Ab initio quantum mechanical simulation of systems with helical symmetry: carbon and chrysotile nanotubes

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Nanotubes can be characterized by a very high point symmetry (helical groups), comparable or even larger than the one of cubic systems.[1] The helical symmetry is now fully exploited in the CRYSTAL code, so that the computational cost of large-unit-cell nanotubes dramatically decreases.[2]

The nanotube symmetry is exploited at three levels: (a) for the automatic generation of the nanotube starting from a two-dymensional structure; (b) for the calculation of the mono- and bi-electronic integrals; (c) for the diagonalization of the Fock matrix in the reciprocal space.

The modified CRYSTAL code was used for the study (structure, stability, vibrational spectrum, elastic properties, band gap) of a set of carbon nanotubes at different DFT levels (LDA, GGA, hybrids) with Gaussian type basis sets of increasing complexity (from STO-3G to 6-1111(2d1f)), and the results compared with the available experiments and other simulations.[1,3]

A preliminar quantum mechanical ab initio analysis of chrysotile[4] nanotubes ($Mg_3Si_2O_5(OH)_4$, phyllosilicate cylindrically wrapped that can contain hundreds of atoms in the unit cell) was also performed for the first time (DFT, 6-31G* basis sets). The relationship between structure (i.e. radius of the tube and rolling direction of the flat layer) and stability is discussed.[5]

Keywords: helical symmetry, carbon nanotubes, chrysotile.

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