Modulation of L-cysteine adsorption on graphene: the role of the Al, Si, P, S dopant and the vacancy

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Abstract

Promoting the application potential of graphenes in biomolecule adsorption and detection is of great significance in the field of nanobiotechnology. In this paper, the density functional theory calculation was used to study the adsorption and sensing of L-cysteine on graphene-based compounds, single-vacancy and double-vacancy graphenes (XSV and XDV) doped with 3p-bolck elements (Al, Si, P, and S). Along with the dopant changing from Al to S, XSV exhibits decreasing exothermical chemisorption to endothermical chemi-sorption, while XDV exhibits decreasing exothermical chemisorption to endothermical physisorption. L-cysteine adsorption on XDV is weaker than corresponding adsorption on XSV. Valence electron number, and atomic ionization potential, modulated by the 3p-block dopant, and X-C interaction, modulated by the vacancy type, contribute to adsorption mechanism of L-cysteine on XGs. The study could facilitate applications of Al, Si, P and S doped graphenes in biosensing technology, biomolecule immobilization, bioseparation and other fields.

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