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g-SiC and g-SiC_2 siligraphenes as two multifunctional H_2S sensing materials

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Abstract

The main purpose of this article is to investigate the capability of g-SiC and g-SiC_2 siligraphenes in detecting H_2S gas through diverse sensing mechanisms, using density functional theory. Our calculations demonstrate that the adsorption of H_2S molecules onto both siligraphenes is a physical and exothermic process. The physical adsorption process helps sensing materials to recover soon (a few nanoseconds) after gas removal at room temperature. Investigation of geometric and electronic properties of g-SiC and g-SiC_2 in combination with H_2S molecule shows that both materials have the gas-detection ability through thermal- and resistance-based mechanisms. For example, the electrical conductance of g-SiC changes by 38% due to gas adsorption. In addition, the presence of H_2S molecule on the g-SiC surface, changes the type of its majority carriers and makes it possible to use this material in Seebeckeffect-based H_2S sensors. Overall, various sensing mechanisms besides short recovery time, make g-SiC and g-SiC_2 great candidates to be used in H_2S gas sensor as sensing material.

Keywords: g-SiC and g-SiC_2 siligraphenes, H2S sensor, Seebeck effect, density functional theory

For full article, refer to the Persian section