Abstract Submitted
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UV Spectra of rutile and anatase phases of TiO_2 using ABINIT2NBSE[1] H.M. LAWLER, J.J. REHR, U. Washington, S. DALOSTO, Z.H. LEVINE, E.L. SHIRLEY, NIST — We have developed an interface between the electronic structure code ABINIT and the optical spectroscopy code NBSE, developed at NIST. NBSE calculates dielectric spectra at various levels of theory, including iterative solution of the Bethe-Salpeter equation (BSE) for electron-hole states. From a single input file the interface executes a complete calculation, from the self-consistent ground-state to the dielectric spectrum. The interace can also treat momentum-transfer dependence of the dielectric function. As an application, we present calculations of the birefringent spectra of rutile and anatase TiO_2. Not surprisingly, we find that excitonic interactions dominate low-energy features of the spectra. We also address the role of planar-bonding, oxygen π-orbitals near the Fermi level, and the unfilled titanium d-band in the birefingent properties of these systems.

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