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First-principles study of the graphene edges: edge orientation, stability, equilibrium shape, and the effect of hydrogen passivation CHEE K. GAN, DAVID J. SROLOVITZ, Institute of High Performance Computing — We use density functional theory to determine the equilibrium shape of graphene flakes, through the calculation of the edge orientation dependence of the edge energy and edge stress of graphene nanoribbons (see C. K. Gan and D. J. Srolovitz, arXiv:0909.4373 (2009)). The edge energy is a nearly linear function of edge orientation angle; increasing from the armchair orientation to the zigzag orientation. Reconstruction of the zigzag edge lowers its energy to less than that of the armchair edge. The edge stress for all edge orientations is compressive, however, reconstruction of the zigzag edge reduces this edge stress to near zero. Hydrogen adsorption is favorable for all edge orientations; dramatically lowering all edge energies and all edge stresses. It also removes the reconstruction of the zigzag edge. Using the new edge energy data, we determine the equilibrium shape of a graphene sheet (with unreconstructed edges) to be hexagonal with straight armchair edges in the presence and absence of hydrogen. However, zigzag edge reconstruction produces graphene flakes with a six-fold symmetry, but with rounded edges. This shape is dominated by near zigzag edges. The compressive edge stresses will lead to edge buckling (out-of-the-plane of the graphene sheet) for all edge orientations, in the absence of hydrogen. Exposing the graphene flake to hydrogen dramatically decreases the buckling amplitude.

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