Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

Electronic, vibrational dispersions and alkali-halides encapsulation in carbon nanotubes[1] K. CHRIST, Dept. of Mechanical Engr. - Univ. of Wisconsin, H.R. SADEGHPOUR, Harvard-Smithsonian CfA — Density functional calculations of electronic and vibrational dispersion energies for prestine graphite and single-walled carbon nanotubes (SWCNT) are presented. Optimized parameters for nonlocal norm-perserving pseudopotentials which replace the potential field due to core electrons are given and the valence electrons are treated with linear combination of localized atomic orbitals. The effect of encapsulation of carbon nanotubes with alkali-halide matrices is numerically investigated. The electronic band structure of encapsulated SWCNT is noticeably modified and hence its optical properties.

[1]NSF, SI

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Date submitted: 15 Nov 2006 Electronic form version 1.4