MSE 690 SEMINAR SERIES, FALL 2021

FRIDAY, SEP 24TH | 3:30 PM | ARMS 1010

Accelerating innovation with data science tools in nanoHUB: In the era of "data is the new oil", let's stop treating materials data as dirt

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Abstract: This talk will discuss how data science is accelerating progress in experimental and computational research in the field of materials science. In addition, I will provide a short tutorial on modern tools to manage and model data participants will be able to easily adopt in their research.

I will discuss recent progress by our team in the **combination of multi-fidelity experiments and physics-based modeling with machine learning** with the ultimate goal of designing refractory complex concentrated alloys with unprecedented combination of high-temperature strength and oxidation resistance. Specifically, I will discuss the integration of information from disparate sources into predictive models and these models to accelerate the discovery of new materials.

In the second part of the talk, I will introduce data science and cloud computing resources in nanoHUB, an open cyberinfrastructure for cloud scientific computing that seeks to maximize the impact of simulations and data in education and research. This hands-on tutorial will introduce participants to modern tools to manage, organize, and visualize data as well as machine learning techniques to model data and make decisions. We will discuss learning modules designed to introduce students and researchers to the fundamentals as well as resources for advanced practitioners.

Highly recommended pre-seminar activity: sign up for a few nanoHUB account (https://nanohub.org/register/) and bring a laptop or tablet.

Biography: Alejandro Strachan is a Professor of Materials Engineering at Purdue University Director, DoD ONR MURI "Predictive Chemistry and Physics at Extreme Conditions", PCP@Xtreme, and the Deputy Director of NSF's nanoHUB. 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 the development of predictive atomistic and multiscale models to describe materials from first principles and their combination with data science to address problems of technological or scientific importance. Areas of interest include: high-energy density and active materials, metallic alloys for high-temperature applications, materials and devices for nanoelectronics and energy, as well as polymers and their composites. In addition, Strachan's scholarly work includes cyberinfrastructure to maximize the impact of and democratize access to models and data for research and education. Prof. Strachan has published over 180 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, his induction as a Purdue University's Faculty Scholar (2012-2017), and the R&D 100 award in the category of software and services for nanoHUB.