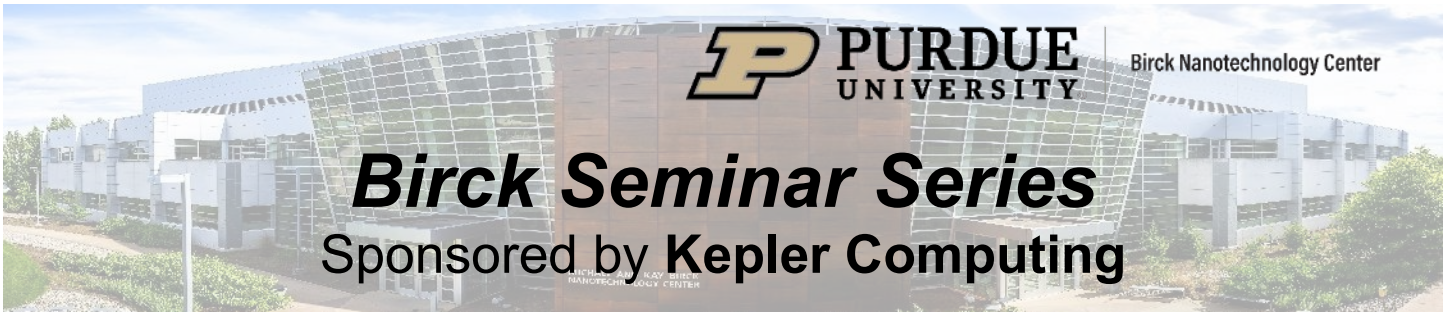


# Smart Science with AI: FAIR Data, Digital Twins, and Autonomous Agents

**Alejandro Strachan**

*School of Materials Engineering*

**TUESDAY, April 14th @ 2:00 pm in BRK 1001**

*Coffee and snacks served before seminar*

**also on MS Teams**

**Abstract:** Artificial intelligence is transforming research by partnering with humans to generate ideas, design experiments, run simulations, and interpret results. For AI to contribute effectively—whether assisting a scientist or leading a discovery—it needs reliable, easy-to-access information from past studies, data repositories, and tools to generate new data. This information must follow the FAIR principles: Findable, Accessible, Interoperable, and Reusable.

In this talk, I will present our work at Purdue and nanoHUB—a widely used open platform for online simulation and data—to create an integrated ecosystem that connects experimental data, computational models, and AI.

- Experimental data is captured directly from instruments or field studies and automatically organized to be AI-ready using FAIR standards.
- Accessible Simulation tools on nanoHUB are published with unique digital identifiers (DOIs), metadata for interoperability, and containerized environments to ensure reproducibility and reuse.
- These resources can be seamlessly called upon by researchers or by AI agents to answer questions and carry out research.

I will showcase real-world examples, including:

- Accelerating materials discovery by combining simulations, data, and AI-driven design;
- Creating smart digital twins that mirror physical systems and predict their behavior;
- Powering nanoRA, an AI research assistant that plans and executes scientific workflows using a growing library of community-contributed tools.

Join us to see how this infrastructure is enabling faster, more collaborative, and more reproducible science—open to experts and AI alike.

**Bio:** ***Alejandro Strachan*** is the Reilly Professor of Materials Engineering at Purdue University, the Co-Director of nanoHUB, and Purdue's Office of Research Fellow for Intelligent Twins and Digital Innovation. Before joining Purdue, he was a Staff Member in the Theoretical Division of Los Alamos National Laboratory and worked as a Postdoctoral Scholar and Scientist at Caltech. He received a Ph.D. in Physics from the University of Buenos Aires, Argentina. Prof. Strachan's research focuses on predictive atomistic and multiscale models grounded on first principles to advance our ability to understand, design, and deploy materials. His recent work integrates machine learning and artificial intelligence with physics-based modeling to tackle critical scientific and engineering challenges in areas such as energy, electronics, and manufacturing. In addition, Strachan's scholarly work includes cyberinfrastructure to make simulations, models, and data widely accessible and useful in research and education to accelerate innovation. nanoHUB has served over 200,000 simulation users and reached 800+ US institutions of higher education. Prof. Strachan has published over 200 peer-reviewed scientific papers and his contributions to research and education have been recognized by several awards, including the Early Career Faculty Fellow Award from TMS in 2009, an R&D 100 award in the category of *software and services* for nanoHUB (2020), and the Reilly Chair Professorship in 2023.

Host: Neil Dilley, Research Manager | Email: ndilley@purdue.edu