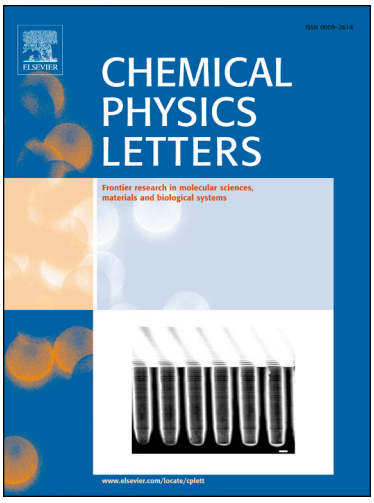

Research paper

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Toxic gases molecules (NH_3, SO_2 and NO_2) adsorption on GeSe monolayer with point defects engineering

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Abstract

First-principles calculations are performed to study the structure, stability, density of states and work function of toxic gases (NH_3, SO_2 and NO_2) molecules adsorption on GeSe monolayer with point defect engineering, including Ge/Se mono-vacancy, anti-site defect, and P atom substituted defect. Our results on the adsorption energy, charge transfer and electron localization function show that the interaction between gas molecules and point defects in GeSe monolayer is sensitive, which causes significant modification to the electronic structure and work functions of GeSe monolayer.

Keywords: monolayer GeSe; point defect; first-principles; work function