

# Reactions, Couplings, and Dynamics: Symposium Celebrating the Life and Work of Martin Karplus

Organizers: Charles Brooks, Q. Cui, Alexander Mackerell, J. E. Straub  
March 22-24, 2026

## Sunday AM

Georgia World Congress Center | B309

### Free Energy Calculations and Applications

C. L. Brooks , Q. Cui, A. D. Mackerell, J. E. Straub, Organizers | A. Szabo, Presiding

**8:00 AM.** Opening Remarks.

**8:25 AM.** Ultra-high throughput free energy calculations with multi-site lambda dynamics.  
**C.L. Brooks**

**8:50 AM.** Graph neural networks for molecular dynamics simulations. **A. Dinner**

**9:15 AM.** Structure-based prediction of dynamic protein interaction networks. **B. Honig**

**9:40 AM.** Intermission.

**10:20 AM.** Exploring fitness and free energy landscapes of kinase family proteins.  
**R.M. Levy**

**10:45 AM.** Studies of the potassium channel: Ion conduction, activation and inactivation mechanisms. **B. Roux**

**11:10 AM.** High-throughput AI and free energy methods for drug discovery. **D.M. York**

**11:35 AM.** Evolution of solution-phase free-energy calculations. **W.L. Jorgensen,**  
J. Tirado-Rives

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### Enzyme Catalysis and Mechanistic Insights

Q. Cui, A. D. Mackerell, J. E. Straub, Organizers | C. L. Brooks, Organizer, Presiding

**2:00 PM.** Pinning down the structural dynamics of k-ras by NMR and MD. X. Xiang, M. Basnet, P. Ma, E. Fagerberg, C. Yuan, L. Bruschiweiler-Li, **R. Bruschiweiler**

**2:25 PM.** Plexin and Eph receptors: The view from computational modeling on protein-protein and protein-membrane interactions. **M. Buck**

**2:50 PM.** Ability of enzymes to preserve reactive conformations during enzyme-catalyzed reactions can be an important factor for efficient catalysis. **H. Guo**

**3:15 PM.** Allosteric connections across the Ras/Raf dimer enhanced in B Raf versus C Raf. **C. Mattos**, K. Pathirage, T. Cookis

**3:40 PM.** Intermission.

**4:20 PM.** Unravelling the coupling between chemistry and motion in enzyme function. **K. Nam**

**4:45 PM.** Phosphorylation influence on protein kinase function: elucidating atomistic mechanisms with simulation and NMR. **C.B. Post**

**5:10 PM.** Substrate turnover simulations identify chemical characteristics that promote enzyme catalysis and guide redesign for increased specific activity. **B. Tidor**

**5:35 PM.** Adaptive capacity of a DNA polymerase clamp loader complex. **J. Kuriyan**

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### **Force Field Development and Application**

C. L. Brooks, Q. Cui, A. D. Mackerell, J. E. Straub, Organizers | C. Mattos, Presiding

**8:00 AM.** CHARMM additive and Drude polarizable force field parametrizations for cytochrome p450 Fe(III) heme. **O. Guvench**

**8:25 AM.** Role of water in the structure, stability, and dynamics of amyloid protein fibrils. **J.E. Straub**, C.B. Abraham, F. Mon, S.P. Nayak

**8:50 AM.** Electronic polarization in nucleic acids: From small RNAs to ribosomes. **J.A. Lemkul**

**9:15 AM.** Classical Drude oscillator polarizable force field: Ongoing developments and role of electronic polarizability in conformational heterogeneity. **A.D. Mackerell**

**9:40 AM.** Intermission.

**10:20 AM.** Machine Learning-Based approaches to chemical reactivity and discovery. **M. Meuwly**

**10:45 AM.** Polarizable Drude force field for gas adsorption. **Y. Nan**

**11:10 AM.** Curvature-dependent adaptive solvation shell model for biomolecules with arbitrary shape. **V. Ovchinnikov**

**11:35 AM.** Molecular simulation, AI and the circular bioeconomy. **J. Smith**

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### **QM/MM and Hybrid Methods**

C. L. Brooks, Q. Cui, A. D. Mackerell, J. E. Straub, Organizers | X. Liu, Presiding

**2:00 PM.** CHARMM, an accomplished product of the research group of Martin Karplus, its past, present, and future. **B. Brooks**

**2:25 PM.** Multiscale simulations for protein design and engineering. **A. Mulholland**

**2:50 PM.** From free energy component analysis to multistate density functional theory. **J. Gao**

**3:15 PM.** How do TIM barrels do it all? The evolvability of catalytic loops. **S.C. Kamerlin**

**3:40 PM.** Intermission.

**4:20 PM.** Analysis of enzyme catalysis and ion transport with classical and QM/MM methods. **Q. Cui**

**4:45 PM.** Power in numbers. C. Huang, R. Workman, **B.M. Pettitt**

**5:10 PM.** Development and applications of gaussian process regression enhanced qm/mm simulations. **J. Pu**

**5:35 PM.** My 20+ years with charmm: Qm/mm, drug discovery, and beyond. **H.L. Woodcock**

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## Tuesday AM

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### **Structural and Integrative Biochemistry and Cell Biology**

C. L. Brooks, Q. Cui, A. D. Mackerell, J. E. Straub, Organizers | Y. Nan, Presiding

**8:00 AM.** All-atom molecular simulations of disordered proteins and biomolecular condensates. **R.B. Best**

**8:25 AM.** Towards accurate simulation of protein/RNA phase separation. **J. Chen**

**8:50 AM.** Dynamics of biomolecules in concentrated environments. **M. Feig**

**9:15 AM.** Molecular modeling and simulation of the Mycobacteria cell envelope. **W. Im**

**9:40 AM.** Intermission.

**10:20 AM.** Induced ordered domains, PIP<sub>2</sub>/PLD2 rafts, and general anesthesia. **R. Pastor**

**10:45 AM.** Integrative mapping reveals molecular features underlying the mechanism of nucleocytoplasmic transport. **A. Sali**

**11:10 AM.** Multiscale simulations of peptide liquid-liquid phase separation. **J.E. Shea**

**11:35 AM.**  $\gamma$ -subunit rotation mechanism of  $f_1$ -ATPase in different substrate-bound states. **Y. Sugita**

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### **Biomolecular Structure, Sampling, Kinetics and Dynamics**

C. L. Brooks, Q. Cui, A. D. Mackerell, Organizers | J. E. Straub, Organizer, Presiding

**2:00 PM.** Slow kinetics of biomolecules from fast sampling of rare conformational transitions. **I. Andricioaei**

**2:25 PM.** Mechanical force as a cofactor of t cell ligand recognition and activation: Diverse behaviors of t-cell receptors revealed by molecular dynamics simulation. **W. Hwang**

**2:50 PM.** Withdrawn

**3:15 PM.** Accessing protein conformational landscapes and dynamics in the era of AI. **J. Huang**

**3:40 PM.** Intermission.

**4:20 .** Register-shifted structures in uracil: Adenine and uracil: Guanine base paired DNA. **A. van der Vaart**

**4:45 PM.** Road to AlphaFold and beyond: A perspective through the legacy of Martin Karplus. **Y. Zhou**

**5:10 PM.** Towards efficient peptide design using multisite  $\lambda$  dynamics. **X. Liu**

**5:35 PM.** Accurate enhanced sampling of long-timescale protein conformational transitions. **W. Yang**