Interaction of H_2 and CO with zinc oxide nanotubes

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Zinc oxide is a material widely used as a gas sensor, varistor, photoelectric cell as well as other semiconductor, optical and catalytic applications. Consequently, the ZnO nanotubes are widely used in the scientific-technological environment. In this work we have analyzed the interaction of armchair and zigzag ZnO nanotubes with diatomic molecules H_2 and CO. We have used semi-empirical (AM1) method to study our nanotube model with 8 units of ZnO (n) and 8 levels(k). We look into the interaction of ZnO armchair and zigzag nanotubes ZnO (SWNT) with H_2 and CO on the surface of the nanotubes at localized sites in the middle and extremity of the nanotubes. We observe adsorption of the hydrogen molecules and the carbon monoxide on the surface of the nanotubes, both in the middle as well as the extremity. The molecules H_2 and CO do not dissociate upon adsorption by the nanotube. Both nanotube models become more stable when they adsorb the molecules. The armchair nanotube energy gap does not vary remaining an isolator whereas the zigzag energy gap lowers becoming a semiconductor. The charge transfer is larger in CO than in H2.

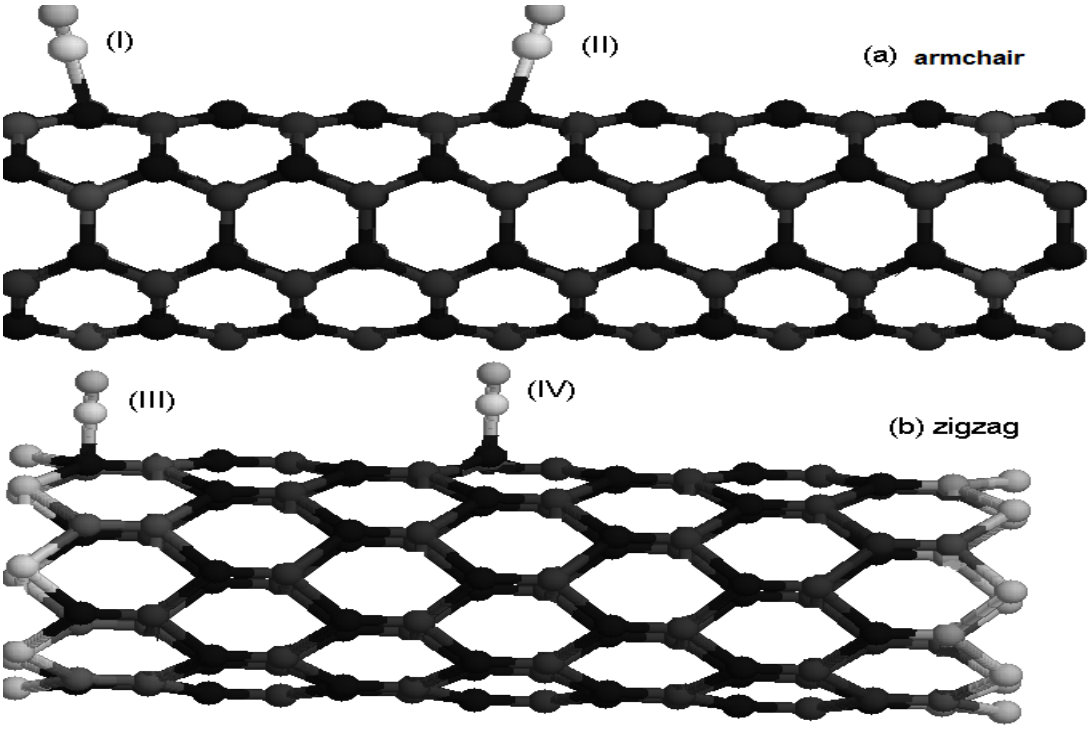

Fig. 1 Interaction of CO and H_2 with a) armchair and b) zigzag nanotubes.

References

[1] J. D. Santos, E. Longo, C. A. Taft, Journal of Molecular Structure 538 (2001) 211.