Abstract Submitted
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Real-space Green's Function Calculations including Hubbard Contributions[1] TOWFIQ AHMED, J. J. KAS, J. J. REHR, U. Washington — Hubbard model contributions are introduced into the real space Green's function formalism in terms of an effective self-energy, based on the LDA+U method of Anisimov et al.[2] The effective self-energy is then applied to localized d-states in a material, e.g. at the metal sites of transition metal oxides. The approach is implemented in an extension of the FEFF9 spectroscopy code and leads to an efficient procedure for including strong correlation effects in the electronic structure and x-ray spectra of d-electron materials, such as transition metal oxides and high T_c cuprates. Calculations are presented for the angular momentum projected density of states of MnO, NiO and $La_{(2-x)}Sr_xCuO_4$ and for the K-edge x-ray absorption and emission spectra of the O atoms in these materials, and the results are found to be in reasonable agreement with experiment.

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[2]V. I. Anisimov, F. Aryasetiawan, and A. I. Lichtenstein, J. Phys.: Condens Matter 9, 767 (1997)

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