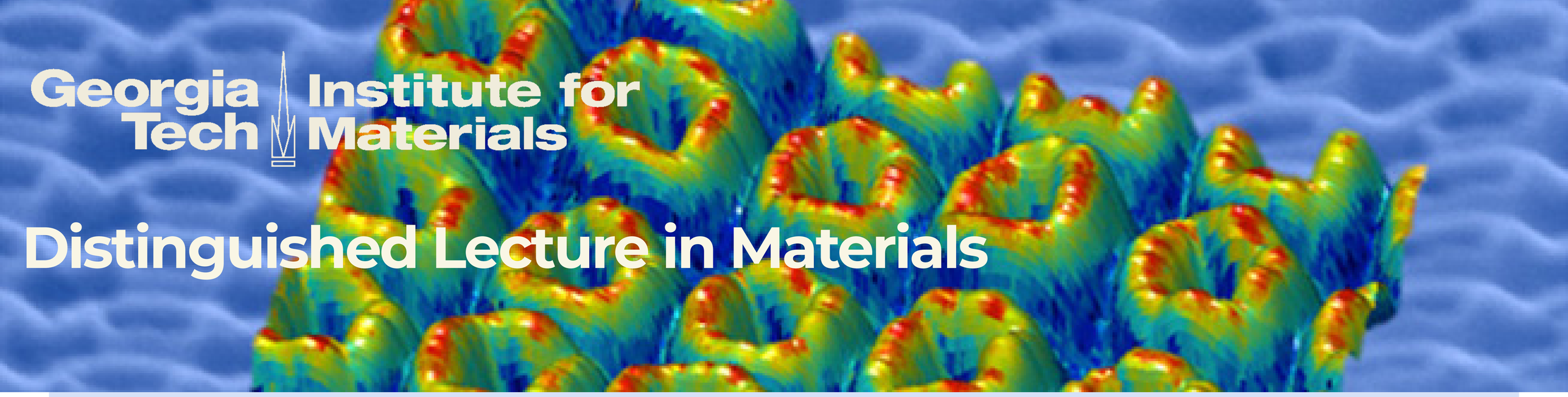

Georgia Tech Institute for Materials

Distinguished Lecture in Materials

Machine Learning and First-Principles Prediction of New Superhard Ternary & High-Entropy Borides

Professor Cheng-Chien Chen | Department of Physics,
University of Alabama at Birmingham

Tuesday September 21, 2021 | 2:00PM EDT
Virtual Event | Access Via RSVP Link

Abstract: Super-hard materials exhibit a Vickers hardness H ≥ 40 GPa, and they have extensive industrial and technological applications. Due to the huge search space of possible element combinations, it is challenging to explore new superhard ternary or quaternary materials. In this talk, I will first discuss machine learning (ML) discovery of new superhard B-C-N and B-N-O compounds. The ML results are validated by evolutionary structure prediction and density functional theory (DFT). In particular, the proposed BC10N has a low formation energy and a high hardness H ~ 86 GPa only next to diamond. In the second part of the talk, I will discuss calculations of entropy formation ability (EFA) using both DFT and ML for 5-metal hexagonal high-entropy borides. The calculations indicate that EFA serves as a good descriptor for the synthesizability of high-entropy materials, some of which have superior mechanical properties promising for applications in extreme environments.

Bio: Cheng-Chien Chen received his Ph.D. in Physics from Stanford University in 2011. Afterwards she became a Postdoctoral Scholar at the SLAC National Accelerator Laboratory and later an Aneesur Rahman Postdoctoral Fellow at the Argonne National Laboratory. He joined the Department of Physics at the University of Alabama at Birmingham (UAB) as an Assistant Professor in 2016. He is currently a Leadership Resource Allocation (LRAC) Awardee to use the NSF-funded Frontera Supercomputer and an NSF EPSCoR Research Fellow. Dr. Chen's expertise lies in using quantum many-body simulations, first-principles calculations, and machine learning approaches to model and predict the properties of various quantum and functional materials.

Please register by September 15th to access the seminar.

Register at: tinyurl.com/IMatDLfall1

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