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Chemical versus Thermal Folding of Graphene Edges[1]

NINGHAI SU, MIAO LIU, FENG LIU, Department of Materials Science and Engineering, University of Utah — Using molecular dynamics (MD) simulations, we have investigated the kinetics of the graphene edge folding process. The lower limit of the energy barrier is found to be ∼380 meV/Å (or about 800 meV per edge atom) and ∼50 meV/Å (or about 120 meV per edge atom) for folding the edges of intrinsic clean single-layer graphene (SLG) and double-layer graphene (DLG), respectively. However, the edge folding barriers can be substantially reduced by imbalanced chemical adsorption, such as of H atoms, on the two sides of graphene along the edges. Our studies indicate that thermal folding is not feasible at room temperature (RT) for clean SLG and DLG edges and is feasible at high temperature only for DLG edges, whereas chemical folding (with adsorbates) of both SLG and DLG edges can be spontaneous at RT. These findings suggest that the folded edge structures of suspended graphene observed in some experiments are possibly due to the presence of adsorbates at the edges.

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Ninghai Su
Department of Materials Science and Engineering, University of Utah

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