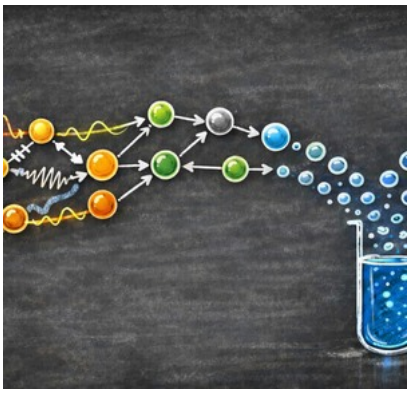
institute for pure & applied mathematics

Artificial Intelligence in Materials Science

SEPTEMBER 13 - DECEMBER 17, 2027



Scientific Overview

Data-driven modelling in the physical sciences has shifted existing paradigms, emerging as the fourth scientific pillar (after experiments, theory, and simulation). The next major step for this field is to embed modern machine learning more deeply into the processes of simulation, theory building, and experiment, so that it can evolve from an accelerating tool into a genuine driver of discovery. To that end, this program aims to develop AI methods that suggest novel principles, mechanisms and structures.

The program is timely, positioned to capitalize on three concurrent revolutions: First, understanding electronic structure from a modern data driven perspective, including the novel parametrization, and the generation of surrogates both for electronic and atomic degrees of freedom. Second, the rapid evolution of generative AI, including diffusion and flow-based models, has opened unprecedented opportunities for the inverse design of molecules and materials. Third, the emergence of “self-driving laboratories” (SDLs) is transforming experimental science by integrating robotics and AI to create closed-loop, autonomous platforms for synthesis and characterization. There is a growing recognition that these powerful data-driven and automated tools must be deeply integrated with robust physical theories to ensure reliability, move beyond simple interpolation, and enable true discovery.

In all themes, the program will focus on the integration of physical laws and constraints into the core of next-generation AI/ML architectures, and the challenge of extrapolation and out-of-distribution generalization. We will bring together leading researchers from applied mathematics, materials science, computer science, and theoretical chemistry and physics, to address the fundamental challenge of integrating first-principles simulation with data-driven discovery, synthesis and autonomous experimentation.

Long Program Schedule

- Workshop I: Quantum Chemistry and Electronic Structure: September 27 - 30, 2027
- Workshop II: Reduced Order Models: October 18 - 22, 2027
- Workshop III: Generative Models and the Challenge of Extrapolation: November 1 - 5, 2027
- Workshop IV: The Mathematics and Automation of Chemical Synthesis: November 15 - 19, 2027

Organizers

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Christoph Ortner
University of British Columbia
Anatole von Lilienfeld
University of Toronto

Participation

This long program will involve senior and junior researchers from several communities relevant to this program.

You may apply for financial support to participate in the entire 14-week program, or a portion of it. We prefer participants who stay for the entire program.

Applications will be accepted through **April 16, 2027**, but offers may be made up to one year before the start date. We urge you to apply early.

Mathematicians and scientists at all levels who are interested in this area of research are encouraged to apply for funding.

Supporting the careers of junior researchers is an important component of IPAM's mission and we welcome their applications.

More information and an application is available online.

NSF UCLA

For program details and registration:

Scan the QR code or visit ipam.ucla.edu/AIM2027