June 29 – July 1, 2026
ROSENTHAL PAVILION
NEW YORK UNIVERSITY

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Monday, June 29

11:00 am	Arrival and Check-in, Hemmerdinger Hall, Silver Ctr. for Arts & Science, 31 Washington Pl.
11:30 am	**Welcome Lunch and Poster Session**
1:30 pm	Break
2:00 pm	Arrival and Check-in, Rosenthal Pavilion, Kimmel Center, 60 Washington Sq. South
Session I	**Chair: Glen Hocky, New York University**
2:10 pm	Welcoming Remarks: Stefano Martiniani, ChemAI co-Organizer, Assoc. Prof. of Physics, Chemistry and Math James Canary, Dean for Science Juan de Pablo, Exec VP for Global Science and Tech, Exec Dean of the Tandon School of Engineering
2:40 pm	Andrew White, Edison Scientific *Training a scientific reasoning model for chemistry*
3:15 pm	Shuwen Yue, Cornell University *Physics Informed Active Learning for Machine Learning Interatomic Potentials*
3:50 pm	Break
4:10 pm	Carles Domingo-Enrich, Microsoft Research *Rare Event Analysis via Stochastic Optimal Control*
4:30 pm	Jan-Willem van de Meent, University of Amsterdam *Title TBA*
5:05 pm	Ge Sun, New York University *HiPoly: A hierarchical polymer-native AI framework for property prediction and generative design*
5:30 pm	Break
6:00 pm	**C&EN Welcome Reception and AI Panel Discussion** Join *Chemical & Engineering News* for networking and an off-the-record discussion about translating chemistry AI research to the commercial realm. Register here by June 20. White Oak Tavern, 21 Waverly Pl.
8:30 pm	Adjourn

Tuesday, June 30

9:00 am	Continental Breakfast, Informal networking
Session IIa	**Chair: Yingkai Zhang, New York University**
9:20 am	Welcoming Remarks: Gregory Weiss, NYU Chemistry Department Chair
9:30 am	Connor Coley, MIT *Chemistry-tailored AI for small molecule design, synthesis, and analysis*
10:05 am	Peter Bolhuis, University of Amsterdam *Transition path sampling-based learning of reaction coordinates and MLIPs for molecular rare events*
10:40 am	Philipp Höllmer, New York University *Open Materials Generation with Inference-Time Reinforcement Learning*
11:00 am	Break
Session IIb	**Chair: Yuanqing Wang, New York University, University of Toronto**
11:20 am	Ellen Zhong, Princeton University *Atomic Diffusion Models for Small Molecule Structure Elucidation from NMR Spectra*
11:55 am	Victor Batista, Yale University *Title TBA*
12:30 pm	Mark Tuckerman, New York University *Title TBA*
1:05 pm	Recess
Session IIIa	**Chair: Muhammad Hasyim, New York University**
2:20 pm	Mohammed AlQuraishi, Columbia University *Latents-Based Conformational Control in OpenFold3*
2:55 pm	Marta Skreta, Mila / Université de Montréal *General Multimodal Protein Design Enables DNA-Encoding of Chemistry*
3:15 pm	Pilar Cossio, Flatiron Institute *Inferring probability distributions of RNAs using cryo-EM simulation-based inference*
3:50 pm	Michael Chen, New York University, University of Kentucky *Sampling Free Energy Landscapes of Ionic Colloidal Crystal Systems using Machine-Learned Proxy Collective Variables and Potentials*
4:10 pm	Break
Session IIIb	**Chair: Rui Wang, New York University, Rochester Institute of Technology**
4:30 pm	Justin Smith, NVIDIA *Building accelerated AI infrastructure for chemistry and materials simulation*
5:05 pm	Adam Lahouari, New York University *From Foundation Models to Free Energies: An Automated Pipeline for Machine Learning Interatomic Potentials*
5:25 pm	Chatipat Lorpaiboon, Flatiron Institute *Towards a foundational model for the committor*
5:45 pm	Boris Kozinsky, Harvard University *Machine Learning Foundation Models of Microscopic Interactions in Materials*
6:20 pm	Adjourn

Wednesday, July 1

9:00 am	Continental Breakfast
Session IVa	**Chair: Stefano Martiniani, New York University**
9:20 am	Welcoming Remarks
9:30 am	Kirill Neklyudov, Mila *Steering Generative Models: From Mathematics to Biomolecular Design*
10:05 am	Bettina Keller, Freie Universität Berlin *A Machine-Learned Symbolic Committor for a Chemical Reaction: Retinal Isomerization*
10:40 am	Liwei Chang, Schrödinger, Inc. *Leveraging the principles learned by AlphaFold for protein folding pathway predictions and beyond*
11:00 am	Break
Session IVb	**Chair: Mark Tuckerman, New York University**
11:20 am	Stefan Chmiela, Technische Universität Berlin *Accelerating Molecular Dynamics with Implicit Machine Learning*
11:55 pm	Joseph A. Morrone, IBM T.J. Watson Research Center *Multi-View Biomedical Foundation Models for molecular property prediction*
12:15 pm	Rocío Mercado Oropeza, Chalmers University of Technology *The data bottleneck in AI-driven molecular design: from agentic extraction to structured benchmarks*
12:50 pm	Minhuan Li, Flatiron Institute *Beyond Pixel Overlap: Optimal Transport for Reconstructing Flexible Biomolecules from Noisy Data*
1:10 pm	Recess
Session V	**Chair: Michael Chen, New York University, University of Kentucky**
2:40 pm	John Chodera, Achira *Title TBA*
3:15 pm	Todd Martinez, Stanford University *Learning For and From Excited State Molecular Dynamics*
3:50 pm	Benjamin Miller, Meta *Modern approaches in symmetry for crystals and enhanced sampling for molecules*
4:30 pm	Adjourn