

## عنوان مقاله:

Computational studies on the Li-B12N12 as potential adsorbent for aniline from environment

## محل انتشار:

چهارمین کنفرانس علوم و فناوری شیمی کاربردی حسگرها و زیست حسگرها (سال: 1399)

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## خلاصه مقاله:

Aniline ( $C_6H_5NH_2$ ) is an important organic compound due to its wide applications in the manufacturing of dyestuffs, rubbers, pesticides, plastics and paints. Aniline is released throughout the environment by industrial wastewater and/or through degradation of some of the above mentioned compounds. Adsorption of aniline molecule on the surface of Li-encapsulated B12N12 nanocage is scrutinized using at Density functional theory (DFT) calculations to investigating its potential as chemical adsorbent. DFT calculations at the B3LYP /6-31G\* level were performed in terms of energetic, geometric, and electronic properties. People had shown that piristin nanocages are weak absorbents. In order to improve the properties of the nanocage adsorbent, Li encapsulating process was investigated. The obtained results show that encapsulating process changes electrical properties of B12N12 dramatically. It was found that aniline is more likely adsorbed via its nitrogen atom on the Li-B12N12 surface. The adsorption energy of aniline on the nanocage in the most stable state is -45.06 kcal/mol and about 0.38|e| is transferred from the aniline molecule to the nanocage. It is expected that Li-encapsulated B12N12 acts as new potential nanosensor for toxic aniline molecules from environmental systems.

## کلمات کلیدی:

Boron nitride nanocage, aniline, adsorbent, electronic structures

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