Treatment of Electrostatics and Polarization in the Simulation of Materials, Biomolecules and Interfaces

Organizers: Wanlu Li, Jesse McDaniel and Qiang Cui
August 24-26, 2026

Monday AM

McCormick Place Convention Center W183a
W. Li, *Organizer, Presiding*

8:00 AM. Converging protein–ligand interaction energies with the many-body expansion. **J.M. Herbert**, P. Bowling, D.R. Broderick

8:30 AM. Explicit treatment of electronic polarizability in molecular simulations using the classical Drude oscillator force field. **A.D. Mackerell**

9:00 AM. Effect of dispersion corrections to density functionals on the predicted free energy profile of chorismate mutase catalysis. S. Ranasinghe, R. Van, A. dos Santos, Y. Mao, **Y. Shao**

9:20 AM. Break.

9:45 AM. Modeling electrostatic and polarization effects with the polarizable Gaussian multipole force field. Z. Huang, Y. Duan, T. Lee, X. Wu, **R. Luo**

10:15 AM. Protein electron transport in photosynthesis, electrochemistry, and extracellular respiration: The role of active-site polarizability and protein electric field. **D.V. Matyushov**

10:45 AM. Break.

11:10 AM. Electrostatics and polarization in bulk materials and complex interfaces: predictive molecular simulation with IFF and IFF-R. **H. Heinz**, I. Armstrong, C. Zhu

11:40 AM. Long-range electrostatics and configuration ensembles are key to predicting electrolyte redox potential trends: Insights from MD and QM/MM simulations. K. Alam, S. Patel, A. Bano, L. Wu, N. Shpigel, **D.T. Major**

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Monday PM

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Y. Mao, *Presiding*

2:00 PM. Correcting implicit solvation at metal/water interfaces: The role of competitive water adsorption. **J.R. Schmidt**

2:30 PM. Advances in physical force fields and machine learned interaction potentials for molecular simulation. **T.L. Head-Gordon**

3:00 PM. Ion-pair speciation in aqueous alkali fluorides from nuclear magnetic resonance of ^{19}F through multiscale modeling. **D. Riccardi**, M. Musial, C. Suiter, J. Widegren

3:20 PM. Break.

3:45 PM. Effective treatment of polarization in classical simulations of gas adsorption at open metal sites in metal–organic frameworks. **H. Chen**

4:15 PM. Ionics in amorphous chlorides. **D. Jiang**

4:45 PM. Break.

5:10 PM. Importance of polarizability in simulations of ionic liquids. **A. Yethiraj**

5:40 PM. Accelerating QM/MM simulations of enzyme catalysis: Multiscale treatment of electrostatics using MTS and machine learning. **K. Nam**

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Tuesday AM

McCormick Place Convention Center W183a
H. Chen, *Presiding*

8:00 AM. Machine-learning-based treatments of electrostatics for condensed phase simulations. **M. Meuwly**

8:30 AM. Evaluating water's contribution to interfacial dielectric effects with classical molecular dynamics simulation. **A. Willard**

9:00 AM. Hydrogen-bond networks and cavitation energetics governing electrostatic environments at electrochemical interfaces. **W. Li**

9:20 AM. Break.

9:45 AM. Unified electric-field theory for biomolecules. **V. Vaissier Welborn**

10:15 AM. Computing molecular properties with a polarizable embedding: The case of the optical rotation of camphor in ethanol. **F. Lipparini**, M. Bondanza, B. Mennucci

10:45 AM. Break.

11:10 AM. Development and application of hybrid machine learning force field for molecular systems. **K. Yu**

11:40 AM. Embedded many-body perturbation theory and the generalized Poisson equation for high-fidelity interfacial electrostatics and polarization. **S. Kim**

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Tuesday PM

McCormick Place Convention Center W183a
R. Sun, *Presiding*

2:00 PM. Machine learning interatomic potential can infer electrical response. **B. Cheng**

2:30 PM. Advancing QM/MM simulations with the polarizable density-based Gaussian electrostatic model (QM/GEM). **J.P. Madriaga**, G.A. Cisneros

3:00 PM. Polarizable molecular dynamics simulations of buried protein environments: Free energy method, enhanced sampling and functional implications. **J. Deng**

3:20 PM. Break.

3:45 PM. Elucidating the role of electrostatic interactions in enzyme catalysis and vibrational spectroscopy. **Y. Mao**

4:15 PM. Electrostatics, polarization, and ion specificity across phases: A data-driven many-body perspective. **F. Paesani**

4:45 PM. Break.

5:10 PM. One decade of the 12-6-4 metal ion model: Triumphs, tensions, and limits. **P. Li**

5:40 PM. Modeling electronic polarization and correlations via surface charges of dielectric medium. **A. Foerster**, O. Obolensky, T. Doerr

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Wednesday AM

McCormick Place Convention Center W187c
Q. Cui, W. Li, J. G. McDaniel, *Organizers* | C. Son, *Presiding*

8:00 AM. Nuclear delocalization and polarization in materials, biomolecules, and interfaces. **S. Hammes-Schiffer**

8:30 AM. Present and future of the molecular modeling of porous materials, lessons for biosimulation. **B. Space**, A. Hogan

9:00 AM. Impact of electronic polarization in ion transport and post-translational modification in proteins. Z. Wan, **Q. Cui**

9:20 AM. Break.

9:45 AM. Polarizable 3DRISM implicit solvent model for chemical and biological molecules. S. Cao, P. Swanson, B. Eder, P. Si, P. Ren, **X. Huang**

10:15 AM. Polarizable embedding method for excited state multi-reference quantum chemistry. **C. Song**

10:45 AM. Break.

11:10 AM. Free energies of redox half-reactions with polarizable QM/MM methods. **K.B. Bravaya**

11:40 AM. Simulation study of the hypergolicity of cyanoborohydride ionic liquids in the liquid phase. **R. Sun**

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Wednesday PM

McCormick Place Convention Center W187c
J. Deng, *Presiding*

2:00 PM. Polaritonic chemistry through the lens of electrostatic catalysis. **N. Hoffmann**

2:30 PM. Classical and quantum charge transport in Li^+/proton conducting electrolytes for advanced electronic materials. **C. Son**

3:00 PM. Modulating primary charge separation in Photosystem II variants: A multiscale investigation of protein-induced electrostatic effects. **S. Bhattacharjee**, I. Gordiy, A. Sirohiwal, D. Pantazis

3:20 PM. Break.

3:45 PM. Strongly heterogeneous and dynamic intra-protein electric fields as drivers of enzymatic catalysis. **A. Alexandrova**, P. Ajmera, A. Goswami

4:15 PM. Role of polarization in modeling energy and charge transfer in photosynthetic complexes. **L.V. Slipchenko**

4:45 PM. Break.

5:10 PM. Demystifying solvation radii in continuum models. J. Filser, B. Gadjagboui, **O. Andreussi**