

Abstract Submitted
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Photoabsorption spectrum of the Xe@C₆₀ endohedral fullerene¹

ZHIFAN CHEN, ALFRED Z. MSEZANE, Clark Atlanta University — Photoabsorption spectrum of the Xe@C₆₀ endohedral fullerene has been studied using the time-dependent-density-functional-theory (TDDFT), which represents the dynamical polarizability of an interacting electron system by an off-diagonal matrix element of the resolvent of the Liouvillian superoperator and solves the problem with the Lanczos algorithm. The method has been tested with the photoabsorption cross sections of the free Xe atom and C₆₀ fullerene. The result for the Xe@C₆₀ confirms the three main peaks observed in the recent measurement in the energy region of the Xe *4d* giant resonance [1] and shows the possibility that the Auger decay of the Xe⁺ has been greatly suppressed if the ion is encapsulated inside C₆₀. It is suggested to perform the same measurement around 22 eV to check this possibility.

[1] A L D Kilcoyne et al, Phys. Rev. Lett. 105 213001 (2010).

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