USING THE TIGHT-BINDING MODEL TO DERIVE A DISPERSION RELATION FOR GRAPHENE ENERGY

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Abstract

We solve the problem of accounting for varying graphene-based nanostructure parameters by means of conducting numerical simulations. To solve the Schrödinger equation, we used the tight-binding model as an alternative to molecular dynamics simulation. We describe implementing this method for the case of π electrons in a graphene layer. We derive a dispersion relation for graphene energy. It is possible to use the results presented to determine the band structure of single-walled carbon nanotubes and to study their electronic properties

Keywords

Carbon nanotubes, graphene, graphene conductivity, tight-binding model, dispersion relation for energy, Bloch functions, Brillouin zones, Dirac points

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