University at Buffalo
Department of Materials Design and Innovation
School of Engineering and Applied Sciences
College of Arts and Sciences

CAS / SEAS SEMINAR

Computational and Statistical Models to Inform Materials Design and Discovery

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Abstract: The design and discovery of optimal or new materials using computation, machine learning and other data-driven methodologies offers the promise of a dramatic acceleration of advances in materials science. This ultimately results in faster "lab-to-market" deployment of advanced materials for consumer, industrial and defense uses. In this talk, I will detail my work in the computational and statistical modeling of material systems, and how such models are used in materials design and discovery, with a strong emphasis on the link between theoretical work and experiments. On the computational front, I will present my work in the development of a high-performance kinetic Monte Carlo (KMC) code, which elucidated the fundamental mechanisms in GaAs quantum dot and nanoring formation under Liquid Droplet Epitaxy. On the statistical and machine learning front, I will describe my work in Optimal Learning, which couples physical models with Bayesian statistics, regression modeling, and decision theory to design a strategic sequence of experiments in order to determine design parameters that maximize a material property of interest. I will highlight my recent collaborations with the Air Force Research Laboratory in applying this methodology to optimizing carbon nanotube growth within the ARES project, a robot scientist that autonomously plans, executes and characterizes experiments. Lastly, I will close with future directions for my research that build upon these projects.

Bio: Kris Reyes received his Ph.D. from the University of Michigan in 2013, where he was joint-advised by the Math and Materials Science departments. There, he developed computational and analytical models for nanostructure formation, with a main thrust in the simulation of GaAs quantum dot and nanoring synthesis. After receiving his Ph.D., he became a postdoctoral research associate in the Department of Operations Research and Financial Engineering (ORFE) at Princeton University. At Princeton, he led a research effort that applied the statistical/machine learning capabilities of the ORFE Department toward problems in materials science, chemistry and biology. In addition to academia, Kris has held positions at the National Security Agency and on Wall Street. In 2015, he founded Meru Apps, whose mission was to make cloud-based data more accessible and user friendly. In 2016, Meru Apps was selected as the winner of the NIST Reference Data challenge after developing a cloud-based infrastructure for the retrieval and visualization of NIST reference data.

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