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PII: S0167-7322(17)31041-3  
DOI: doi: [10.1016/j.molliq.2017.05.020](https://doi.org/10.1016/j.molliq.2017.05.020)  
Reference: MOLLIQ 7312

To appear in: *Journal of Molecular Liquids*

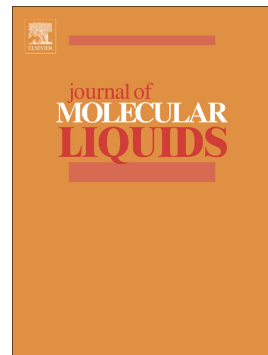
Received date: 9 March 2017

Revised date: 27 April 2017

Accepted date: 6 May 2017

Please cite this article as: Ali Shokuhi Rad, Khurshid Ayub , Adsorption of thiophene on the surfaces of X<sub>12</sub>Y<sub>12</sub> (X=Al, B, and Y=N,P) nanoclusters; A DFT study, *Journal of Molecular Liquids* (2017), doi: [10.1016/j.molliq.2017.05.020](https://doi.org/10.1016/j.molliq.2017.05.020)

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## Adsorption of thiophene on the surfaces of $X_{12}Y_{12}$ ( $X=Al, B$ , and $Y=N,P$ ) nanoclusters; A DFT study

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### Abstract

Density functional theory (DFT) calculations are performed to study the response of  $X_{12}Y_{12}$  nanoclusters ( $Al_{12}N_{12}$ ,  $Al_{12}P_{12}$ ,  $B_{12}N_{12}$ , and  $B_{12}P_{12}$ ) towards adsorption of thiophene molecule. The interaction energies of thiophene on nanoclusters are evaluated with long range and dispersion corrected ( $\omega$ B97XD and M06-2X), and conventional non-corrected (B3LYP) methods in order to estimate the dispersion effects. The dispersion corrected ( $\omega$ B97XD) binding energies of thiophene on  $Al_{12}N_{12}$  and  $Al_{12}P_{12}$  are  $-60.4$  and  $-45.0$  kJ mol<sup>-1</sup>, respectively. The corresponding non-corrected binding energies calculated at B3LYP method are  $-43.6$  and  $-30.3$  kJ mol<sup>-1</sup>, respectively. Thiophene is physisorbed on B-containing surfaces where binding energies are  $-10.4$ ,  $-8.3$  ( $\omega$ B97XD) and  $-6.3$  and  $-4.1$  (B3LYP) kJ mol<sup>-1</sup> for  $B_{12}N_{12}$  and  $B_{12}P_{12}$ , respectively. Changes in electronic properties such as HOMO-LUMO gap, Fermi level and densities of states are also analyzed to realize the sensing ability of nanoclusters for thiophene molecule. Among all the studied nanoclusters,  $Al_{12}N_{12}$  is the strongest adsorbent for thiophene whereas  $B_{12}N_{12}$  shows the highest change in the electronic structure when a thiophene molecule is adsorbed.

**Keywords:** Nanocluster; Thiophene; Sensor; Electronic properties; Density functional theory

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