

Magnesium doped helium nanodroplets

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We have studied the structure of ^4He droplets doped with magnesium atoms using density functional theory[1]. We have found that the solvation properties of this system strongly depend on the size of the ^4He droplet. For small drops, Mg resides in a deep surface state, whereas for large size drops it is fully solvated but radially delocalized in their interior. We have studied the $3s3p\ ^1P_1 \leftarrow 3s^2\ ^1S_0$ transition of the dopant, and have compared our results with experimental data from laser induced fluorescence (LIF).[2] Line broadening effects due to the coupling of dynamical deformations of the surrounding helium with the dipole excitation of the impurity are explicitly taken into account. We show that the Mg radial delocalization inside large droplets may help reconcile the apparently contradictory solvation properties of magnesium as provided by LIF and electron-impact ionization experiments.[3] The structure of ^4He drops doped with two magnesium atoms is also studied and used to interpret the results of resonant two-photon-ionization (R2PI) and LIF experiments. We have found that the two solvated Mg atoms do not easily merge into a dimer, but rather form a weakly-bound state due to the presence of an energy barrier caused by the helium environment that keep them some 9.5 Å apart, preventing the formation of the Mg_2 cluster. From this observation, we suggest that Mg atoms in ^4He drops may form, under suitable conditions, a soft “foam”-like aggregate rather than coalesce into a compact metallic cluster. Our findings are in qualitative agreement with recent R2PI experimental evidences. We predict that, contrarily, Mg atoms adsorbed in ^3He droplets do not form such metastable aggregates.

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