عنوان مقاله:

Carbon Monoxide Gas Sensor Based on ZrSe۲ monolayer nanosheet

محل انتشار:

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خلاصه مقاله:

Recently, the semiconducting electronicproperties of different compounds of two-dimensional(۲D) materials have been explored. One of the mostimportant members of this family (ZrSe۲; Zirconiumdiselenide) is used to substitute the silicon in Nanoelectronics because of its considerable bandgap.Moreover, this material seems to have potentialapplication in sensing some toxic gases. In this research,we have investigated the adsorption ability of ZrSe۲nanosheet structure when the CO and CO۲ gas moleculesare applied to the nanosheet surface. The simulationresults show appropriate and considerable sensingproperty of this structure in presence of CO gas moleculewith stable configuration and prominent changes inamount of current after gas adsorption. The CO gasmolecule shows a stable and considerable adsorption onthe ZrSe۲ structure which indicates that the ZrSe۲nanosheet structure is a proper case for gas sensingapplications. I-V calculations illustrate a selectivesensitivity to this especial gas molecule.

کلمات کلیدی:

transition metal dichalcogenides, ZrSe۲ nanosheet, CO gas molecule, Density functional theory