Pande
5:00 (152). Statistical mechanics of protein-protein association.
D. Kozakov, S.E. Mottarella, S. Vajda

TUESDAY MORNING
Michael Feig, Presiding

8:00 (201). Ensemble refinement methods using molecular dynamics simulations and their relation to free energy calculations and long-time sampling.
G. Hummer, J. Koefinger
8:30 (202). New biological problems enabled by multi-dimensional replica exchange molecular dynamics simulations.
D.M. York
9:00 (203). Variational approach to enhanced sampling and free energy calculations.
M. Parrinello
9:30 INTERMISSION
9:45 (204). Calculation of protein-ligand binding affinities via free energy perturbation methods.
A.F. Voter
10:15 (205). Constant pH simulations in biomolecular systems.
A.E. Roitberg
10:45 INTERMISSION
11:00 (206). Orthogonal sampling of slow responses to enable efficient biomolecular simulations.
W. Yang
11:30 (207). Integrated computational-experimental-Bayesian approach to quantify conformation ensembles of unstructured peptides.
Y. Zhang

WEDNESDAY MORNING
Adrian E. Roitberg, Presiding

8:00 (266). Exploring energy and fitness landscapes of proteins for binding and allostery.
R.M. Levy
8:30 (267). Computational thermodynamics of noncovalent binding.
M.K. Gilson, A. Fenley, K. Gao, N.M. Henriksen, T.P. Kurtzman, H. Muddana, C.N. Nguyen, J. Yin
9:00 (268). Multi-resolution modeling of protein unfolding and function in a pH-dependent chaperone.
C.L. Brooks
9:30 INTERMISSION
J.A. McCammon, Y. Miao
J. Vilseck, J. Tirado-Rives, W.L. Jorgensen
10:45 INTERMISSION
11:00 (271). Relative binding energies by the direct method.
C.B. Post
H. Jang, R. Nussinov