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First-principles calculation of electronic structure and optical absorption of BN ZnO XIAO ZHANG, ANDRE SCHLEIFE, Univ of Illinois - Urbana — The α-BN structure of ZnO, a nonequilibrium phase with a transition pressure of 25 GPa, has been found in nano structures of ZnO. The structural difference between the BN structure and the equilibrium wurtzite structure can play an important role for applications of nanostructured ZnO. In order to understand the difference, first principles calculations have been performed on both phases. The electronic structure is computed using the *GW* method based on Density Functional Theory and HSE hybrid functional calculations. The *GW* method includes the quasiparticle effects due to the screened electron-electron interaction which gives an accurate description of the electronic band structure and density of states. After that, by solving the Bethe-Salpeter Equation for the optical polarization function, which take excitonic effects into account, we have achieved an accurate description of optical absorption spectra for both structures. We find a good agreement with experimental and previous computational results for WZ structure, and predict the absorption for the BN structure. The BN structure shows a larger band gap and we found a very large optical anisotropy: The gap for extraordinary light polarization is almost 0.7eV larger than that for ordinary light polarization.

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