



Chemical Theory Center

Monthly Newsletter

September 2025

AWARDS and Recognition:

- Prof. Ilja Siepmann was named the inaugural Thomas Allen Gregory Chair in Physical Chemistry
- Prof. Melissa Ramirez and her team were awarded the ACS Ignition Grant
- Prof. Chris Bartel was featured in *Materials Horizons* Emerging Investigator Series
- Lauren Way was recognized for achieving a 4.0 GPA
- Mikayla Fahrenbruch was awarded the Robert L. Ferm Outstanding Graduate TA Award
- PH Minh was awarded the Wayland E. Noland Excellence Fellowship



Seminars and Community:



- Prof. Jiali Gao gave our first CTC seminar of the academic year with a talk titled "Multistate density functional theory" on September 11th
- Prof. John Herbert gave a Departmental Seminar hosted by Prof. Boyn
- Prof. Jeetain Mittal gave the Bryce L. Crawford, Jr. Memorial Lecture hosted by Prof. Sarupria

NEW PAPERS

- N. Jiang, S. Velliyyarat, C.-Y. Lien, H.L. Nguyen, J. Hofmann, J.-H. Chen, A. Ramanathan, A.S. Filatov, H.S. La Pierre, S. Patel, K.W. Chapman, J.-N. Boyn, and J.S. Anderson, Pre-synthetic redox control of structure and properties in copper ttftt coordination polymers. *Chemical Science*, 2025.
- D. Gibney and J.-N. Boyn, Tunable aromaticity and biradical character in tetrathiafulvalene and tetraselenafulvalene derivatives. *Journal of Physical Chemistry A*, 2025.
- Y. Lu and J. Gao, Multistate Density Functional Theory: Theory, Methods, and Applications, *Wiley Interdisciplinary Reviews: Computational Molecular Science* 15 (5), 2025.
- T. Martinon, A. Sinha, A.W. Schlimgen, A. Persell, T. Garner, K. Peterson, J.-I. Siepmann, and V. Pierre, "Selective Bicarbonate Receptors for Direct Ocean Capture of CO₂", *Journal of the American Chemical Society Au*, 2025.



WHAT WE'RE LOOKING FORWARD TO IN OCTOBER

- Upcoming seminars:
 - ▷ Oct. 7th 9:45AM: Prof. Rebecca Lindsey from the University of Michigan, Department of Chemistry Seminar in Smith 331 (hosted by Prof. Siepmann)
 - ▷ Oct. 16th 12:30PM: Prerna and Pragya Parihar from the Siepmann group, CTC Seminar in Smith 117/119
 - ▷ Oct. 21st 11:15AM: Prof. Anastassia Alexandrova from the University of California Los Angeles, Quantum Information Science Seminar in Tate 201-20 (hosted by Prof. Head-Marsden)
- Preprints:
 - ▷ F. Formalik, B. Jia, B. Mazur, P. Prerna, Z. Li, H.-F. Liu, P. Parihar, R.Q. Snurr, and J.-I. Siepmann Understanding Differences in Water Adsorption Isotherms: Structural Variations, Force Fields, and Monte Carlo Simulation Approaches. *ChemRxiv*, 2025
 - ▷ J.W.P. Zajac, I. Tohidian, P. Muralikrishnan, S.L. Perry, C.L. Heldt, and S. Sarupria. Cracking the Capsid Code: A Computationally-Feasible Approach for Investigating Virus-Excipient Interactions in Biologics Design. *BioRxiv* :2025.09.04.674344, 2025
 - ▷ J.R. Canavan, R. Daga, J. Hopkins, U.R. Gaillard, A. McCormick, M. Neurock, O.A. Abdelrahman, and P.J. Dauenhauer, Isopotential Electron Titration of Ammonia Charge Transfer on Metal Catalysts. *ChemRxiv*, 2025
 - ▷ P. Muralikrishnan, J.W.P. Zajac, C.L. Heldt, S.L. Perry, and S. Sarupria. Thermodynamic Basis of Sugar-Dependent Polymer Stabilization: Informing Biologic Formulation Design. *arXiv:2509.04301*, 2025