

Edges of Low-dimensional Materials: Structures, Energies, and Applications

Y. Liu, V. I. Artyukhov, X. Zou, and B. I. Yakobson

*Department of Mechanical Engineering and Materials Science, Department of Chemistry,
and the Smalley Institute for Nanoscale Science and Technology,
Rice University, Houston, TX 77005, USA.*

Edges and interfaces play important roles in the morphologies and properties of low-dimensional materials. Based on first-principles calculations, we present that (i) the energies of graphene edge, and its implication to nanotube chirality [1]; (ii) the thermodynamics and kinetics of graphene growth is determined by its edge [2]; (iii) the interfacial structures and properties of merging graphene domains, i.e. grain boundaries [3]; (iv) the structures and properties of grain boundaries in two-dimensional (2D) boron nitride (BN) [4]; (v) the energies of single crystalline 2D BN edges, and interfaces of graphene quantum dot embedded in BN matrix with electronic and magnetic properties modulation [5]; (vi) The crack propagation is determined by energies of graphene edge [6]. Our studies enrich the understanding of edges and interfaces in low-dimensional materials.

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