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**From graphene to graphite: A first-principles study**[1] BI-RU WU, Department of Nature Science, Center for General Education, Chang Gung University — The multilayer graphene and graphite are systematic studied via a first-principles method based on density functional theory and general gradient approximation. The hexagonal, Bernal and rhombohedral stacking types are considered. The total energy, the electronic structure and the strength of the multilayer graphene and graphite are analyzed to study the process of graphene to graphite. We predict the number of graphene multilayers shall be greater than 15 layers to behave as a graphite bulk.

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