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Boron-rich enhanced ambient CO2capture and storage of boron–carbon–nitride hybrid nanotubes

Increasing carbon dioxide (CO2) 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 CO2 have been applied to capture and reduce the CO2 effect on the atmosphere. To this end, we study the adsorption of CO2 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 BC2NNT, BC4NNT, and parallel BCN (p-BCN) nanotubes are investigated as hosts for the capture.