Boron-rich enhanced ambient CO_2 capture and storage of boron–carbon–nitride hybrid nanotubes

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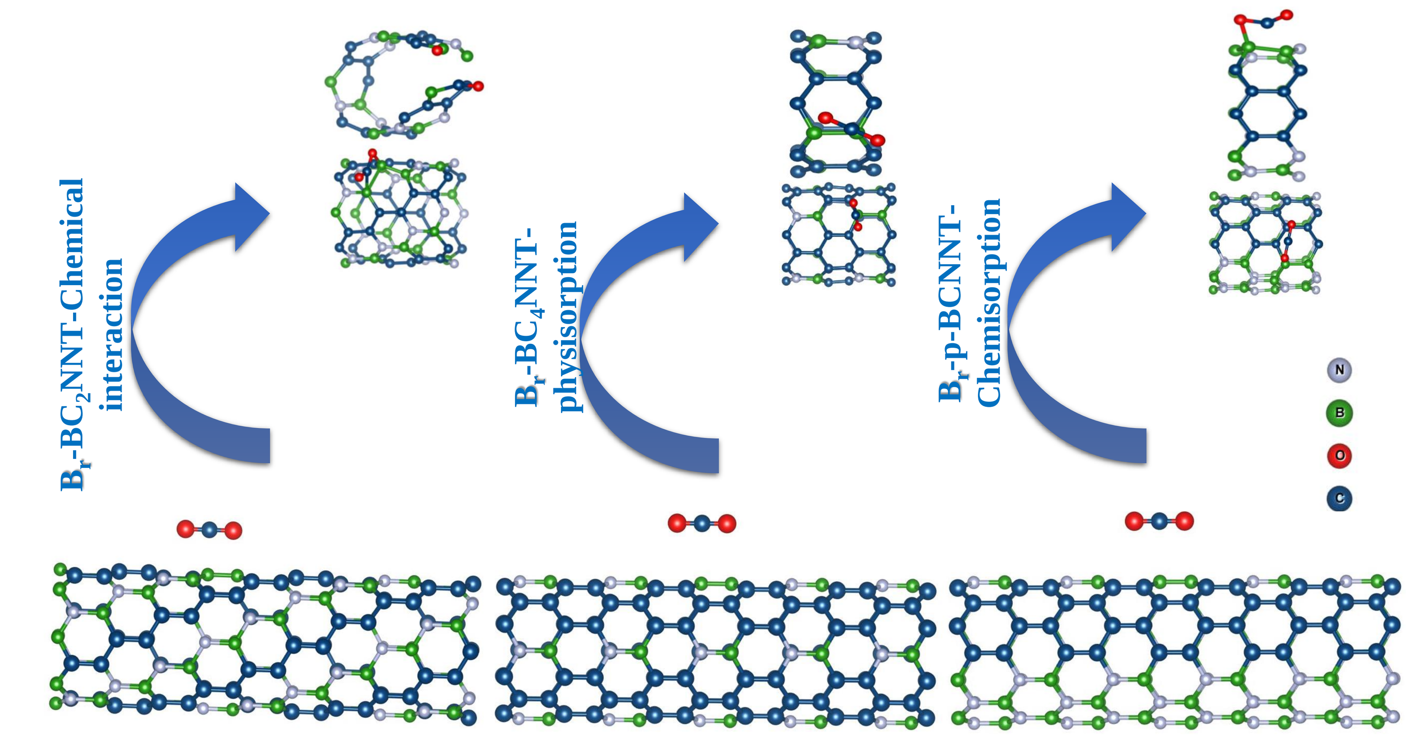
Abstract

Increasing carbon dioxide (CO_2) emissions as the most challenging greenhouse gas is considered as a major cause of global warming and ocean acidification. Different strategies against anthropogenic emissions of CO_2 have been applied to capture and reduce the CO_2 effect on the atmosphere. To this end, we study the adsorption of CO_2 on boron-rich structures of boron–carbon–nitride (BCN) hybrid nanotubes by the implementation of an ab initio approach based on density functional theory (DFT). Three different boron-rich BC_2NNT, BC_4NNT, and parallel BCN (p-BCN) nanotubes are investigated as hosts for the capture and sequestration of CO_2. The analysis of calculations shows that the boron-rich BC_4N nanotube adsorbs CO_2 physically, while in the boron-rich BC_2N and p-BCN nanotubes, both chemisorption and physisorption occurred. In the chemisorption process, a linear CO_2 molecule is bent over, and a new bond is formed between oxygen and boron antisite (BN) in boron-rich nanotubes due to electron back donation between CO_2 and nanotubes as a result of orbital mixing of oxygen and boron atoms. Moreover, our findings show that the sensitivity factor (SF) and adsorption energy for boron-rich BC_2N nanotubes are higher than those of other hybrid nanotubes and CO_2 free energy at room temperature. Elaborating on the stability and recycling of host material challenges suggests that the boron-rich hybrid nanotubes could be a good candidate for capturing CO_2 under ambient conditions



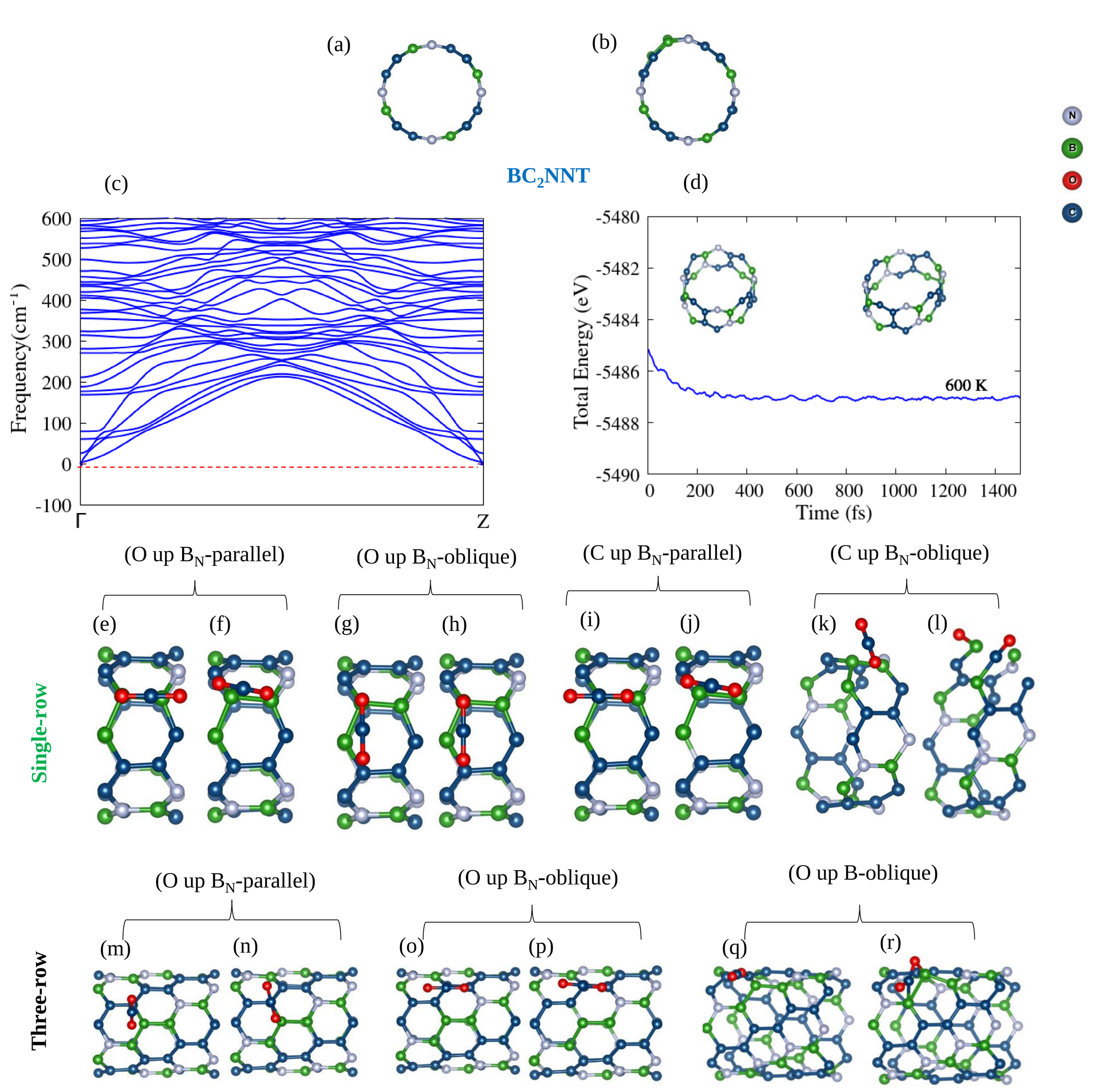
Graphical Abstract

Objectives

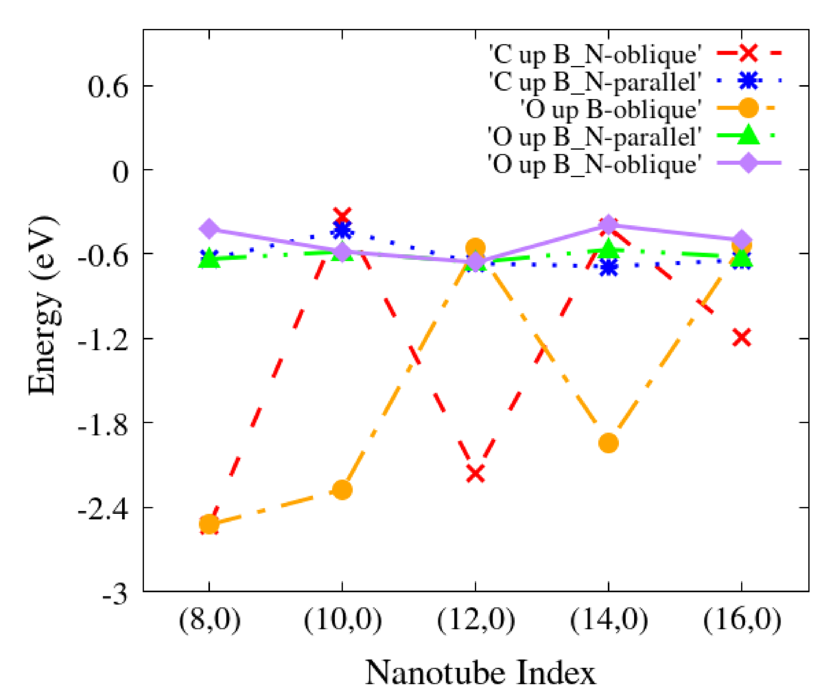
Investigating the hybrid nanotubes (boron-carbon-nitride) as ambient CO_2 adsorbents.

Materials & Methods

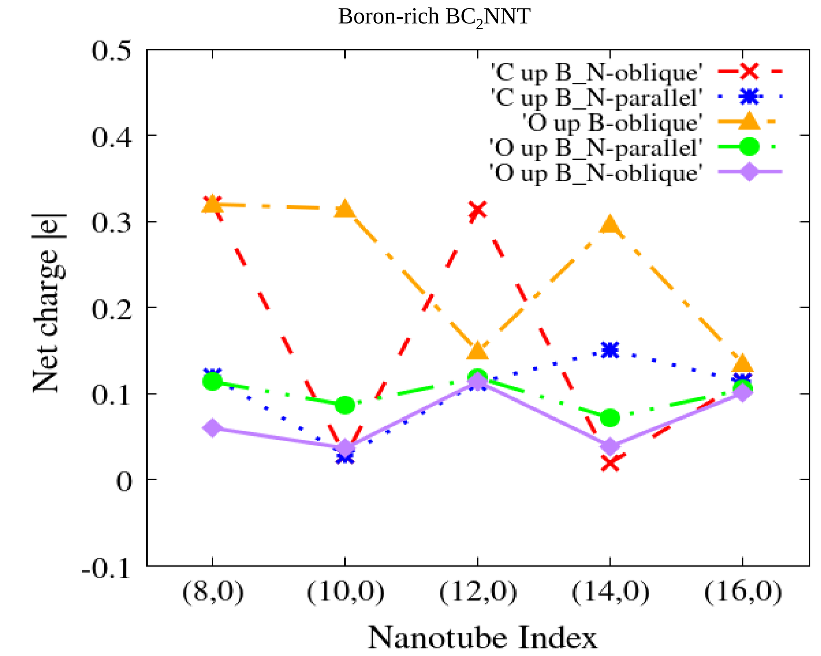
- Boron rich BC_2N, BC_4N and p-BCN nanotubes
- Density Functional Theory (DFT)



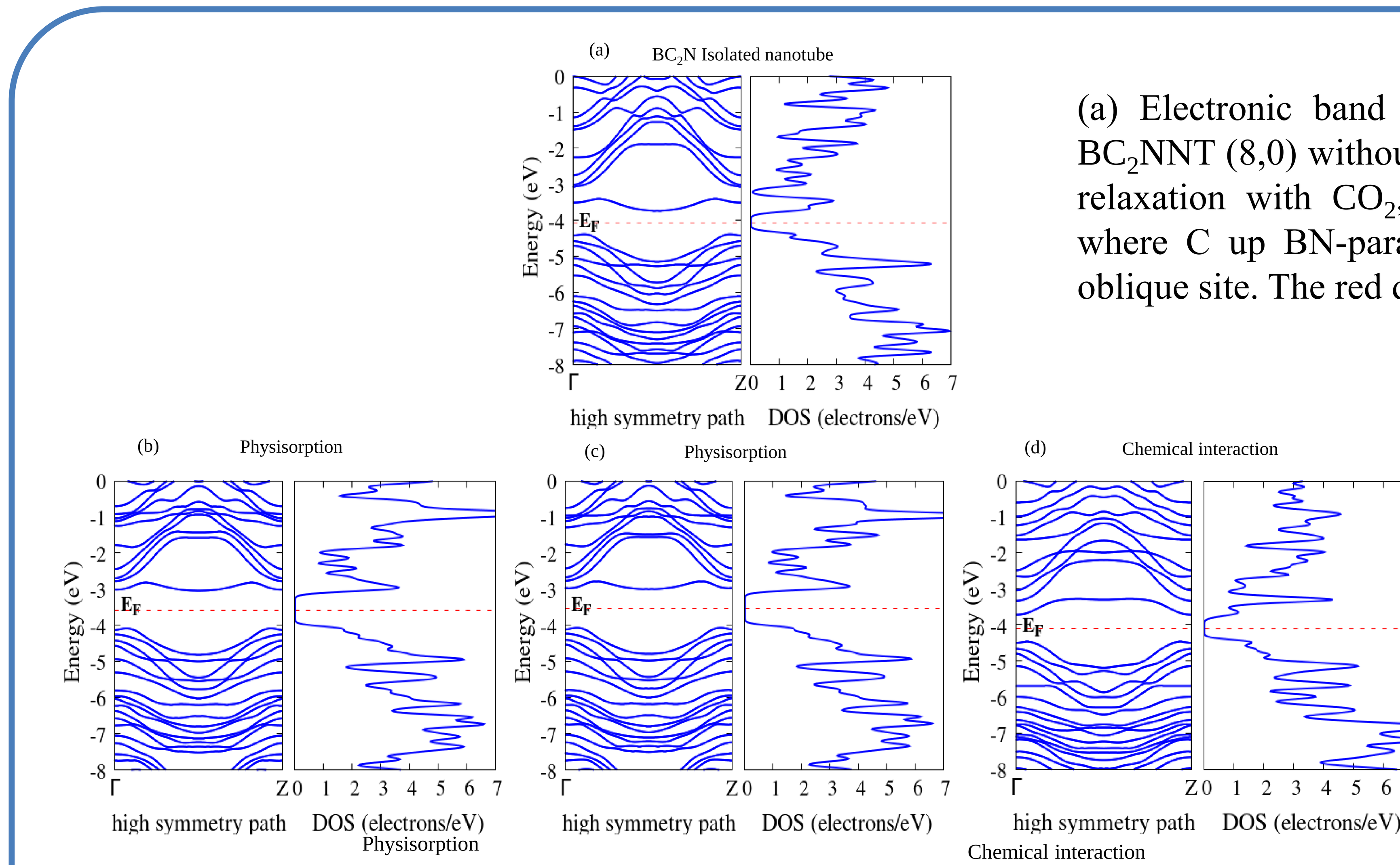
The geometric configuration of single-row and three-row BC_2NNT (8,0) before and after adsorption.



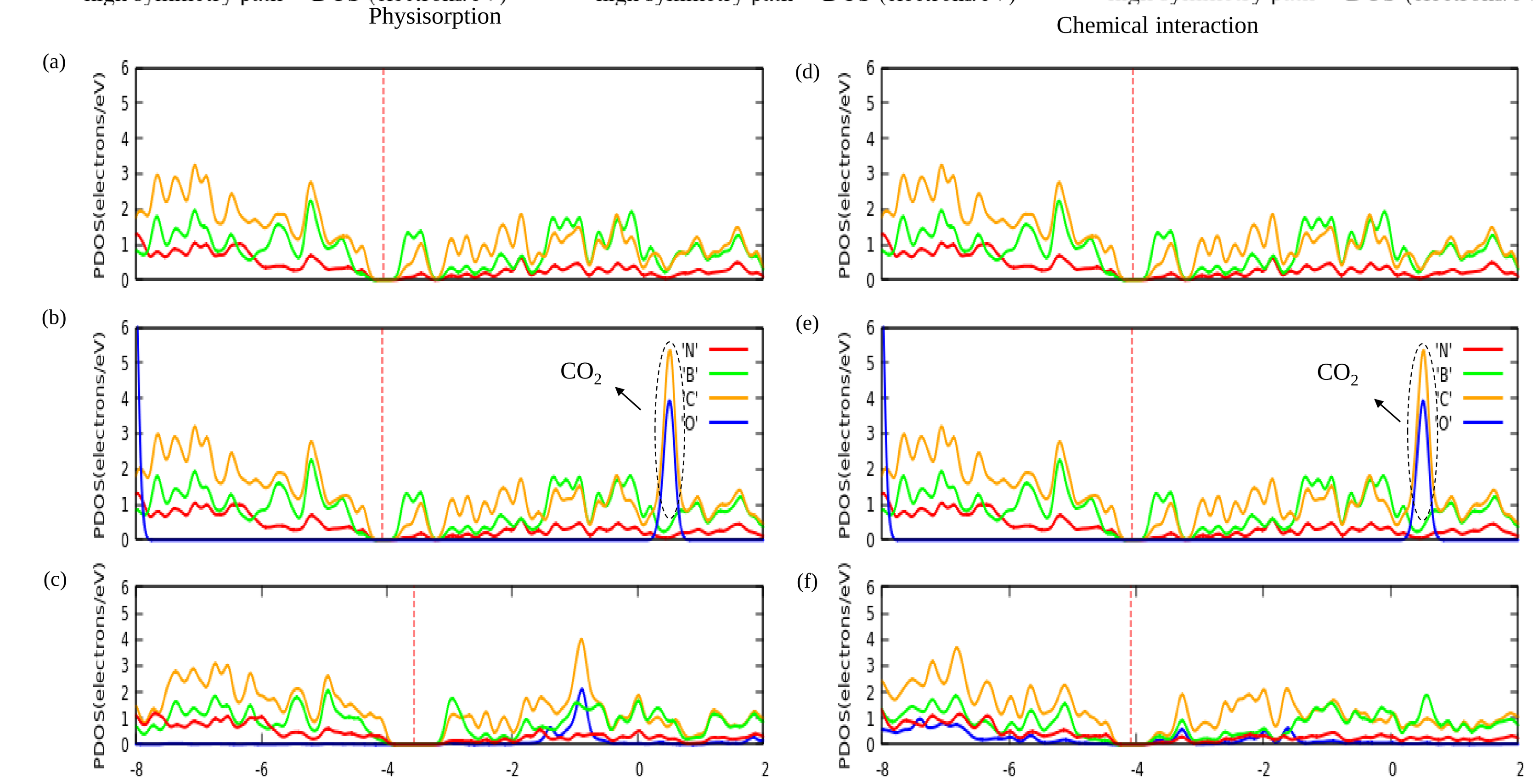
Variation of adsorption energy at different radii and sites of boron-rich BC_2NNT



The amount of charge transferred between CO_2 molecule and BC_2NNT



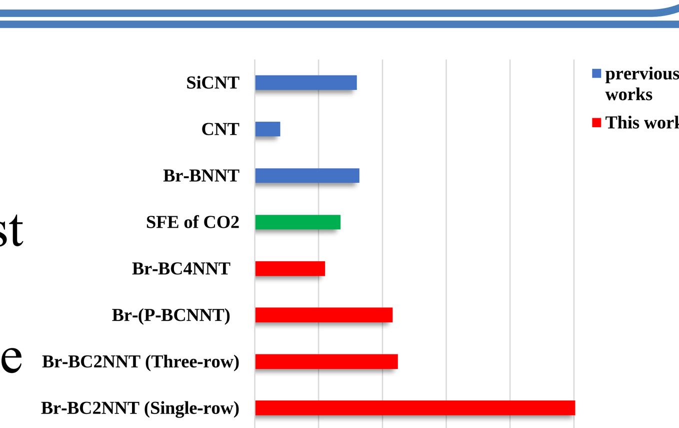
(a) Electronic band structure and TDOS of boron-rich BC_2NNT (8,0) without CO_2 before relaxation and (b) after relaxation with CO_2, where O up BN-parallel site, (c) where C up BN-parallel site, and (d) where C up BN-oblique site. The red dashed lines show the Fermi level



PDOS of boron-rich BC_2NNT (8,0) nanotubes for (a) and (d) isolated nanotubes, (b) and (e) where CO_2 is placed at 7.4 Å far from the nanotube, (c) for the physisorption process, where O up BN-parallel site, and (f) for chemical interaction, where C up BN-oblique site. The red dashed lines show the Fermi level

Conclusions

- This work proposes new three hybrid nanotubes based on B-C-N for CO_2 adsorption.
- The structural stability, adsorption energy and charge transfer were calculated by first principles method.
- The calculations indicate that chemisorption occurred in BC_2NNT and p-BCN, while physisorption happened in BC_4NNT adsorption process..



Reference:

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