Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

Density Functional Theory (DFT) study of Li adsorption on the CNT-C60 hybrid system WONSANG KOH, JI IL CHOI, SEUNG SOON JANG, Georgia Institute of Technology — With a rapidly increasing demand of better electrochemical materials for high energy storage density, various types of Li intercalation materials have been exploited to promote Li adsorption. In this study, we investigate a new type of hybrid system consisting of carbon nanotubes (CNTs) and fullerenes (C60) using the first-principles computational methods such as quantum mechanics and molecular dynamics simulation, aiming at improving electrochemical characteristics such as adsorption capabilities and charge transfer. This hybrid system makes use of C60s as the electron acceptor from Li in the presence of CNT that act a role as a charge transport channel to electrode. We investigate adsorption energy as well as electronic properties such as band structure, density of states (DOS) and charge distribution through the density functional theory (DFT). The performance of the system during charging and discharging process will be discussed. From the calculation, we find that the adsorption energy of Li on the hybrid system is increased comparing with that on pristine CNT. We believe this complex not only improve Li adhesion but also utilize CNT as an electrode for better electron transport.

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Date submitted: 01 Dec 2009 Electronic form version 1.4