

Abstract Submitted
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The quantum confinement resonances of a Xe atom encapsulated inside fullerenes¹ ZHIFAN CHEN, ALFRED Z. MSEZANE, Clark Atlanta University — The quantum confinement resonances of a Xe atom encapsulated inside C₆₀, C₈₀, C₁₈₀, and C₂₄₀ have been investigated. The geometric optimization for these fullerenes was performed using the DMol₃ software package with the GGA PBE exchange-correlation functional along with all electron double numerical basis sets as implemented in the software package [1]. The measured average radii of the C₆₀, C₈₀, C₁₈₀, and C₂₄₀ are respectively, 3.5 Å, 4.1 Å, 6.3 Å, and 7.1 Å. Each optimized structure was then introduced into a supercell. The linear response of the ground state to an external perturbation by an electric field was evaluated using the TDDFT method. The locations of the peaks for the confinement resonances calculated by the TDDFT method were compared with the locations estimated using the equation $E(eV) = 67.55 + (\frac{12.25n}{2r})^2$, where r is the radius in Å of the fullerene and $n = 2, 3, 4, 5$, etc. The results demonstrate that if the radius of a fullerene equals to an integer (≥ 2) \times the half wave length of the photoelectron, then at this photon energy we may be able to observe a confinement peak.

[1] DMol₃, Accelrys Software (Inc., San Diego, CA 2010)

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