عنوان مقاله:

DFT investigation of the para-nitrophenol adsorption on phosphorus-doped polypyrrole

محل انتشار:

ششمین کنگره ملی شیمی و نانو شیمی از پژوهش تا توسعه ملی (سال: 1402)

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خلاصه مقاله:

In this study, the adsorption of para-nitrophenol on phosphorus-doped polypyrrole was investigated using density functional theory (DFT). Calculations are performed at two levels b۳lyp/۶-۳۱+G(d, p) and wb۹۷xd/۶-۳۱+G(d, p), for two orientations of adsorbate molecule. The correlation-exchange function wb۹۷xd shows more negative adsorption energy for the adsorption of these compounds. Evaluation of energy level changes, hardness, chemical potential, softness, electrophilicity, diploe moment, charge transfer by Molliken method and natural bond orbitals (NBO), adsorption energy, the density of states (DOS) diagrams, molecular electrostatic potential (MEP), Intermolecular distances and analysis of non-covalent interactions (NCI) have been performed. Analysis of non-covalent interactions shows more van der Waals interactions between adsorbent and adsorbate in the wb۹۷xd correlation-exchange function compared to b۳lyp.

کلمات کلیدی:

Adsorption, para-nitrophenol, phosphorus -doped polypyrole,Density functional theory