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First-Principles study of the optical properties of BN nanotubes and h-BN CHEOL HWAN PARK, CATALIN SPATARU, STEVEN LOUIE, UC Berkeley and Lawrence Berkeley National Laboratory — We present first-principles calculations of the effects of quasiparticle self-energy and electron-hole interaction on the optical properties of single-walled BN nanotubes (both zigzag and armchair tubes) and bulk h-BN. Excitonic effects are shown to be even more important in BN nanotubes than in carbon nanotubes, giving rise to excitons with binding energy larger than 2 eV for the zigzag (8,0) BN nanotubes. Moreover, unlike the carbon nanotubes, theory predicts that these exciton states are comprised of coherent supposition of transitions from several different subband pairs, giving rise to novel behaviors. Our calculatioins are in quantitative agreement with available experimental data. We also compare the optical properties of single-walled BN nanotubes with those of bulk h-BN. This work was supported by the NSF under Grant No. DMR04-39768, and the U.S. DOE under Contract No. DE-AC03-76SF00098. Computer time was provided by NERSC and NPACI.

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