Gas molecule sensing (CO) with defect silicene monolayer: a turbo Energy Electron Loss Spectroscopy study

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Abstract

Increasing demand for highly sensitive, selective, affordable, low-consumption, durable and portable sensors has led to extensive research into the use of two-dimensional materials. Two-dimensional materials are very suitable for making gaseous sensors due to good optical clarity, high flexibility, high mechanical strength, and special electronic and optoelectronic properties. In this paper, the electronic, optical and magnetic properties of pure and defected silicene monolayer in the presence of carbon monoxide gas has been studied using first principles calculations based on density functional theory and time-dependent density functional theory. According to the investigations, we find that the optical and electronic properties of the system are altered by the absorption of the gas molecule and the vacancy defect. Here, the electron energy loss spectroscopy for pure silicene monolayer in the presence of gaseous molecule and vacancies defect have been investigated. The spectrum associated with them indicates that the plasma peak changes (Collective modes).

Keywords: Two-dimensional materials, Time-dependent density functional theory, Collective modes, Electron energy loss spectroscopy

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