Metal Atoms and Ions in Helium Clusters

M. Lewerenz

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

Many metal atoms M have binary interaction potentials with helium such that the dopant location inside liquid helium clusters M@He_n depends on a delicate balance between the potential energy and the quantum mechanical kinetic energy contribution. Reliable theoretical predictions of dopant locations therefore require accurate microscopic many body quantum calculations. The diffusion quantum Monte Carlo (DMC) method in combination with advanced electronic structure methods is an excellent tool to accomplish this goal.

After a brief discussion of the particularly challenging case of Mg atom solvation and recombination inside helium we will discuss the modelling of metal containing ionic clusters which are produced by electron impact or laser ionisation of neutral precursors. The strong electrostatic interaction leads to an unambiguous dopant location but a number of new challenges arise due to open electronic shells and the possibility of the appearance of magic cluster sizes. M^{k+}@He_n, $k > 1$, compounds have been proposed as possible candidates for the highest coordination numbers in chemistry. In collaboration with P. Slavíček we have developed an accurate non-additive potential model for Pb^{2+}@He_n clusters based on extensive ab initio calculations which has been used for studies of shell closure effects by DMC. An extension of this model to Pb^+ ions requires the inclusion of spin-orbit effects. DMC calculations with and without spin-orbit coupling show the importance of this effect on binding energies and structures of Pb^+@He_n. Analoguous calculations are reported for the electronically much simpler Mg^+@He_n system.