

4 documents have cited:

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

Saadh M.J., Mirzaei M., Abdullaeva B.S., Maaliw III R.R., Da'i M., Salem-Bekhit M.M., Akhavan-Sigari R.

(2023) Physica B: Condensed Matter, 671 , art. no. 415445

Search within results...

Refine results

Limit to Exclude

Open Access

All Open Access (2)

Gold (2)

Learn more

Year

2024 (2)

2023 (2)

Author name

Da'i, M. (3)

Mirzaei, M. (3)

Maaliw, R.R. (2)

Saadh, M.J. (2)

Salem-Bekhit, M.M. (2)

Ahmed, H.H. (1)

Al Zahrani, S. (1)

Alhabib, N.A. (1)

Alwan, M. (1)

Dhiaa, S.M. (1)

View less View all

Subject area

Materials Science (4)

Physics and Astronomy (4)

Chemistry (3)

Biochemistry, Genetics and Molecular Biology (2)

Engineering (2)

Document type

Article (4)

Source title

Chemical Physics Impact (2)

Diamond And Related Materials (1)

Materials Science In Semiconductor Processing (1)

Analyze search results

Show all abstracts Sort on: Date (newest)

All

Export

Download

View citation overview

View cited by

Save to list

	Document title	Authors	Year	Source	Cited by
<input type="checkbox"/> 1	A novel pentagonal BCN monolayer for sensing and drug delivery of nitrosourea and hydroxyurea anticancer drugs: A DFT outlook	Rahimi, R., Solimannejad, M.	2024	Materials Science in Semiconductor Processing 173,108109	0
<div>Hide abstract View at Publisher Related documents</div> <div><p>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.</p></div>					
<input type="checkbox"/> 2	Density functional theory assessments of an iron-doped graphene platform towards the hydrea anticancer drug delivery	Saadh, M.J., Mirzaei, M., Dhiaa, S.M., (...), Da'i, M., Salem-Bekhit, M.M.	2024	Diamond and Related Materials 141,110683	1
<div>View abstract View at Publisher Related documents</div>					
<input type="checkbox"/> 3	Computational assessments of sumanene-hydroxyurea conjugations for proposing a novel drug design and delivery platform	Saadh, M.J., Mirzaei, M., Ahmed, H.H., (...), Maaliw III, R.R., Da'i, M.	2023	Chemical Physics Impact 7,100365	0
<div>View abstract View at Publisher Related documents</div>					
<input type="checkbox"/> 4	Metal-doped fullerenes as promising drug carriers of hydroxycarbamide anticancer: Insights from density functional theory	Salem-Bekhit, M.M., Al Zahrani, S., Alhabib, N.A., (...), Da'i, M., Mirzaei, M.	2023	Chemical Physics Impact 7,100347	3
<div>View abstract View at Publisher Related documents</div>					

Display: 20 results per page

1

Top of page