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Energetical Stability of Near-Armchair Carbon Nanotubes: A Systematic First-Principles Study KOICHIRO KATO, TAKASHI KORETSUNE, SUSUMU SAITO, Department of Physics, Tokyo Institute of Technology — We perform the systematic first-principles study of 57 kinds of carbon nanotubes (CNTs) and investigate the energetical stability of so-called "near-armchair" CNTs. The density functional theory computational code which utilizes the helical symmetry and has been developed in our group is extensively used in the present work. Because the computational effort can be drastically reduced by using the helical symmetry of CNTs, the systematic study of fully-optimized CNTs including the experimentally abundant CNTs was finally achieved in this work. As a result, it is found that "near-armchair" CNTs including (6,5) and (7,5) CNTs are energetically more stable than other CNTs. This result corresponds well with the high abundance of these near-armchair CNTs experimentally reported so far. In addition, by performing the systematic analysis of CNT bond-lengths and angles, the presence of the geometrical family pattern after their structural optimizations has been revealed for the first time. It is also confirmed that the geometrical optimization plays a very important role in predicting electronic structures of chiral CNTs as well as achiral CNTs. The fundamental gap corrections associated with the geometrical optimizations are sizable even in one nm diameter CNTs.

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