Ab-Initio Simulations of the Growth of Short Carbon Nanobells

G.L. ZHAO, Southern University and A&M College; Visiting Fellow, Princeton University, D. BAGAYOKO, Southern University and A&M College — We performed ab-initio density functional simulations to study the structural and growth properties of short carbon nanobells. We used a real space approach and the linear combination of atomic orbitals (LCAO) formalism. In the nitrogen-doped carbon nanobells, the nitrogen atoms that are attracted to the open-edge sites of the carbon nanobells play an important role in the growth of the short carbon nanostructures. We also present the calculated electronic structure of the short nanobells. The calculated local density of states of the nanobells revealed field emission characteristics that agree with experimental observations. Acknowledgments: this work was funded in part by NASA (Award No. NCC 2-1344), NSF (Award No. 0508245), and ONR (Grant No: N00014-05-1-0009).

G. L. Zhao
Southern University and A&M College; Visiting Fellow, Princeton University

Date submitted: 28 Nov 2005