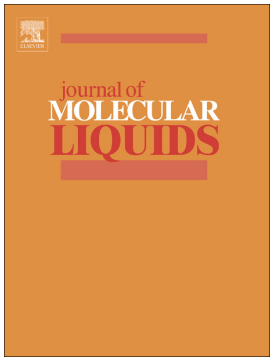

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Adsorption of thiophene on the surfaces of $X_{12}Y_{12}$ (X=Al, B, and Y=N,P) nanoclusters; A DFT study

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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 (ωB97XD and M06-2X), and conventional non-corrected (B3LYP) methods in order to estimate the dispersion effects. The dispersion corrected (ωB97XD) binding energies of thiophene on $Al_{12}N_{12}$ and $Al_{12}P_{12}$ are −60.4 and -45.0 kJ mol^{-1}, respectively. The corresponding non-corrected binding energies calculated at B3LYP method are -43.6 and -30.3 kJ mol^{-1}, respectively. Thiophene is physisorbed on B-containing surfaces where binding energies are −10.4, -8.3 (ωB97XD) and -6.3 and -4.1 (B3LYP) kJ mol^{-1} 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*