Multiscale Modelling of Complex Interfaces

There has been a significant interest in the bilayer systems (such as Ceria (CeO_2)/yttria-stabilized zirconia (YSZ)) for the development of solid oxide fuel cell (SOFC) technology. Multiple studies have explored the composing materials of the bilayer systems individually, however, the interface formed by them remain largely unexplored due to its complex nature.

Density functional theory (DFT) and molecular dynamics (MD), the commonly used techniques to study complex materials, are also insufficient to provide complete and accurate information of these interfaces when used individually. DFT fails to analyze all the possibilities of nature, location and concentration of dislocation arrays and associated defects present at the interfaces as it is limited by the model size. Whereas, MD although capable of handling bigger models of the interfaces, cannot provide the much-required insights into their electronic properties.

In this study, we combined both DFT and MD calculations to extract the atomic- and electronic-level details of the YSZ/CeO_2 bilayer system. First, a YSZ/CeO_2 interface model containing all the important micro-structural features of the real interface such as dislocations, point defects, diffusion, and lattice strains was prepared by using classical MD simulations. Then, DFT was implemented to analyze the electronic properties of the realistic YSZ/CeO_2 interface model prepared by MD. This work resulted in the long-sought explanation for the experimentally observed insulating layer at the YSZ/CeO_2 interface, details of which will be presented in this talk along with the model preparation details.