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Abstract

CO2 switching on g-B4N3 nanosheet for industrial applications: Decorated by alkaline earth elements

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Abstract:
The adsorption and desorption of carbon dioxide (CO2) molecule based on switching process along with graphite boron nitride (g-B4N3) nanosheet with additional group II elements have been analyzed in support of density functional theory (DFT) calculations with long-range correlation (DFT+D2). The Graphite boron nitride (g-B4N3) nanosheet with additional group II elements is like sorbent materials, which have been implemented to understand the switchable process of CO2 molecule. The electron mobility, electronic properties, charge accumulation, charge transfer (e-) and adsorption energy (Kcal/mol) have also been computed to understand the switching process. The gB4N3 nanosheet yields a high carrier mobility (8020 cm2 V-1s -1) at 300 K and formation energy (-6.67 eV/atom). The switching of CO2 can be easily controlled by positive adatoms on the nanosheet of gB4N3 and the greenhouse gas CO2 capture/release gets spontaneously without any external energy. Therefore, due to the weak absorption of CO2, it makes possible to uncharged the g-B4N3 nanosheet and show switching process. In contrast, these negatively charged g-B4N3 nanosheets are highly selective for switching CO2.

Biography:
Shivam Kansara has his expertise in computational material science to work in the novel materials in major society applications. Mainly he is working on a low dimensional system for energy applications. He had done various work on strain engineering, optical and magnetic materials, etc. His current project is a Hydrogen fuel cell and charge storing for energy applications. He is focused on the electronic, optical, thermal, transport, electrochemical properties, etc. of materials. The dynamic stability of low-dimensional materials will be impacted toward the next generation which is one of the key issues in energy saving, energy transfer, compact designs, and different operational properties.

Publication of speakers:

- Shivam Kansara et al ; Free-standing Pt and Pd nanowires: strain-modulated stability and magnetic and thermoelectric properties, 2018 Nov 14.
- Shivam Kansara et al ; Modeling of diameter-dependent Fe and Co ultrathin nanowires from first-principles calculations, 2017 Jun 14.
- Shivam Kansara et al ; Toward dental caries: Exploring nanoparticle-based platforms and calcium phosphate compounds for dental restorative materials, 2018 Dec 18.
- Shivam Kansara et al ; Monitoring characteristics and genotoxic effects of engineered nanoparticle-protein corona, 2017 Oct 17.
- Shivam Kansara et al ; Synthesis of biocompatible iron oxide nanoparticles as a drug delivery vehicle, 2018 Mar 15.

Webinar on Nanomaterials, November 28, 2020; Dubai, UAE.

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