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Off center effect on the photoabsorption spectrum of the Xe@C_{60} endohedral fullerene[1] ZHIFAN CHEN, ALFRED Z. MSEZANE, Clark Atlanta University — The absolute differential oscillator strengths (DOS's) for the photoabsorption of the Xe atom encapsulated at different locations of the C_{60} have been evaluated using the time-dependent-density-functional-theory. The calculations are performed in the energy region of the Xe $4d$ giant resonance with the locations of the Xe atom at the center and 0.2 Å, 0.3 Å, 0.4 Å, 0.5 Å, 0.8 Å, 1.5 Å, 2.0 Å away from the center. The results demonstrate that the main confinement resonances result only when the Xe atom is located in a very small region of the C_{60}. This region is about 0.3 Å around the center of the C_{60} (3.5 Å is the C_{60} radius). These results explain the absence of the confinement resonances in the photoionization of the encapsulated lanthanide atoms such as Ce@C_{82} [1], Pr@C_{82} [2] as these atoms (Ce, Pr) are usually located 1.8-2.0 Å off the center of the C_{82}.

[1] K Mitsuke et al, J. Chem. Phys. **122** 064304 (2005)
[2] H Katayanag et al, J. Quant. Spectrosc. Radiat. Transfer, **109** 1590 (2008)

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