عنوان مقاله:

(Investigating the Influence of Doping Graphene with Silicon and Germanium on the Adsorption of Silver (I

محل انتشار:

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نویسندگان:

Mohammad Reza Jalali Sarvestani - *Young Researchers and Elite Club, Yadegar-e-Imam Khomeini (RAH) Shahr-e-Rey Branch, Islamic Azad University, Tehran, Iran*

Roya Ahmadi - *Department of Chemistry, Yadegar-e-Imam Khomeini (RAH) Shahre-rey Branch, Islamic Azad University, Tehran, Iran*

خلاصه مقاله:

In this study, the impact of doping graphene with silicon and germanium on the adsorption of Ag+ was evaluated by density functional theory. At the outset, the structures of silver, adsorbents and their derived products at ten different configurations were optimized geometrically. Then, IR and frontier molecular orbital calculations were implemented on them and some important parameters such as adsorption energy, Gibbs free energy changes, enthalpy variations, the thermodynamic equilibrium constant, specific heat capacity, chemical hardness, energy gap and electrophilicity were obtained and inspected. The achieved results indicate that by doping graphene with silicon and germanium the adsorption process has become more spontaneous, exothermic and experimentally feasible. The influence of temperature on the adsorption procedure was also checked out and the results indicate that 298.15 K is the optimum temperature for the desired process at all of the evaluated configurations. The HOMO-LUMO related parameters reveal that the pure and also doped nano-adsorbents are not appropriate sensing material in the construction of conductometric sensors but they can act as an eminent neutral ion carrier in the development of a potentiometric ion selective electrode for determination of silver (I) cations.

کلمات کلیدی:

Adsorption, Ag+, density functional theory, Graphene