Linear Augmented Cylindrical Wave Method For Nanotubes Electronic Structure

The main ideas and results of application of the linearized augmented cylindrical wave (LACW) method for the electron properties of the single-walled, double-walled, embedded, and intercalated nanotubes are discussed [1]. We start with the simplest case of the achiral single-walled (n, 0) and (n, n) tubules having small translational unit cells. Then, the electron properties of chiral (n,m) nanotubes having very large translational cells are discussed with account of the tubules rotational and screw symmetries. Based on the LACW and Green’s function techniques, the ab initio numerical approach to calculating the electron local densities of states of the substitutional impurities in the nanotubes is presented. The relativistic version of LACW theory is described and applied to calculating the effects of spin–orbit coupling on bands of the tubules.


Vljudno vabljeni! / Kindly invited!

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