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Impact of defect state in the structural, electronic and spectroscopic properties of graphene quantum dot by substituting heavy elements on the surface

Quantum dots are nanostructured semiconductor materials whose dimension is comparable to the de Broglie wavelength of free electrons. Due to the quantum confinement effect, the motion of the electrons present in the quantum dots is restricted in all three dimensions and the electronic energy states become quantized as compared to their bulk counterparts. This quantization of energy states gives rise to significant changes in the electronic properties of the material. Here, in this work, we have designed graphene quantum dots and studied their electronic and spectroscopic properties. In addition to that we have also introduced a defect state in the graphene surface by introducing heavy elements in its lattice structure. The density functional theory (DFT) is applied to design, optimize (in the gas phase), and investigate the impact of the defect state in the graphene surface, which is the most widely used electronic structure method in the material science community (the significant importance of DFT in physics and chemistry is evidenced by the 1998 award of the Nobel Prize). Results obtained from the present investigation signify that the incorporation of heavy elements not only produces structural distortion but also has the capability to induce lattice defects on the graphene surface. This deformation occurs due to the difference in electronegativities and covalent radii of the heavy elements and the carbon. Furthermore, we have noticed some additional energy states that appear near the fermi energy level as a result of the creation of the defect states. These energy levels significantly impact the density of states, orbital coupling, overall conductivity etc. of the graphene quantum dots.

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