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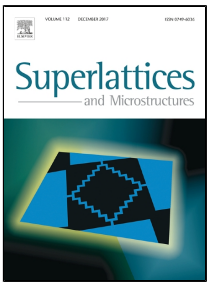

Optical Graphene Quantum Dots Gas Sensors: Theoretical Study

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Optical Graphene Quantum Dots Gas Sensors: Theoretical Study

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Abstract:

In this work, we theoretically studied the changes of graphene quantum dots (GQD) absorption spectra under the influence of different gases to indicate optical gas sensing features of GQDs. The adsorption of gas molecules such as CO_2, N_2 and Ar on GQDs have been theoretically investigated through time-dependent density functional theory (TDDFT) calculations. Our study revealed that UV-Vis absorption spectrum of GQDs in the presence of CO_2 undergoes considerable changes than that of N_2 and Ar. The shift of maximum absorption wavelength for adsorption of CO_2, N_2 and Ar in same distance from GQD in addition to density of state (DOS) and orbital analyses have been obtained. To verify our theoretical results, comparison with experimental study has been done and good agreement has been observed. Comparing with electrical property of GQD, optical properties showed an efficient tool to be implemented in gas adsorption and paves the way towards GQD optical gas sensors.

Keywords: Time Dependent Density Functional Theory, Graphene Quantum Dot, Optical absorption, Optical Gas Sensing.

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