Machine Learning in Materials Science: Reality, Hype, Opportunities and Pitfalls

THURSDAY October 10 | 4 P.M. | HILL HALL 202

Shyue Ping Ong
University of California, San Diego

Dr Shyue Ping Ong is an Associate Professor of NanoEngineering at the University of California, San Diego. He obtained his PhD from the Massachusetts Institute of Technology in 2011. His group, the Materials Virtual Lab, is dedicated to the interdisciplinary application of machine learning and first principles computations to accelerate materials design. He is a key developer of the Materials Project and the globally-used Python Materials Genomics (pymatgen) materials library. Dr Ong is also a recipient of the US Department of Energy Early Career Research Program and the Office of Naval Research Young Investigator Program awards.

Machine learning (ML) has garnered substantial interest as a potential tool to address many challenges in materials science, from materials discovery to simulation of complex materials. In this talk, I will discuss the potentially transformative impact that ML can have on materials research, from providing new chemistry insights that will greatly improve our ability to “guess” new materials with superior properties to accessing large length / time scales at near DFT accuracy to even interpreting experimental characterization. I will highlight major recent advances in materials ML models, focusing in particular on graph-based deep learning that has achieved state-of-the-art performance in the prediction of many properties. Nevertheless, many challenges remain and I will share my perspectives on major limitations in current materials ML models and potential opportunities.