

Abstract Submitted
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Ab initio calculations of the dielectric functions of semiconductors and alloys including excitonic effect via LASTO method HYEJUNG KIM, YIA-CHUNG CHANG, Department of Physics, University of Illinois at Urbana-Champaign, Urbana IL and Research center for Applied Sciences, Academia Sinica, Taipei, Taiwan — We calculate dielectric functions of semiconductors and alloys 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. The electron-hole interaction is computed with a sufficiently dense k-point mesh, which shows good convergence. Point group symmetry has been utilized to speed up the computation significantly. Dielectric functions of alloys are calculated by the configurational average of special quasirandom structures. The inclusion of the electron-hole interaction both shifts the peak positions and changes peak heights of the imaginary part of the dielectric functions, resulting in better agreement with ellipsometry data than the spectra obtained without including the electron-hole interactions.

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