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Real Space Multiple-Scattering Calculations of Optical Properties¹ M.P. PRANGE, J.J. REHR, A.L. ANKUDINOV, U. of Washington, J.A. SOININEN, U. of Helsinki — We present a method for *ab initio* calculations of the dielectric function which is applicable for periodic and non-periodic materials alike. Our approach is a generalization to finite momentum transfer of that implemented in the real space multiple-scattering code FEFF8 and is the real-space analog of the KKR method. The approach includes self-consistent potentials, an energy dependent self-energy and screened core-hole effects. The method yields the dynamic structure factor $S(\vec{q}, \omega)$ over a broad spectrum from the optical to x-ray energies, and in the long-wavelength limit, yields various optical constants. Results for several materials are presented and compared with experiment.

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