Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

Ab initio study of the quasiparticle band structure and opticalproperties of bulk h-BN and BN nanotubes. CHEOL HWAN PARK, CATALIN D. SPATARU, STEVEN G. LOUIE — In the crystalline phase, different stacking of the hexagonal basal layers affects the electronic properties of bulk h-BN significantly. We have studied this stacking effect by first performing calculations on the Kohn-Sham band structure within the local density approximation to the density functional theory. Next, we compute the quasiparticle band structure by including electron self-energy effects within the GW appromixation. Finally, we obtain the optical excitation spectrum including electron-hole interaction (excitonic) effects by solving the Bethe-Salpeter equation. For single- walled boron-nitride nanotubes, we have also carried out a similar series of calculations to obtain the optical response of these tubes as a function of diameter and chirality. This work was supported by the NSF under Grant No. DMR0087088, and the U.S. DOE under Contract No. DE-AC03-76SF00098. Computer time was provided by NERSC and NPACI.

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Date submitted: 22 Dec 2004 Electronic form version 1.4