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DFT/TDDFT Investigation of Electronic, Magnetic, and Optical Properties of Graphene Containing Different Values of Se Impurity

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The electronic, magnetic, and optical properties of graphene (gr) containing selenium impurities of 2, 3, 5.5, and 12.5% were calculated by DFT. By increasing the percentage of Se impurity, the energy gap decreases from about 0.3 eV for the gr + Se (2%), to about 0.1 eV for gr + Se (3%) monolayer. Continuing this trend leads to metallic property for gr + Se (5.5%) and gr + Se (12.5%) cases. By decreasing the percentage of Se impurity as a non-thermal control parameter, the magnetization started from zero and gradually increased so that the phase transition occurred. By calculating optical properties, using TDDFT, we found that in the absorption spectrums, a visible peak appeared for the cases of Se (3%) and Se (5.5%), and in the gr + Se (12.5%) layer, there exist an infrared shoulder. Also, except for gr + Se (3%), other cases have one peak in the UVA range. Finally, in the gr + Se (2%) case, for all optical variables, the peaks are sharper and stronger, therefore this case could behave as a quantum dot.

Keywords: graphene, Se impurity, density functional theory (DFT), semiconductor, time-dependent density functional theory (TDDFT).