Strain-induced stacking transition in bilayer graphene

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Abstract
Strain, both naturally occurring and deliberately engineered, can have considerable effects on the structural and electronic properties of 2D materials like graphene [1-3]. For example, uniaxial or biaxial heterostrain in bilayer graphene (BLG) modifies the stacking arrangement from the ground state AB stacking, with subsequent effects on the electronic structure of the bilayer. Here, we use Density Functional Theory (DFT) calculations to investigate the interplay between strain and stacking in BLG. We are particularly interested in determining how strain applied to one layer is transferred to the second layer, and at what critical strain the AB stacking is disrupted. To overcome limitations introduced by periodic boundary conditions [4], we consider an approximate system consisting of an infinite sheet and a graphene nanoribbon. Strain is applied to the continuous layer, and we determine whether that strain is transferred to the ribbon layer or if it is more energetically favorable for the ribbon to remain unstrained, despite the disruption in stacking. We find that above a critical strain of about 1% the ribbon prefers to be unstrained, indicating a transition between uniform AB stacking and non-uniform mixed stacking. This is in agreement with a simple model estimate based on the individual energy contributions of strain and stacking effects. Our findings suggest that small amounts of strain provide a platform to reversibly engineer stacking order and Moire features in bilayers, providing a viable alternative to twistronics to engineer topological and exotic physical phenomena in such systems.

References

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Figures

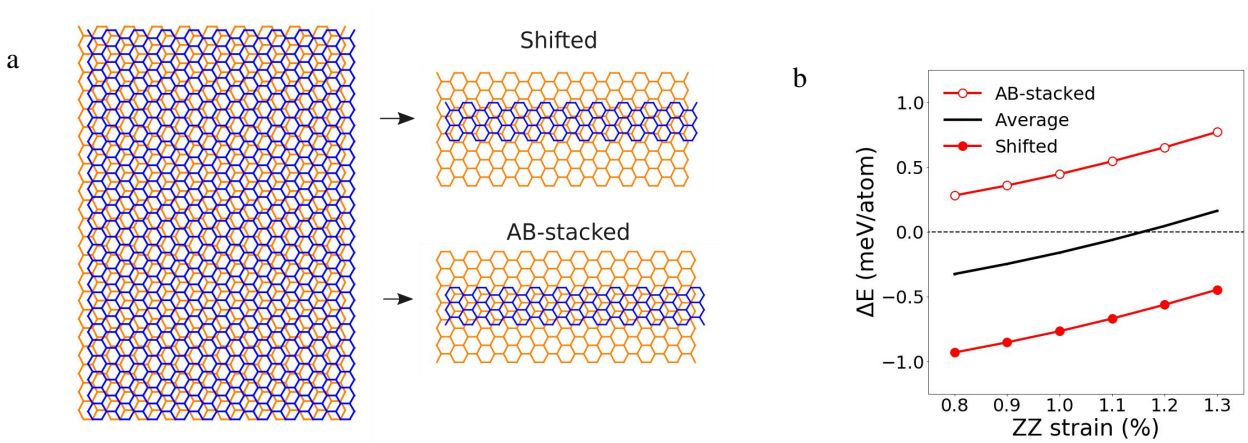

Figure 1: (a) Structure of BLG when only one layer is strained by 15% uniaxial strain and the nanoribbons that are used for the approximation, that correspond to the two extremes of energy in terms of stacking. (b) Plot of the energy difference $\Delta E = E_{strained} - E_{unstrained}$, where $E_{strained}$ refers to the total energy when both layers are strained and $E_{unstrained}$ to the total energy that only one layer is strained, as a function of the uniaxial strain that is applied. If $\Delta E<0$, the ribbon layer prefers to be strained, while when $\Delta E>0$ the ribbon layer prefers to be unstrained. In the second case stacking changes and it is not AB-stacked anymore.