Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

Nitrogen doped carbon nanotubes for dioxygen reduction from ab initio simulation[1] SHIZHONG YANG, LONI Institute/Southern University, GUANG-LIN ZHAO, EBRAHIM KHOSRAVI, Southern University — Nitrogen substitutionally doped short carbon nanotubes (CNTs) has potential application for metal-free efficient oxygen reduction reactions(ORRs). We have performed *ab initio* density-functional-theory (DFT) calculations to simulate nitrogen substitutionally doped short (10, 0) CNTs. Our calculated results show that nitrogen prefers to stay at the open-edge of the short CNTs. Dioxygen O_2 can adsorb and partially reduce on the carbon-nitrogen complex site (Pauling site) and on carbon-carbon long bridge sites at the open-edge of the CNTs. The results of the spin polarization calculations show that the carbon atoms on the open-edge of the CNT can possess a magnetic moment of about 0.59 μB/atom, while those carbon atoms in the inner wall of the CNT do not have a magnetic moment. The doped nitrogen in the CNT does not have a magnetic moment. The chemisorption of dioxygen O_2 on the open-edge of the short CNT reduces the magnetic moments of the carbon atoms to nearly zero.

[1]This work is funded in part by NASA LaSPACE(subcontract No. 28538, contract No. 35879), LONI institute, NSF(Award No. CBET-0754821), and the Air Force Office of Scientific Research (Award No. FA9550-09-1-0367).

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Date submitted: 20 Nov 2009 Electronic form version 1.4