Modification of the rutile plane of $[(SnO_2)_n]_m$ to a nanotube

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Abstract

One-dimensional (1D) nanomaterials, such as nanotubes and nanowires, are promising materials and they show novel physicochemical properties and potential applications in many new technologies. SnO_2 is a semiconductor with a band gap of 3,62 eV at room temperature [1].
Nanotubes of tin oxide have been widely studied. SnO_2 nanotubes are known for different applications, e.g., gas sensors, transistors, and solar cells [1, 2]. This semiconductor has been obtained as nanomaterial with a large number of morphology and properties [2, 3].There has been reported computed MgF2 nanotubes using Hartree-Fock and B3LYP methods using Huzinaga basis set [3].

The Hartree-Fock and DFT using 3-21G and Huzinaga basis set was used in order to optimize the d_{Sn-Sn}, d_{O-O}, d_{Sn-O} interatomic distances in the nanotubes SnO2 constructed using the structure [110] plane of the rutile crystal.The Figure 1 presents the various stages of doubling the SnO_2 [110] plane which optimized are stabilized forming nanotubes.

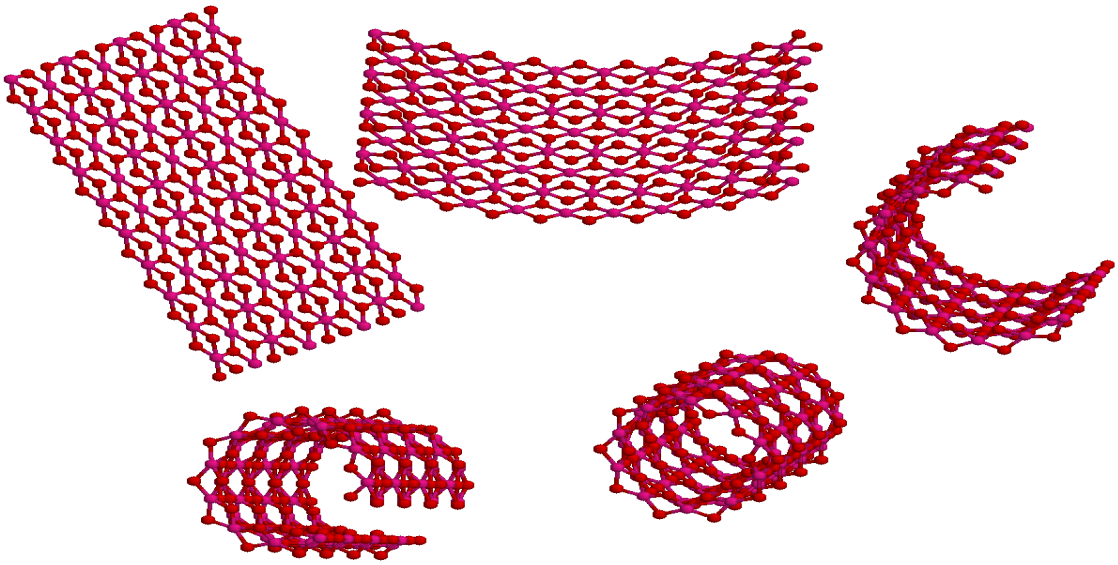

Figure 1: A modification of the (110) plane of SnO_2 for the nanotube

References

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