Efficient adsorption of super greenhouse gas (tetrafluoromethane) in carbon nanotubes

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IS. Infinite Bundle of Single-Walled Carbon Nanotubes

To simulate the adsorption of tetrafluoromethane in an infinitely long bundle of SWNTs we adopted a cubic simulation box of size: $m \cdot n \cdot 10\sigma_{ff}$ ($\sigma_{ff} = 4.7$ Å, n and m box sizes were adjusted to keep the intra-tube distance) with periodic boundary conditions in all directions (1,2), as displayed in Figure 1S. For the computation of molecular interactions we used the minimum image convention (1,2). In the cubic simulation box we placed an idealized hexagonal bundle of investigated SWNTs consisting of 11 rigid tubes (3), as shown on Figure 1S. Following the previous studies and experimental reports we used a van der Waals gap of 4 Å between the individual SWNTs (3). On the Figure 1S we presented correct as well as incorrect construction of the simulation model for idealized hexagonal bundle of SWNTs. Note that due to applied periodic boundary conditions and minimum image convention only case (E) represents the idealized hexagonal arrangement of carbon nanotubes. The total number of carbon tubes composed our simulation model is six, as displayed on Figure 1S. However, it is not mean that these hexagonally arranged carbon nanotubes are equivalent to six isolated ones since besides the presence of interstitial channels our adsorbed molecules exerted an additional potential from molecules adsorbed in other places of the bundle as well as from all cylindrical carbon surfaces. Moreover, in an idealized SWNTs bundle the ratio of inaccessible spaces to the total pore volume is different in comparison to isolated nanotubes. Models form (A) to (B) present some other arrangement of individual SWNTs characteristic for defected hexagonal assembly.

References

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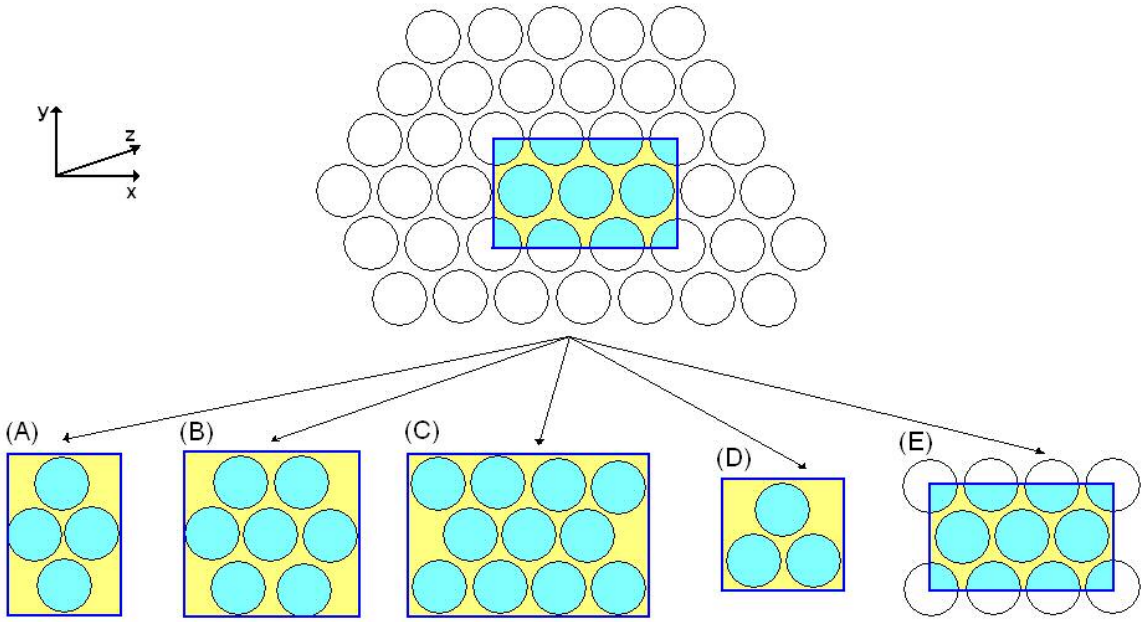

Figure 1S. Idealized model of SWNTs bundle composed of infinitely long cylindrical nanotubes arranged into hexagonal lattice. The incorrect construction of the simulation model of hexagonally assembled SWNTs is displayed on panels (A)-(D). Panel (E) showed correct construction of an idealized hexagonal SWNTs assembly used in the current theoretical study.

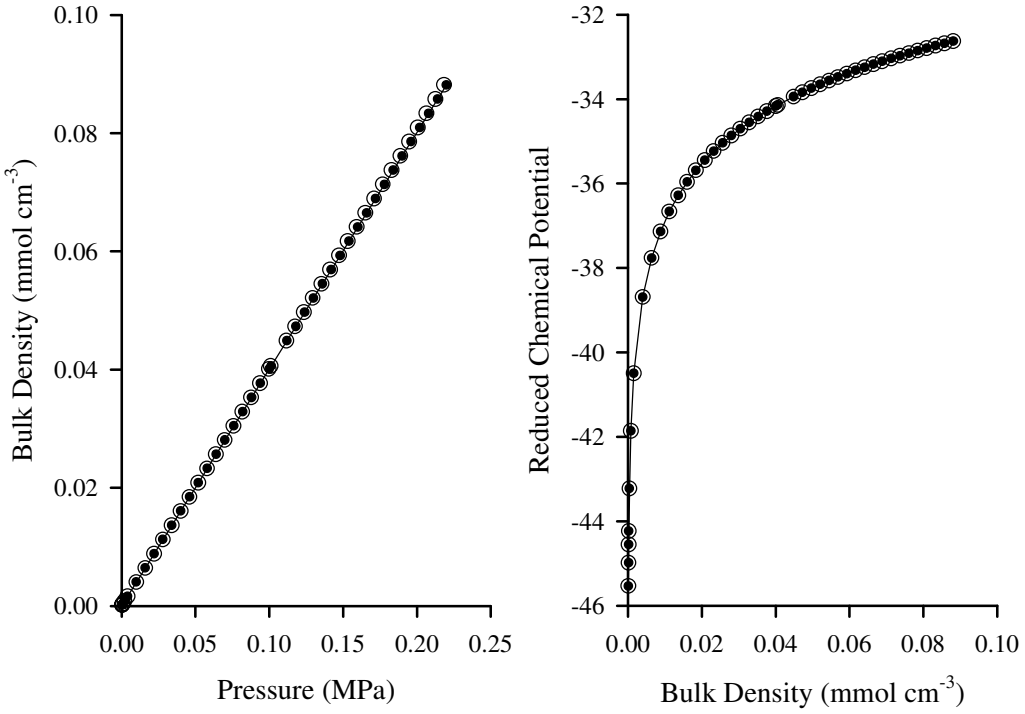

Figure 2S. Phase diagram (left panel) and variation of chemical potential versus bulk density (right panel) for carbon tetrafluoride at 300.15 K computed from modified Benedict-Webb-Rubin equation of state (filled circles) and Widom's particle insertion method (open circles).