THE MATERIALS SCIENCE AND ENGINEERING DEPARTMENT SPRING COLLOQUIUM SERIES PRESENTS:

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Towards an Efficient Exploration of the Materials Design Space

Over the last decade, there has been a paradigm shift away from labor-intensive and time-consuming materials discovery methods, and materials exploration through informatics approaches is gaining traction at present. Current approaches are typically centered around the idea of achieving this exploration through high-throughput (HT) experimentation/computation. Such approaches, however, do not account for the practicalities of resource constraints, which eventually result in bottlenecks at various stages of the materials discovery/design workflow. Regardless of how many bottlenecks are eliminated, the fact that ultimately a human must make decisions about what to do with the acquired information implies that HT frameworks face hard limits that will be extremely difficult to overcome. Recently, this problem has been addressed by framing the materials discovery process as an optimal experiment design problem. In this talk, I will discuss the need for optimal experiment design, the challenges in its implementation and finally discuss some successful examples of materials discovery via experiment design. Specifically, I will discuss some recent examples in which my group and collaborators have demonstrated: (i) Multi-objective materials discovery and design; (ii) Bayesian optimization under model uncertainty (BOMU); (iii) Multi-source information fusion Bayesian optimization for materials design; (iv) Batch Bayesian optimization applied to microstructure sensitive design of materials.

Raymundo Arróyave is a Professor, Presidential Impact Fellow and Chancellor's EDGES Fellow in the Department of Materials Science and Engineering at Texas A&M University. He received his PhD in Materials Science from the Massachusetts Institute of Technology in 2004. After completing a postdoctoral stay at Penn State, he joined the department of Mechanical Engineering at Texas A&M University in 2006, becoming a founding faculty of the Department of Materials Science and Engineering in 2013. His main areas of interest include: 1) computational thermodynamics and phase stability in structural and functional materials; 2) kinetic processes and microstructure evolution simulation; 3) multi-scale computational materials science; 4) simulation-assisted materials design; 5) machine learning and artificial intelligence-enabled materials discovery; 6 Integrated Computational Materials Engineering in Additive Manufacturing. He has worked on a number of materials classes including structural and functional alloys, thin films, and nano materials with applications in energy, transportation, etc. He has received several honors and distinctions including the NSF CAREER Award and the TMS 2019 Brimacombe Medal. He has authored or co-authored over 180 peer-reviewed articles and conference proceedings. He currently is the Chair of the Alloy Phase Diagram Committee of ASM International. He is also the Chair of the Functional Materials Division of TMS and serves on the Board of TMS as well as in its Executive Committee.

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