عنوان مقاله:

Compariso n of H۲, C H۴ and C O۲ gas adsorption o n Boron N itride Nanoscrolls

محل انتشار:

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خلاصه مقاله:

Nanomet ric structures have be en intensively studied during the last years. Carbon-base d materials are among the most investigated in literature, but science ۱۹۶۰s there are very few works on Carbon Nanoscroll (C NSs).In principle, CNSs and boron ni tride nanoscroll (BNSs) can be form ed by rollin g up graphite and boro n nitride layers. Nano scrolls can be formed tubular and conical, al so depend o n wrapping angle of s heet aroun d the axis, we can have three for ms: (armchair, chiral an d zigzag).As we know, one i mportant cha racteristic is that nanos crolls occupy consider able high an d fully accessible surfa ce area. Th ese features are potentially advantage to adsorption storage of gases. B ecause of the novel scro ll topology, their prope rties differ from single wall or multi wall nan otubes. On the basis of the previous works, it seems that nanoscrolls with a n expansion of interla yer spacin g could be very promising materials for gas storage, for hydrogen storage the highest binding energy was found for the ۲Å distance.

کلمات کلیدی:

DFT, BN nanoscroll, Gas stora ge, MPW۱P۹۱

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