Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Chirally - Selective Growth of Single Walled Carbon Nanotube on Fe_{13} Nanocatalyst[1] ANTENEH TEFERA, MOGUS MOCHENA, Florida A&M University — Controlled growth of single - walled carbon nanotubes with desired chiral indices remains the holy grail of single walled carbon nanotube synthesis. We performed ab initio molecular dynamics calculation of the nucleation and early stage growth of (5,0) SWCNT in the low temperature range where the nanocatalyst is a solid. We show that a zigzag formation of carbon atoms is possible when the surface of the pentagonal pyramid of Fe_{13} icosahedron is exposed to ambient carbon atoms or carbon atoms and dimers or a ring of ten carbon atoms. The possibility of anomalous cap formation resulting from competing repulsive and attractive forces is presented.

[1]This work was supported by NSF grant: DMR-0804805. This research was supported in part by the NSF through TeraGrid resources provided by NCSA under grant number TG-DMR100055.

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Date submitted: 15 Nov 2013 Electronic form version 1.4