Designing interfaces for energy materials: atomistic modelling, chemical heuristics and machine learning

Materials for energy-related applications, which are crucial for a sustainable energy economy, rely on combining materials that form complex heterogenous interfaces. Simultaneously, progress in computational materials science in describing complex interfaces is critical for improving the understanding and performance of energy materials. In this presentation I will give an overview of computational approaches for understanding and tailoring interfaces for renewable energy applications. Density functional theory (DFT) has been a crucial tool for understanding the atomic and electronic structure of surfaces and interfaces and I will show how insights from DFT calculations have allowed us to propose new designs to tailor interfaces for bespoke applications. Computational screening also offers the possibility of virtual screening of materials for optimal pairs to satisfy different criteria, I will present a scheme that allows rapid searching of known materials to identify mechanically stable and electronically optimal interfaces for photovoltaics. One of the limiting factors for virtual screening of interfaces is the lack of data on electronic energy levels. Recent advances in machine learning promise the ability to predict properties in a fraction of the time required for DFT calculations, thereby facilitating virtual screening, but the lack of reliable data hinders the training of such models. I will consider two approaches to overcoming this problem, first using simple chemical heuristics to estimate energy levels and second developing active learning techniques that can facilitate the generation of sparse yet representative databases of interface properties.