Structure and Dynamics of Magnesium Doped Helium Clusters

M. Elhiyani, M. Lewerenz

Université Paris-Est
Laboratoire Modélisation et Simulation Multi Echelle,
MSME FRE3160 CNRS,
5 bd Descartes, 77454 Marne-la-Vallée, France

Helium clusters have proved to be a very versatile environment for the cooling and controlled assembly of molecular and metallic aggregates for spectroscopic studies and, more recently, also for the investigation of reactive processes. Alkaline and alkaline earth metal atoms have extremely weak van der Waals interactions with helium with well depths even weaker than the He-He value of about 7.6 cm^{-1}. In spite of their extreme shallowness these potentials seem to support at least one bound state even for alkali atoms. The competition between this weak interaction and the cohesive energy of helium allows only surface bound states for single alkali atoms but leads to a more ambiguous situation for alkaline earth atoms, where experimental evidence exists for solvation of magnesium and for a more delicate 'neither surface nor bulk' situation for calcium. The interactions between individual alkaline earth atoms are of van der Waals type. This effect might explain the observation of atomic transitions in large helium clusters doped with more than one magnesium atom. We have performed extensive ab initio calculations for the binary magnesium-helium interaction with coupled cluster techniques and large diffuse basis sets and including core correlation. Our potential and previously published ones support bound states for all mixed $Mg@He_n$ clusters, starting at $n = 1$. An analytical representation of the Mg-He interaction is combined with accurate He-He pair potentials and used for diffusion quantum Monte Carlo (DMC) calculations of the binding energy and the structure of clusters with up to 200 helium atoms. DMC calculations with geometrical constraints show that the effective radial potential for Mg atoms inside the He_n droplet is very shallow. We present first results on the recombination dynamics of two Mg atoms inside He_n using an effective potential method.