

Abstract Submitted  
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**Correlation Study of Endohedrally Confined Atoms (A@C<sub>60</sub>):  
Alkaline Earth Metal Elements**<sup>1</sup> MUHAMMET F. HASOGLU, HSIAO-LING  
ZHOU, STEVEN T. MANSON, Georgia State University — Effects of endohedral  
confinement on the correlation energy of Be, Mg, and Ca have been investigated us-  
ing a modified Hartree- Fock (HF) and Multi-Configuration Hartree-Fock (MCHF)  
method. In this method, an atomic endohedral system (A@C<sub>60</sub>) is approximated  
as an atom enclosed in an attractive spherical potential well of inner radius  $r \sim 5.8$   
and thickness of  $\Delta \sim 1.89$  a.u., and correlation energies are studied as a function of  
the depth of the confining potential ( $0 \leq U_0 < 2$  a.u.). In order to calculate single-  
and multi- configuration wave functions, we have modified the MCHF codes [1] by  
adding a well potential in addition to the internal atomic potential. Single- and  
multi-configuration wave functions are obtained from the solution of HF and MCHF  
equations with the extra potential self-consistently. In general, we have found that  
valance electrons diffuse outward in the presence of extra potential, which causes  
the electrons to be further apart. As a consequence, the electron correlations get  
smaller. In conclusion, our studies has showed that the correlation effects in endo-  
hedrally confined atoms gets less important than the free atoms.

[1] C. Froese Fischer et al., Comput. Phys. Commun. **176**, 559 (2007).

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