Division of Physical Chemistry
American Chemical Society

Bridging Theory and Experiment with AI

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Organizers

Walter E. Washington Convention Center
see schedule for room locations

19-21 August 2025

PHYS Programs also available online:

TUESDAY AFTERNOON

Room 152A | O. Isayev, *Presiding*

2:00 PM. Opening.

2:10 PM. Revolutionizing molecular MLIPs with a novel large-scale dataset and comprehensive model evaluations. D.S. Levine, M. Shuaibi, M.G. Taylor, E.W. Spotte-Smith, M.R. Hasyim, A.S. Rosen, S. Raja, A. Krishnapriyan, P. Eastman, J.A. Rackers, N. Frey, S. Vargas, I. Batatia, G. Csanyi, Z. Ulissi, C. Zitnick, **S. Blau**, B.M. Wood

2:35 PM. Leveraging AI hardware and graph theory for real-world scale quantum simulations. **M. Kulichenko**, C. Negre, A. Niklasson

3:00 PM. Crash testing machine learning force fields for molecules, materials, and interfaces. **I. Poltavsky**

3:25 PM. Exploring potential-energy surfaces with on-the-fly Bayesian learning: From ground state structures to excited state dynamics. **J. Bao**

3:45 PM. Intermission.

4:30 PM. Active Learning Framework (ALF): Modular, extensible and crafted to explore vast chemical space. **N. Fedik**, V. Grizzi, B.T. Nebgen, S. Tretiak

4:55 PM. Combing active learning machine learning with transfer learning: Building better interatomic potentials for nuclear fuels. **E. Stippell**, L. Alzate-Vargas, R. Messerly

5:15 PM. Unified deep learning framework for many-body quantum chemistry via Green's functions. **T. Zhu**, C. Venturella, J. Li, C. Hillenbrand, X. Leyva Peralta, J. Liu

5:35 PM. Machine-learning accelerated construction of the self-energy operator. **A. Chakraborty**

WEDNESDAY MORNING

Room 153 | L. Madureira, *Presiding*

8:00 AM. Exploring the property space of materials with self-driving labs. **K. Tsuda**

8:25 AM. ARES™ autonomous experimentation for accelerated research. **B. Maruyama**

8:50 AM. Operational system approach for autonomous chemical research. **G. Gomes**, R. MacKnight

9:15 AM. Synergy of machine learning and DFT calculations in predicting physical and chemical properties of Lewis acid-base adducts. **H. Phan**, H. Huynh, E.A. Jarvis, M. Holcomb, S. Forli

9:35 AM. Intermission.

9:50 AM. Active learning for the halide perovskite discovery: Co-navigating literature and experimental synthesis. **M. Ahmadi**

10:15 AM. Vision-based automation in chemistry: A Python framework for self-driving labs. **R. El-Khawaldeh**, J. Hein

10:40 AM. Feature engineering in predicting catalysis reaction efficiency and selectivity. **J. Ma**

11:00 AM. Machine learning assisted synthesis condition exploration for mixed metal oxides. **Y. Liu**, M. Ansari, R. Black, J. Hattrick-Simpers

11:20 AM. Computational quantum chemistry search for electronic features governing performance of heteroleptic Ir(III) complexes in photocatalytic hydrogen evolution reaction. Y. Wang, E. Lopato, C. Collins, S. DiLuzio, L. Dong, C. Shao, D. Yaron, S. Bernhard, **T. Kowalewski**

WEDNESDAY AFTERNOON

Room 153 | D. Eremin, *Presiding*

2:00 PM. Property-networking deep learning model for predicting experimental material properties. **S. Kim**

2:25 PM. Polybot: An AI-guided robotic laboratory advancing polymer innovation. **J. Xu**

2:50 PM. High-throughput robotic platforms for investigating electrochemical and chemical doping of conjugated polymers. **C.G. Bischak**

3:10 PM. Quantum chemical analysis of the nature of copper-halogen bond in transition metal complexes used in atom transfer radical polymerization (ATRP). **L. Madureira**, T. Kowalewski, K. Matyjaszewski

3:30 PM. Automation and AI enable precision and reproducibility in organic semiconductor function. **M. Seifrid**

3:55. PM Intermission.

4:10 PM. Continuous flow chemistry and bayesian optimization to functionalize poly(4-vinylpyridine) and facilitate polymer wrapped carbon nanotubes. **L. Baldwin**

4:35 PM. Polymer discovery using a combination of automation and machine learning. **F.A. Leibfarth**, O. Isayev

5:00 PM. Detecting thermodynamic phase transition via explainable machine learning of photoemission spectroscopy.
X. Chen, Y. Sun, E. Hruska, V. Dixit, J. Yang, Y. He, Y. Wang, **F. Liu**

5:20 PM. Predicting the chemical (dis)order in multicomponent materials with high-throughput simulations and representation learning. **J. Peng**

5:40 PM. Inversely assigning the electronic absorption spectral features of highly conjugated organic macromolecules with machine learning. **H.A. Moran** , J. Nicholson, S. Kempel, Q. Michaudel, D.P. Tabor

THURSDAY MORNING

Room 153| F. Liu, *Presiding*

8:00 AM. Hypothesis testing approach to cryo-EM. **J. Rhodes**, E. Thiede

8:20 AM. Deep learning of protein energy landscape and conformational dynamics from experimental structures in PDB using DeepConformer. Y. Tang, M. Yu, X. Li, G. Bai, Y. Xu, **B. Ma**

8:40 AM. Teaching machines MicroED: Fully autonomous structure determination. **D. Eremin**, K. Jha, D.A. Delgadillo, J. Rodriguez, H. Nelson

9:00 AM. Probing and engineering of regulatory mechanisms in signalling proteins by targeted allosteric modulators: A dynamic view through the lens of network biology and AI. **G.M. Verkhivker**

9:20 AM. AlphaFold2-RAVE: Protein ensemble generation with physics-based sampling. **D. Teng**, V. Meraz, A. Aranganathan, X. Gu, P. Tiwary

9:40 AM. Intermission.

10:00 AM. Learning to correct biomolecular simulations from cryo-EM images. J. Xiang, -. Kawamura, **E. Thiede**

10:20 AM. Learning conformational ensembles from cryo-EM data via stochastic inverse modeling. **D. Sanchez Espinosa**, E. Thiede, Y. Yang

10:40 AM. Scalable multi-temperature free energy sampling of the alchemical space. **P. Tuo**, Z. Zeng, J. Chen, B. Cheng

11:00 AM. AI-enabled ultra-low-power smart gas sensing for wearable devices. **S. De**, F. Diallo, J. Collins, S. Joshi, H. Upadhyay, R. Fernandez

11:20 AM. Confident AC assignment using statistics of VCD spectral similarity index. **J. Shen**