

Dr. Boris I. Yakobson

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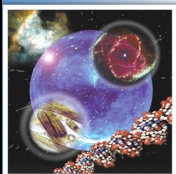
3:15 p.m. - 4:15 p.m.

BB 3.04.06

**Equilibrium at the Edge: From Nanotubes to
Graphene and the Other Flat Materials**

We will discuss the developments in theory of graphene growth [1], its similarities and contrasts with nanotubes, including the dynamics of defect healing [2]. Comprehensive DFT computations allow one to build a “nanoreactor” diagram of all important energy states, and then to evaluate the rate of carbon addition, the growth speed in different directions and thus the shape of growing islands. Their misorientation causes the formation of grain boundaries, which display their own interesting mechanics [3]. Non-carbon 2D-materials may also be considered: “white-graphene” h-BN with its peculiar grain boundaries [4], pure boron [5], and metal-disulfides.

[1] Artyukhov et al. Proc. Natl. Acad. Sci. (2012) doi:10.1073/pnas.1207519109.
[2] Rao et al. Nature Mater. 11, 213 (2012); Yuan, et al. Phys. Rev. Lett. 108, 245505 (2012). [3] Ajayan and BIY, Nature Mater. 10, 415 (2011); BIY and Ding, ACS Nano 5, 1569 (2011). [4] Liu et al. ACS Nano, doi:10.1021/nn302099q (2012). [5] E. Penev et al. Nano Lett. 12, 2441 (2012).

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