

Abstract Submitted
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The origins of nanotube chirality: Is the edge-catalyst in control?

EVGENI PENEV, YUANYUE LIU, BORIS YAKOBSON, Rice University — The chance for a nanotube of a chiral angle c to emerge from the “primordial soup” of carbon atoms on the catalyst is determined by their relative energies. Massive computations allow one to evaluate the “elastic” energies of the caps, and the energies of their edges [1], $G(c+C)$, which appears to be dominating. Importantly, the latter contains a “chemical phase shift” C , so that the probability of different chiralities is determined by the chemical conditions at the edge. Preference for specific chirality can be achieved by tuning chemical potential of edge terminating chemical. This offers a rational way to control the tube chiral symmetry, a tantalizing yet so far elusive goal.

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

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