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An enhanced adsorption of paracetamol drug using the iron-encapsulated boron carbide nanocage: DFT outlook

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Abstract

By various importance of paracetamol (PMOL) drug adsorption from environmental issues to drug overdose abasement, the current work was done to recognize the capability of an iron-encapsulated boron carbide (FBC) nanocage for working as a suitable adsorbent. Density functional theory (DFT) calculations were performed to stabilize the structures for being analyzed regarding the structural and electronic features. Accordingly, the results indicated a higher strength of formation for the PMOL@FBC complex in comparison with the PMOL@BC complex. Additionally, the variations of molecular orbital features indicated a higher sensitivity of detection of PMOL substance by the assistance of FBC nanocage. As a final remark, this claim "the iron-encapsulation yielded an enhanced boron carbide nanocage for better adsorbing the paracetamol drug" was affirmed by both of structural and electronic analyses revealing the importance of iron-encapsulation for approaching a better result of PMOL drug adsorption by the assistance of FBC nanocage. © 2023 Elsevier B.V.

Author keywords

Boron carbide; Drug detection; Molecular adsorption; Nanocage; Paracetamol

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This research explores how two-dimensional honeycomb materials can be used in advanced electronics, focusing on zigzag honeycomb nanoribbons. These nanoribbons can create zero-energy band gaps, enabling helical spin current edge states. The study investigates the quantum spin Hall state, showcasing the adaptability of the Kane-Mele model in various honeycomb lattices. In addition to the theoretical discussions, this study presents a detailed Hamiltonian, performs band structure computations, and introduces a novel spin-filtering technique for zigzag nanoribbons. This method enhances our understanding of edge-localized quantum states and can revolutionize spintronics. By revealing the quantum states in honeycomb nanoribbons, this study contributes to the advancement of electronics and offers a promising path for highly efficient spin-based technologies.

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Quantum spin hall effect on pseudo-graphene zigzag nanoribbons

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Abstract

This research explores how two-dimensional honeycomb materials can be used in advanced electronics, focusing on zigzag honeycomb nanoribbons. These nanoribbons can create zero-energy band gaps, enabling helical spin current edge states. The study investigates the quantum spin Hall state, showcasing the adaptability of the Kane-Mele model in various honeycomb lattices. In addition to the theoretical discussions, this study presents a detailed Hamiltonian, performs band structure computations, and introduces a novel spin-filtering technique for zigzag nanoribbons. This method enhances our understanding of edge-localized quantum states and can revolutionize spintronics. By revealing the quantum states in honeycomb nanoribbons, this study contributes to the advancement of electronics and offers a promising path for highly efficient spin-based technologies. © 2024 The Authors.

Author keywords

Haldane Model; Kane-Mele Model; Pseudo-Graphene; Quantum Spin Hall Effect; Topological Insulator; Two-Dimensional Honeycomb Materials; Zigzag Nanoribbon

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