Abstract Submitted
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Ab initio Anderson impurity approach to x-ray absorption spectra of transition metal complexes[1] DANIEL L. COX, Department of Physics, University of California, Davis, CA 95616, ARND HUBSCH, Max-Planck-Insitut für Physik komplexer Systeme, Nöthnitzer Str. 38, 01187 Dresden, Germany, MONTIAGO X. LABUTE, Theoretical Biology and Biophysics, Los Alamos National Laboratory, Los Alamos, NM 87545 — We present a generic Anderson impurity approach to transition metal molecules that allows to study correlation effects beyond the usual electronic structure calculations. Here, first principle density functional theory calculations (using SIESTA) are employed to determine the parameter of the model Anderson impurity Hamiltonian. We use the Lanczos algorithm to diagonalize the model Hamiltonian within a restricted set of basis states that is built up in the spirit of of the Gunnarsson Schönhammer trial wave function for heavy fermion compounds. The presented approach is applied to the K-edge x-ray absorption spectra of the valence tautomer molecule Co(3,5-DTBSQ)$_2$(phen).

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