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Intrinsic Twisting and Electronic Properties of Carbon Nanotubes : A First-Principles Study KOICHIRO KATO, TAKASHI KORETSUNE, SUSUMU SAITO, Department of Physics, Tokyo Institute of Technology — We report the energetics and electronic structures of twisted single-walled CNTs in the framework of the density functional theory (DFT) with the local density approximation. As for very thin CNTs, we use conventional plane-wave DFT computational code. In order to utilize the periodic boundary condition implemented in the plane-wave DFT code, we study CNTs under several discretized twisting conditions. On the other hand, in the case of thicker nanotubes including experimentally abundant nanotube sizes, we use a real-space DFT computational code which can deal with twisted CNTs with only two atoms per "helical" unit cell. As a result, it is found that chiral CNTs become more stable in slightly twisted geometry. Our results suggest that chiral nanotubes would possess the intrinsic twisting. We also report the twisting-level dependence of the electronic structures. It is found that the fundamental gaps of most kinds of CNTs sensitively depend on twisting level. Importantly, the directions of the intrinsic twisting are the same as the directions of enlarging the fundamental gap except for very thin CNTs.

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