Abstract Submitted
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Ab initio **calculations of optical spectra**[1] M.P. PRANGE, J.J. REHR, A.L. ANKUDINOV, U. of Washington — We present a real space approach for *ab initio* calculations of the optical constants of materials. The approach is based on a generalization of the *ab initio* Green's function formalism implemented in the FEFF8 code to include valence and conduction band spectra. This all-electron approach, which is the real-space analog of the KKR method, includes self-consistent potentials, relativistic effects, inelastic losses, self-energy and screened core-hole effects, and multiple-scattering to all orders. Our procedure is based on calculations of the imaginary part of the dielectric function ϵ_2, from which various optical constants can be derived using analytical properties and Kramers-Kronig transforms. Results for several materials are presented and compared with experiment.

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