Off center effect on the photoabsorption spectrum of the Xe@C$_{60}$ endohedral fullerene

Zhifan Chen$^*$, Alfred Z Msezane$^*$

$^*$ Clark Atlanta University, Atlanta GA 30314, USA

Synopsis

DOS’s of Xe atom located at different distances from the C$_{60}$ center have been evaluated. The results indicate that the main confinement resonances result only when the Xe atom is within about 0.3 Å around the center of C$_{60}$.

We have used the recently developed TDDFT method [1] to calculate the absolute differential oscillator strengths (DOS’s) for the photoabsorption of the Xe atom encapsulated at different locations of the C$_{60}$. This method takes three steps to evaluate the spectrum. Firstly, the structure of the C$_{60}$ is optimized. Secondly, the ground state eigenvalues and eigenvectors are created by solving the Kohn-Sham equation self-consistently. Thirdly the linear response of the system to the perturbation by an external electric field is described by the TDDFT. After the C$_{60}$ calculation a Xe atom was introduced into the C$_{60}$ 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 DOS’s of the Xe@C$_{60}$ were evaluated using the same procedure as described for the C$_{60}$. Then the DOS’s for the photoabsorption of the encaged Xe atom were extracted by subtracting the DOS’s of the fullerene from the corresponding DOS’s of the Xe@C$_{60}$.

Fig. 1 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 also explain the absence of the confinement resonances in the photoionization of the encapsulated lanthanide atoms such as Ce@C$_{82}$ [2], as these atoms (Ce, Pr) are usually located 1.8-2.0 Å off the center of the C$_{82}$.

![Figure 1](image1)

Figure 1. Photoabsorption spectrum from bottom up, Xe at the center, 0.2 Å, 0.3 Å and 0.4 Å away from center, respectively

Fig. 2. Solid (red) curve is the DOS’s of free Xe atom, dashed (blue) curve represents the DOS’s of Xe located 2 Å away from the center of C$_{60}$.

![Figure 2](image2)

Figure 2. Solid (red) curve is the DOS’s of free Xe atom, dashed (blue) curve represents the DOS’s of Xe located 2 Å away from the center of C$_{60}$

Fig. 2 indicates that the DOS’s of the Xe atom located far away from the center is almost the same as that of the free Xe atom.

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References

[1] Zhifan Chen and A Z Msezane 2012 Phys. Rev. A 86 063405

[2] A Müller et al 2008 Phys. Rev. lett. 101 133001