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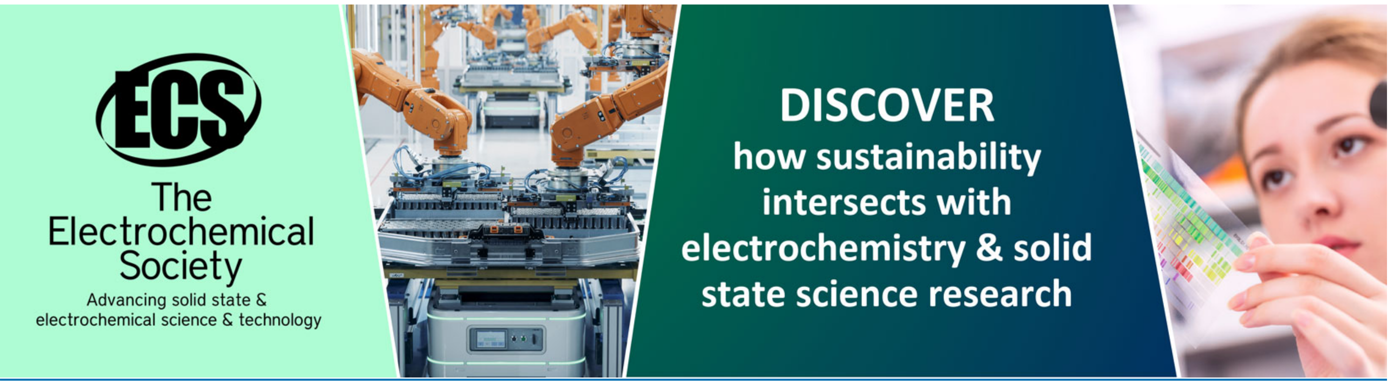

Photoionization of Endohedrally Confined Ca ($Ca@C_{60}$)

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Synopsis Photoionization cross section of endohedrally confined calcium is computed using R-matrix method.

Photoionization of atoms are of great interest in atomic physics as well in astrophysical applications. The photoionization of the outer shell of neutral calcium was studied using different methods in the past. Three-state R-matrix calculations were found to be successful in describing complex resonance structure in free Ca [1]. Here, we report on similar calculations for endohedrally confined Ca, $Ca@C_{60}$. In our calculations, we have formed spectroscopic orbitals, 1s-4p, using the Hartree-Fock method (HF) and correlation orbitals, 4d and 4f, using the Multiconfiguration Hartree-Fock method (MCHF).

In this work, we have modeled C_{60} confinement as an attractive spherical potential well of inner radius $r \sim 5.8$ and thickness of $\Delta \sim 1.89$, and a depth of $U_0 \sim 0.302$ a.u. This confining potential is added to the internal atomic potential to perform the HF and MCHF calculations [2] and also to the one-electron operator in the R-matrix calculations [3].

Calculated energies for confined Ca^+ [Ar]3d ^2D and [Ar]4p $^2P^o$ with respect to [Ar]4s ^2S and the ionization potentials compared to results of previous work for free Ca^+ are presented in Table 1. Our studies show that the confined Ca^+ system gets more bound and also the order of ^2D and $^2P^o$ thresholds switches in the presence of the confining potential.

Table 1. Comparison of energies for free and confined Ca^+ and ionization potentials (IP) in Rydbergs.

	Free Ca		$Ca@C_{60}$	
State	HF[a]	CI[a]	HF	CI
[Ar]4s ^2S	0.0000	0.0000	0.0000	0.0000
[Ar]3d ^2D	0.1524	0.1202	0.1908	0.1807
[Ar]4p $^2P^o$	0.2076	0.2180	0.1206	0.1217
IP	0.4410		0.6173	

[a]Previous work[1].

Our calculations also predict that the threshold energy for confined Ca is about 2 eV higher than the free Ca system, which agrees with the earlier resonanceless photionization study of $Ca@C_{60}$ [4]. This is because the attractive C_{60} potential makes the ground state of Ca more bound.

One-electron radial wave functions for 4s, 3d, and 4p are shown in Fig. 1. In the presence of C_{60} confinement, radial wave functions of outer electrons move into the attractive potential. As a consequence, the outer electron gets further away from the nucleus in the confined cases which makes the correlation effects smaller; note the differences between HF and CI energies in Table 1.

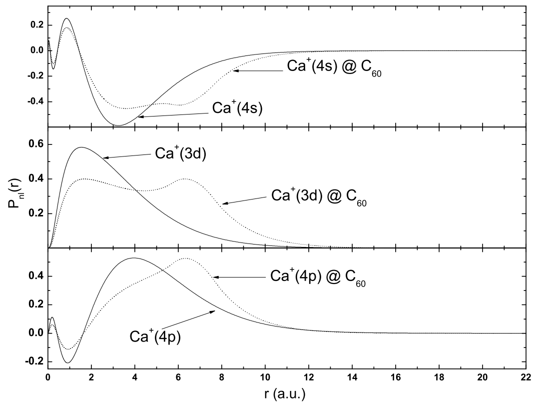

Figure 1. One-electron radial wave-functions for free and confined Ca^+.

References

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