Theoretical models of zinc oxide nanotubes

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With the advent of nanoscience and nanotechnology, zinc oxide has its physical and chemical properties not only dependent on the material, but also on it`s form and structure, which increases the possibilities of technological application. The nanostructures of ZnO have semiconducting, optic, catalytic and piezoelectric properties and can also be used for gas sensors and varistors due to their structural and electronic properties. In this theoretical investigation, a nanotube model of zinc oxide is made via an appropriate algorithm analyzing its`s structural characteristics with relation to height, diameter, Zn and O bonding distance as well as quirality. Charge, polarity, conducting properties and stability are also analyzed. We created models of armchar and zigzag nanotubes using an algorithm that established spatial coordinates of the zinc atoms and oxygens of both nanotubes. We used the semi-empirical and ab-initio methods to determine for the armchair and zigzag models the total energy as well as the positions for the fixed atoms. For each structure we established a configuration of distances and the algorithm generated various structures with the same number of units, levels, configurations of distances in order to obtain the least energy. The surface gradients were also investigated. Our results indicate that increasing the size of the nanotube the Zn-O distance tends to 1.96 and 2.00 Å for armchar and zigzag respectively. Both semi-empirical and ab-initio indicated that the armchair has a greater stabililty that the zigzag structure in most cases. Both the dipole moment as well as the charge distribution indicate that the armchair nanotubes are apolar whereas the zigzag nanotubes are polar.

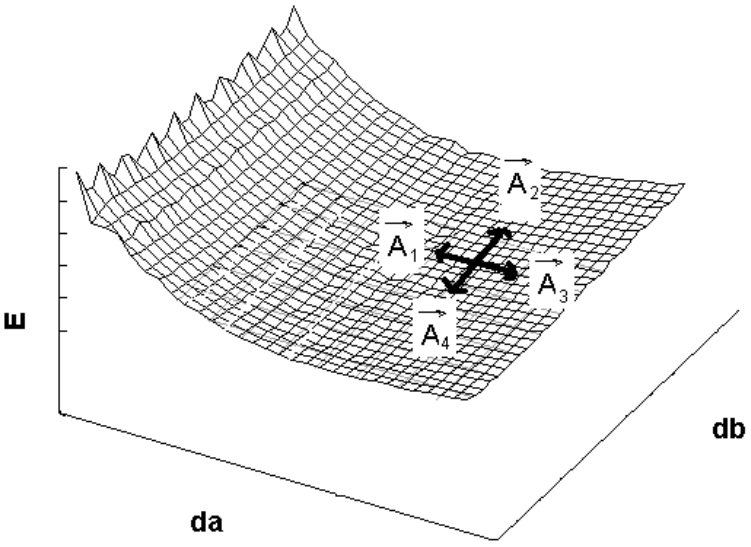

Fig. 1 Optimization surface of zigzag ZnO nanotubes with vetors $\vec{A}_i$.

References

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