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Calculated Electronic Behavior and Spectrum of $Mg^+@C_{60}$ Using a Simple Jellium-shell Model

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Abstract: We present a method for calculating the energy levels and wave functions of any atom or ion with a single valence electron encapsulated in a Fullerene cage using a jelluim-shell model. The valence electron-core interaction is represented by a one-body pseudo-potential obtained through density functional theory with strikingly accurate parameters for Mg^+ and which reduces to a purely Coulombic interaction in the case of H. We find that most energy states are affected little by encapsulation. However, when either the electron in the non-encapsulated species has a high probability of being near the jellium cage, or when the cage induces a maximum electron probability density within it, the energy levels shift considerably. Mg^+ shows behavior similar to that of H, but since its wave functions are broader, the changes in its energy levels from encapsulation are slightly more pronounced. Agreement with other computational work as well as experiment is excellent and the method presented here is generalizable to any encapsulated species where a one-body electronic pseudo-potential for the free atom (or ion) is available. Results are also presented for off-center hydrogen, where a ground state energy minimum of -14.01 eV is found at a nuclear displacement of around 0.1 Å.

Keywords: Encapsulation, confined atoms, magnesium, Fullerenes, spectral shift.
