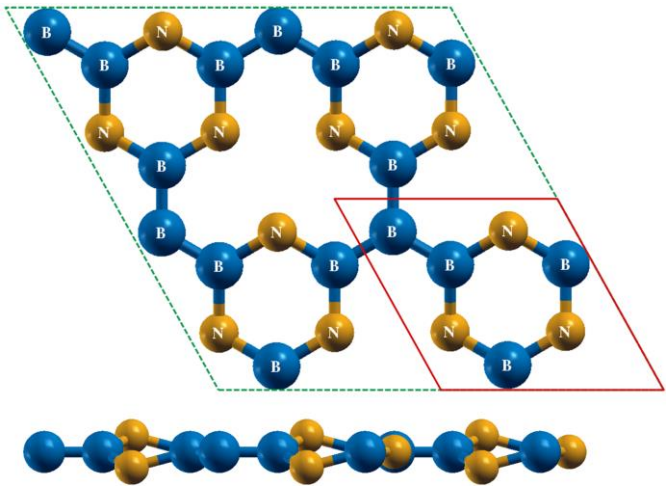
CO_2 switching on g-B_4N_3 nanosheet for industrial applications: Decorated by alkaline earth elements

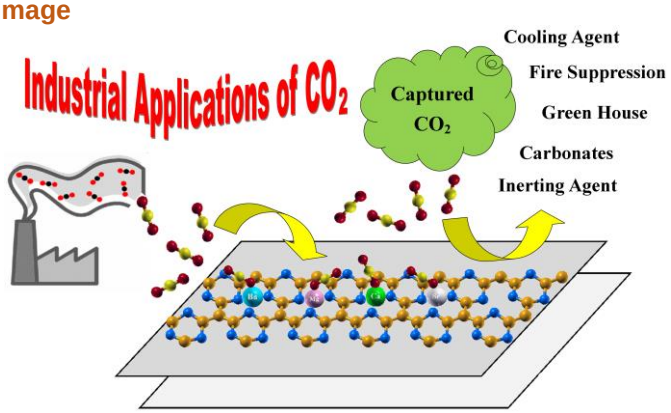
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Abstract

The adsorption and desorption of carbon dioxide (CO_2) molecule based on switching process along with graphite boron nitride (g-B_4N_3) nanosheet with additional group II elements have been analyzed in support of density functional theory (DFT) calculations with long-range correlation (DFT+D_2). The Graphite boron nitride (g-B_4N_3) nanosheet with additional group II elements is like sorbent materials, which have been implemented to understand the switchable process of CO_2 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 g-B_4N_3 nanosheet yields a high carrier mobility (≈8020 $cm^2\ V^{-1}s^{-1}$) at 300 K and formation energy (-6.67 eV/atom). The switching of CO_2 can be easily controlled by positive adatoms on the nanosheet of g-B_4N_3 and the greenhouse gas CO_2 capture/release gets spontaneously without any external energy. Therefore, due to the weak absorption of CO_2, it makes possible to uncharged the g-B_4N_3 nanosheet and show switching process. In contrast, these negatively charged g-B_4N_3 nanosheets are highly selective for switching CO_2.



Image



Recent Publications (minimum 5)

1. Iguchi, S., Hasegawa, Y., Teramura, K., Hosokawa, S., & Tanaka, T. (2016). Preparation of transition metal-containing layered double hydroxides and application to the photocatalytic conversion of CO2 in water. Journal of CO2 Utilization, 15:6-14.
2. Chu, S., & Majumdar, A. (2012). Opportunities and challenges for a sustainable energy future. nature, 488: 294-303.
3. Liu, J., Thallapally, P. K., McGrail, B. P., Brown, D. R., & Liu, J. (2012). Progress in adsorption-based CO 2 capture by metal–organic frameworks. Chemical Society Reviews, 41:2308-2322.
4. Mishra, A. K., & Ramaprabhu, S. (2012). Nanostructured polyaniline decorated graphene sheets for reversible CO 2 capture. Journal of Materials Chemistry, 22:3708-3712.
5. Sun, Q., Li, Z., Searles, D. J., Chen, Y., Lu, G., & Du, A. (2013). Charge-controlled switchable CO2 capture on boron nitride nanomaterials. Journal of the American Chemical Society, 135:8246-8253.
6. X. Tan, L. Kou, H.A. Tahini, S.C. Smith, Conductive Graphitic Carbon Nitride as an Ideal Material for Electrocatalytically Switchable CO2 Capture. Sci. Rep. 5 (2015) 17636.



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.

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