

Abstract Submitted
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Modeling the catalytic action of supersaturated Ni droplets for the initial stage of growth of single-walled nanotubes¹ I. CHAUDHURI, M. YU, C.S. JAYANTHI, S. Y. WU, University of Louisville — Transition metal nanoparticles are the catalysis of choice for the growth of single-walled carbon nanotubes because of the high miscibility of carbon atoms with their supersaturated liquid droplets. This suggests that, at least for modeling the initial stage of growth, the droplets may be represented by the jellium medium and catalytic action of the droplets may be modeled by the electron redistribution for carbon atoms mediated by the medium. We have tested this scenario by comparing stable configurations of cage-structured C clusters in vacuum with those in jellium, with an average charge transfer from the jellium to C atoms $n_{av} \approx 0.2e$ to model the effect of nickel atoms. The structural optimization was carried out using the semi-empirical self-consistent and environment- dependent Hamiltonian in the framework of linear combination of atomic orbitals developed by our group [1]. Our results showed that the pentagons are more stable with substantial charge transfer occurrence in the defects in the vicinity of pentagons, consistent with previous results [2]. We also found that for a cage-structured cluster of a given size, increasing n_{av} tends to elongate the hexagonal rings. Thus it appears that the catalytic action provided by Ni-droplet may be modeled by the charge fluctuations on C atoms mediated by the jellium. [1] S. Y. Wu et.al. *Handbook of Material Modeling* Vol. I, p.2935 (2005). [2] X. Fan et. al. *Phys. Rev. Lett.* **90**, 145501 (2003).

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