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Real-Space Multiple-Scattering X-ray Absorption Spectroscopy Calculations of d- and f-state Materials using a Hubbard Model[1] CHRISTIAN VORWERK, KEVIN JORISSEN, JOHN REHR, Department of Physics, University of Washington, Seattle, Washington 98195 USA, AHMED TOWFIQ, Theoretical Division, Los Alamos National Laboratory, Los Alamos, New Mexico 87545 USA — We present calculations of the electronic structure and x-ray spectra of materials with correlated d- and f-electron states treated with the Hubbard model in a real-space multiple scattering (RSMS) formalism, and using a rotationally invariant local density approximation (LDA+U). Values of the Hubbard parameter U are calculated ab initio using the constrained random-phase approximation (cRPA). The real-space Green's function approach with Hubbard model corrections is an efficient way to describe localized electron states in strongly correlated systems, and their effect on core-level x-ray spectra. The method is shown to give the correct density of states and x-ray absorption spectra for Transition Metal- and Lanthanide-oxides such as Ce2O3 and NiO, where the traditional RSMS calculations fail.

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