Abstract Submitted
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***Ab initio* calculations of the dielectric functions of semiconductors including the electron-hole interactions via LASTO method** HYE-JUNG KIM, YIA-CHUNG CHANG, University of Illinois at Urbana-Champaign and Research Center for Applied Sciences, Academia Sinica, Taipei, Taiwan — We calculate dielectric functions of semiconductors including the electron-hole interactions within the *ab initio* framework. The Bethe-Salpeter equation is constructed using a full-potential linear augmented-Slater-type orbital (LASTO) method [1, 2]. Using the LASTO method allows us to compute optical matrix element for large number of k points efficiently. Due to requirements of a dense k-point mesh, we use quasi-minimum residual (QMR) method to solve the equation. The inclusion of the electron-hole interactions both shifts the peak positions and changes peak heights of the imaginary part of the dielectric functions, resulting in better agreement with experimental data than the spectra obtained without including the electron-hole interactions. The calculated dielectric functions are compared to experimental data of ZnSe, CdSe, CdTe, InP, InAs, AlAs and GaN. The self-energy correctoins are described by an empirical tight-binding formula. [1] J. W. Davenport, Phys. Rev. B 29, 2896 (1984) [2] Y.-C. Chang, R.B.James, and J.W.Davenport, Phys. Rev. B 73, 035211 (2006)

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