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Off center effect on the photoabsorption spectrum of the Xe@C_{60} endohedral fullerene

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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}.

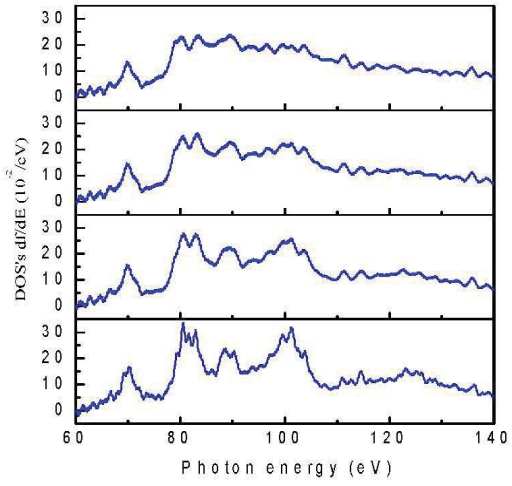

Figure 1. Photoabsorption spectrum from bottom up, Xe at the center, 0.2 Å, 0.3 Å and 0.4 Å away from center, respectively

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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}.

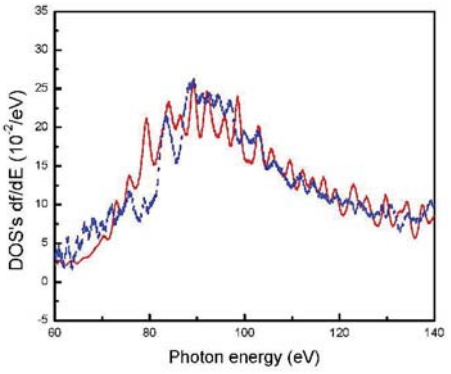

Figure 2. Solid (red) curve is the DOS's of free Xe atom, dashed (blue) curve represents the DOS's of Xe located 2 Å away from the center of C_{60}

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

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