

Equilibrium at the edge: nanotubes' nucleation, steady-state and cooperative growth

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We will discuss the developments in theory of sp^2 -carbon growth [1], the similarities and contrasts between nanotubes and graphene, including the dynamics of defect healing [2]. Comprehensive DFT computations allow one to build a “nanoreactor” model which include all the 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. Nucleation statistics in its possible relation with the edge energy will also be discussed [3-4].

[1] Artyukhov et al. Proc. Natl. Acad. Sci. 109, 15136 (2012). [2] Rao et al. Nature Mater. 11, 213 (2012); Yuan, et al. Phys. Rev. Lett. 108, 245505 (2012). [3] Liu et al. Phys. Rev. Lett. 105, 235502 (2010). [4] Penev et al. in progress.