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# Explorations of structural and electronic features of an enhanced iron-doped boron nitride nanocage for adsorbing/sensing functions of the hydroxyurea anticancer drug delivery under density functional theory calculations

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## Abstract

An iron-doped boron nitride (FBN) nanocage was investigated for adsorbing/sensing the hydroxyurea (Hyd) anticancer for the smart and targeted drug delivery processes. Optimizations were done under density functional theory (DFT) calculations and the properties were obtained. Interaction of Hyd with each of FBN and BN nanocages yielded four configurations of Hyd@FBN and Hyd@BN complexes. The FBN nanocage surface was found better for interacting with the Hyd counterpart; stronger Hyd@FBN complexes than the Hyd@BN complexes were obtained. The electronic frontier molecular orbital features showed a stronger tendency of complex formations for the FBN nanocage by a shorter energy gap for a better interaction with the Hyd substance. The adsorbing features indicated a meaningful recovery time and those of sensing features indicated a meaningful conductance rate for the investigated FBN nanocage. As a consequence, the FBN nanocage was proposed for involving in the drug delivery processes but still requiring further investigations. © 2023 Elsevier B.V.

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Adsorbing; Boron nitride; DFT; Drug delivery; Nanocage; Sensing

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# A novel pentagonal BCN monolayer for sensing and drug delivery of nitrosourea and hydroxyurea anticancer drugs: A DFT outlook

Rahimi, Rezvan<sup>a, b</sup>✉ ; Solimannejad, Mohammad<sup>a, b</sup>✉[Save all to author list](#)<sup>a</sup> Department of Chemistry, Faculty of Science, Arak University, Arak, 38156-8-8349, Iran<sup>b</sup> Institute of Nanosciences and Nanotechnology, Arak University, Arak, 38156-8-8349, Iran[Full text options ▾](#)[Export ▾](#)**Abstract****Author keywords****Indexed keywords****Sustainable Development Goals 2023****SciVal Topics****Metrics****Abstract**

In the present investigation, the capability of the pristine pentagonal BCN (penta-BCN) nanosheet for sensing and drug delivery of the nitrosourea and hydroxyurea anticancer drugs has been examined through the periodic density functional theory. The adsorption and sense effect of these drug molecules on the structural and electronic virtues of the substrate are analyzed. The energy gap has been reduced by 57.63 % and 19.96 % after adsorbing the nitrosourea and hydroxyurea anticancer drugs respectively, so the penta-BCN nanosheet shows an electrical response to the presence of these drugs. The adsorption energy in the gas/water phases for the most stable nitrosourea/BCN and hydroxyurea/BCN complexes are -2.7/-1.21 and -2.53/-1.96 eV, respectively. The solvability of the drug, the surface, and the complexes in the aqueous solvent have also been examined. The thermal and dynamical stability of the structures at room temperature, by results of the NVT module of the molecular dynamics, has been confirmed. The drug release from the substrate near the target cells in an acidic environment has also been simulated. We can propose a pristine penta-BCN substrate as a potential carrier and sensor of nitrosourea and hydroxyurea anticancer drugs. © 2024 Elsevier Ltd

**Author keywords**

Drug delivery; Hydroxyurea; Nitrosourea; Penta-BCN; Sensor

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