

Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Graphene edge from A to Z YUANYUE LIU, SOMNATH BHOWMICK, BORIS I. YAKOBSON, Rice University — We introduce an energy decomposition ansatz, which leads to an analytical expression for the edge energy $G(X)$ of arbitrary direction-cut angle X in two dimensional materials [1]. We further show that thermodynamic conditions at the edge simply add a “chemical phase shift” C , $G(X) = \cos(X + C)$, making the favorable shapes controllable, according to the Wulff construction. Direct atomistic computations and analysis for graphene, as well as 2D boron nitride (h-BN), and zinc oxide (ZnO) support the universal nature of the relationship.

[1] Y. Liu, A. Dobrinsky, and B.I. Yakobson, Phys. Rev. Lett., in press (Dec 10 2010 issue).

Boris I. Yakobson
Rice University

Date submitted: 03 Jan 2011

Electronic form version 1.4