Theoretical studies of impurity solvation in large He nanodroplets frequently employ a helium density functional (He-DF) treatment of the helium solvent. Quantum Monte Carlo studies of impurity solvation in He nanodroplets complement these He-DF studies and make it possible to study, at an atomistic level, the structure of the solvation shells that surround the embedded impurities. He-DF studies of exotic systems such as metastable “atomic foams” [1-3] suggest that these solvation shells play an important role in the structure and energetics of weakly-bound aggregates dissolved in He nanodroplets.

Here we present fully atomistic quantum Monte Carlo studies of weakly bound atomic and molecular clusters embedded in moderately large He clusters with *O*(103) atoms. The clusters of primary interest are Mg2 dimers and (pH2)*n* clusters. Our results shed light on the way in which the He droplet environment modifies the structure and “floppiness” of the embedded clusters.

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