

# APS Scientific Computation Seminar Series

Speaker: John Mitchell  
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Title: Panoramic Synthesis

Date: Tuesday, February 12, 2019

Time: 1:00 p.m.

Location: 401/A1100

Hosts: Nicholas Schwarz and Uta Ruett

## Abstract:

A notable ‘synthesis gap’ exists between what we can now predict with exceptional speed and fidelity (i.e., MGI approaches) and our ability to create these targets in the laboratory. Although high-throughput synthesis is well-established as a technique for optimization, and is now bringing AI/ML to bear in autonomous systems, the underlying synthetic approaches—solid state reaction, flux growth, vapor deposition, etc.—are largely unchanged for decades. A re-imagining of how we discover materials and synthesize them is needed to bridge the synthesis gap; panoramic synthesis bolstered by AI/ML presents one such new pathway to synthesis by design. In this computationally-guided approach to synthesis science, in situ and operando approaches will be leveraged to reveal the fundamental mechanisms of how materials and molecules assemble from atoms or complex building blocks. Multimodal approaches that capture structural and/or electronic signatures will be integrated through ML to create models of the synthesis mechanism itself. Ultimately, responsive, on-the-fly approaches to steering reaction pathways may be achievable in a feedback loop.