Topic:

Accelerated Materials Design by Integrating Multiscale Modelling and Machine Learning

Abstract:

Materials science has been transformed through the applications of Density Functional Theory (DFT) calculations, which is the workhorse method for the computational investigation of materials across four domains of applications, conducted recently in our lab (Energy Materials Modelling Group): (I) Catalysis (II) Energy Storage (III) Semiconductors (IV) High Entropy Materials. (I) Electronic structure calculations help understanding catalytic mechanisms and predicting their activity performance. (II) In the realm of energy storage materials, DFT enables prediction of reversible hydrogen storage materials, with optimum hydrogen adsorption energies and high hydrogen adsorption capacities. DFT is also instrumental in understanding the mechanisms in battery materials to facilitate the design of batteries with enhanced performance, longer cycle life, and higher energy density. (III) For the semiconductor research, DFT predicts the electronic properties of materials by elucidating band structures, carrier mobilities, and doping effects in semiconductors. This information is crucial for optimizing semiconductor materials for various electronic and optoelectronic applications. (IV) For high entropy materials, DFT could predict their structural stability, mechanical properties, and phase behavior, to guide the design of tailored properties. Nowadays, we also see the advent of integration of Machine learning (ML) algorithms with multiscale modelling in various research realms. ML algorithms, trained with accurate DFT-calculated and other simulations outcomes, could enable large-scale modeling and simulations with unprecedented accuracy and efficiency. Thus, we expect to see the synergy of ML and multiscale modelling in the future to play important roles in design and development of materials.