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Atomic Arrangement and Its Effects on Electronic Structures of Graphene from Tight-Binding Description

The electronic structures of pristine graphene can be qualitatively described by tight-binding method. Tight-binding model is a simple method to understand the contributions of each atomic state. The method is helpful to investigate how chemical bonding, atomic arrangement, and structural symmetry reflect to the electronic structure of a system. Structural stability of monolayer graphene with dopants or impurities is able to be systematically investigated by means of first-principles calculations. However, the method is more expensive than simple tight-binding approximation. Tight-binding method provides an insightful of how the interactions between the constituents influence on the characteristic of electronic structure, which is sensitive to the detailed arrangement of the constituents. Tight-binding calculations of several representative ordering patterns including ribbon, superlattice (SL) or stripe, and scattering arrangements are given to illustrate an idea of how to construct Hamiltonian matrix for such systems. These matrix elements are considered as parameters, which are fitted to reproduce certain properties from experimental data or first-principles calculations. The properties of nanoribbons and superlattices along armchair and zigzag direction have been discussed in the context of the tight-binding approximation, as they provide an informative trend of the electronic properties related to edge modification and inversion symmetry of structure.

Ref http://110.170.84.132/ccmp/sirichok/doc/graphene.pdf

Primary author: Dr JUNGTHAWAN, Sirichok (School of Physics, Suranaree University of Technology)

Presenter: Dr JUNGTHAWAN, Sirichok (School of Physics, Suranaree University of Technology)

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