Relative Stability of Bernal and Rhombohedral Stackings in Trilayer Graphene under Distortions

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Stackings in graphene have a pivotal role in properties to be discussed in the future, as seen in the recently found superconductivity of twisted bilayer graphene[1]. Beyond bilayer graphene, the stacking order of multilayer graphene can be rhombohedral, which shows flat bands near the Fermi level that are associated with interesting phenomena, such as tunable conducting surface states[2] expected to exhibit spontaneous quantum Hall effect[3], surface superconductivity[4], and even topological order[5]. However, the difficulty in exploring rhombohedral graphenes is that in experiments, the alternative, hexagonal stacking is the most commonly found geometry and has been considered the most stable configuration for many years. Here we reexamine this stability issue in line with current ongoing studies in various laboratories. We conducted a detailed investigation of the relative stability of trilayer graphene stackings and showed how delicate this subject is. These few-layer graphenes appear to have two basic stackings with similar energies. The rhombohedral and Bernal stackings are selected using not only compressions but anisotropic in-plane distortions. Furthermore, switching between stable stackings is more clearly induced by deformations such as shear and breaking of the symmetries between graphene sublattices, which can be accessed during selective synthesis approaches. We seek a guide on how to better control – by preserving and changing - the stackings in multilayer graphene samples [6].

References

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Figures

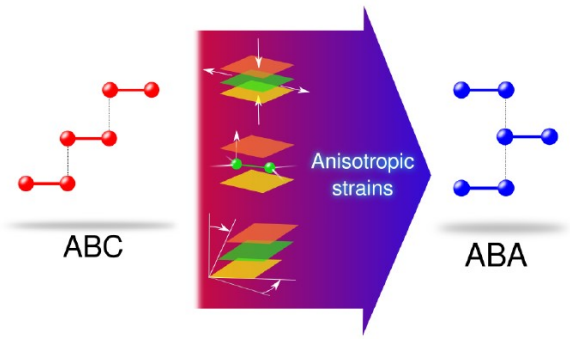

Figure 1: Graphene stacking changes from rhombohedral to Bernal due to small lattice deformations.