ABSTRACT

Modern industrial chemical activities depend on computational technologies. The information supporting many process and product optimization comes from fundamental molecular simulation computations.

In this talk I will briefly discuss two different applications of molecular modelling a) proton transport through perovskites, b) computational investigation of novel lubricant-additives. Perovskites are ceramics with general formula ABO3. High temperature proton conducting properties of perovskites have also recently been used for constructing membranes for cell reactors for catalytic dehydrogenation/ hydrogenation processes. It is known that perovskites with more cubic structure have higher proton mobility. We have used ab-initio molecular dynamics simulations (MD) to compute the diffusion coefficients and the activation energies from trajectories obtained from pure and Yttrium doped BaZrO3 at different concentrations and temperatures. Thermodynamics of proton conductivity in these systems were addressed by performing activation energy barrier calculations for proton hopping transition states using Nudged Elastic Bands (NEB) theory and ab-initio quantum chemical calculations. Finally, we have compared the activation barriers from MD (dynamical energy barriers) with thermodynamic barriers. Apart from this, we have analyzed the MD trajectories for understanding proton conduction mechanism. In the second part, I will discuss about computational investigation of novel lubricant-additives. In this study, we used nonequilibrium molecular dynamics simulations to examine the friction and wear reduction mechanisms of promising carbon nanoparticle friction modifier additives-- carbon nanodiamonds (CNDs) and carbon nano-onions (CNOs). Additives confined between á-iron slabs is probed at a range of coverages, pressures, and sliding velocities. The contribution to the friction coefficient is well predicted by an expression developed for macroscopic indentation by Bowden and Tabor. The results are in experimental agreement.