Abstract Submitted
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Carbon metal interactions and epitaxy in nanotube growth: Towards chirality-selected nanotube production FENG DING, MS&MS Dept., Rice University, 6100 Main street, Houston TX 770005, PETER LARSSON, Condensed Matter Theory Group, Department of Physics, Uppsala University, Box 530, SE-751 21 Uppsala, Sweden, J. ANDREAS LARSSON, Tyndall National Institute, University College Cork, Lee Maltings, Prospect Row, Cork, Ireland, RAJEEV AHUJA, Condensed Matter Theory Group, Department of Physics, Uppsala University, Box 530, SE-751 21 Uppsala, Sweden, ARNE ROSÉN, KIM BOLTON, Physics Department, Göteborg University, SE-412 96, Göteborg, Sweden, BORIS I. YAKONSON, MS&MS Dept., Rice University, 6100 Main street, Houston TX 770005, FENG DING TEAM, GOTHEBURG UNIVERSITY COLLABORATION, UPPSALA COLLABORATION, UNIVERSITY COLLEGE CORK COLLABORATION — The nucleation of carbon nanotubes (CNTs) on catalyst cluster surfaces was studied by both molecular dynamics (MD) simulation and density functional theory (DFT) calculations. The analysis reveals the two important necessary conditions for the CNT growth: (i) weak tube wall-catalyst interaction and (ii) strong carbon dangling bond-catalyst interaction. A model of CNT growth is proposed to explain the efficiency of the catalyst and the chirality-selective nucleation of carbon nanotubes. [1] F. Ding, et al. J. Phys. Chem. B 108, 17369 (2004). [2] F. Ding, et al. J. Chem. Phys. 121, 2775 (2004). [3] F. Ding, et al. Nanotechnology 17, 543 (2006). [4] F. Ding, et al. Carbon 43, 2215 (2005).

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