Light Metal Nanostructures for Hydrogen Storage

Light metal hydrides have the potential for high hydrogen storage uptake (up to 10.6 wt% hydrogen uptake for Al-Li based metal hydrides). Aluminium clusters are of particular interest due to their potential to form alanates. Yarovsky and co-workers have used Density Functional Theory techniques to study the interactions of bare and doped aluminium clusters with hydrogen and identified a candidate cluster with a high hydrogen storage capacity. Furthermore, \((\text{Al}12\text{Mg})2\) was found to spontaneously dissociate a hydrogen molecule, suggesting that doped Al clusters can be used as building blocks for a potential hydrogen storage material.

In order to study the thermodynamic and kinetic processes of large clusters, approximate techniques such as the Embedded Atom Method (EAM) has to be used. While there are many available EAM potentials developed for specific systems consisting of one or more elements, most of these potentials have been constructed by fitting to bulk structures, and hence their reliability and applicability for small clusters are not certain. In this presentation, we compare the performance of several EAM potentials in terms of the thermodynamic behaviour and structural characteristics of the resulting clusters. Using the best-performing potential, we will then explore hydrogen dynamics on the aluminium clusters.