Division of Physical Chemistry
American Chemical Society

Automation & Artificial Intelligence for 2D Materials Discovery

Jeffrey J. Schwartz & Son T. Le
Organizers

Walter E. Washington Convention Center
Room 152B

20-21 August 2025

Wednesday Afternoon | S. T. Le, Presiding

2:00 PM. Accelerating the discovery of 2D quantum materials using AI. **T. Rhone**

2:30 PM. DiffractGPT: Atomic structure determination from X-ray diffraction patterns using a generative pretrained transformer. **K. Choudhary**

3:00 PM. Quality control and expertise integration in autonomous experimentation. **Y. Liu**

3:30 PM. Advancing design and discovery of 2D materials via autonomous high throughput synthesis and characterization. **M. Ahmadi**

4:00 PM. Intermission.

4:15 PM. Machine learning-assisted electron microscopy for advanced characterization of two-dimensional materials. **Y. Han**, C. Shi, X. Yin, Y. Jiang

4:45 PM. Self-driving lab for discovering tunable and soluble organic lasers. **H. Park**, M. Mazaheri, C. Choi, H. Hao, D. Avagliano, A. Aspuru-Guzik

5:00 PM. From bulk effective mass to 2D carrier mobility accurate prediction via adversarial transfer learning. **C. Xinyu**, C. Qian, L. Shuaihua, Z. Qionghua, J. Wang

5:15 PM. Large language model-guided optimization of two-dimensional material synthesis. **X. Mao**

Thursday Morning | J. J. Schwartz, Presiding

8:00 AM. Automated 2D materials fabrication with Quantum material press (QPress). **S. Park**, H. Jang, K. Yager, G. Doerk, A. Stein, J. Sadoski, C. Black

8:30 AM. Heuristic-based approach to 2D material identification. **G. Foster**, M.R. Carbone, S. Park, H. Jang, P. Vora

8:45 AM. Deep learning for wafer-scale optical characterization of 2D materials: From RGB to multispectral imaging. **H.B. Li**, M.S. Rosen

9:15 AM. Nanovision: An integrated platform for two-dimensional material discovery and device assembly–hardware. **S.T. Le**, J. Schwartz, R. Ni, Y. Zhou, K. Grutter, A. Hanbicki, A. Friedman

9:30 AM. Nanovision: An integrated platform for two-dimensional material discovery and device assembly – software. **J.J. Schwartz**, S.T. Le, R. Ni, Y. Zhou, K. Grutter, A. Hanbicki, A.L. Friedman

9:45 AM. Intermission.

10:00 AM. Artificial neuron networks enabled identification and characterizations of 2D materials and van der Waals heterostructures. **Y. Hao**

10:30 AM. AI-driven advances in atomic-scale microscopy for 2D materials and emerging LLM-based experiment-theory coordination. **M. Ziatdinov**

11:00 AM. Artificial intelligence models in biomedical image-based measurements. **P. Bajcsy**

11:30 AM. Ternary halide perovskite nanocrystals balancing stability and surface effects. S. Levy, G. Dosovitskiy, L. Kortstee, **Y. Bekenstein**, I.E. Castelli

PHYS Programs also available online: