

عنوان مقاله:

Titanium Decorated Graphyne As Sensor of Sarin: A DFT-D study

محل انتشار:

نهمین سمینار ملی شیمی و محیط زیست ایران (سال: 1398)

تعداد صفحات اصل مقاله: 1

نویسندگان:

F Mofidi, - *Department of Physical Chemistry, Faculty of Chemistry, University of Kashan, Kashan, Iran*

A Reisi-Vanani - *Department of Physical Chemistry, Faculty of Chemistry, University of Kashan, Kashan, Iran*

خلاصه مقاله:

Sarin ($C_4H_{10}FO_2P$ / isopropyl methyl phosphonofluoridate) is an organo-phosphorus compound, toxic and deadly, which is used in the production of chemical warfare agents (CWAs). It is dangerous in both vapor and liquid states. Finding of the materials for using as sensing, capturing and adsorption of hazardous compounds such as sarin is one of the aims of researchers. Graphyne (GY) is an interesting two dimensional (2D) periodic structure of the carbon allotropes. GY is a planar honeycomb networks contains acetylenic linkages. In this work, the effect of Ti single atom on the structural and electronic properties of GY toward sarin adsorption was studied by density functional theory (DFT) calculations. Seven sites of the GY and different distances of the metal from GY plane were investigated to gain the best structure of Ti-decorated GY. Then, adsorption of sarin on this structure as well as the pristine GY was considered. We examined various directions of sarin molecule onto pristine and Ti-decorated GY. The results showed that H1 (center of 12-membered ring) is the best site for Ti decoration and sarin adsorption. Also, decoration with Ti improves adsorption energy of sarin on GY up to 4.5 times (From -0.500 to -2.228 eV). Among six examined sites of sarin for joining to Ti -decorated GY, oxygen of carbonyl group is the best site. In these systems, charge transfer happens from sarin and metal atom to GY sheet. Finally, our investigation shows that Ti-decorated GY can be used as a promising candidate for sensing and capturing applications of CWAs such as Sarin.

کلمات کلیدی:

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