Metal Clusters in a Helium Matrix

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Capturing atoms in ^{4}He nanodroplets allows to assemble cold nanoclusters in a well controlled step-by-step way. A challenge for the theorist is the multi-scale description of all degrees of freedom of such a system: the electrons of the cluster, the motion of the ions of the cluster and the motion of the ^{4}He atoms surrounding the cluster. We present calculations of small Mg_N clusters within ^{4}He droplets. We employ density functional theory in the local density approximation (LDA) for the electronic structure of Mg_N and Path Integral Monte Carlo simulations for the superfluid ^{4}He droplet. The interaction between the cluster and the surrounding ^{4}He is modeled in a such a way that the known He-Mg interaction is reproduced for the dimer, and the polarization of the Mg valence electrons is treated, consistently with the rest of the system, in the LDA. The Mg_N clusters are annealed including the response of the ^{4}He environment. We discuss the effect of the ^{4}He matrix on the structure and the response of the Mg_N cluster.