Recent Progress and Applications of the Chiral-Symmetry Density-Functional-Theory Program Code for Nanotubes

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We have studied systematically the electronic properties of carbon nanotubes using explicitly the chiral symmetries of the system within the framework of the density functional theory. While in the past CCTN6 symposium, we reported systematically the electronic structure of carbon nantoubes without the geometry optimization [1], we now can optimize the geometries of carbon nanotubes using chiral-symmetry program code [2]. In this talk we report the presence of the "intrinsic twisting" in chiral nanotubes and the effect of the external twisting on the electronic properties of carbon nanotubes. In addition, we will report the extension of the present program code to the boron-nitride nanotubes.

1. Y. Akai and S. Saito, Physica E 29, 555 (2005).
2. K. Kato, T. Koretsune, and S. Saito, Phys. Rev. B 85, 115448 (2012).