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Correlated hybridization in transition metal complexes[1] ARND HUBSCH, Max-Planck-Institut für Physik komplexer Systeme, Nöthnitzer Str. 38, 01187 Dresden, Germany, JONG-CHIN LIN, JIANPING PAN, DANIEL L. COX, Department of Physics, University of California, Davis, CA 95616 — We apply local orbital basis density functional theory (using SIESTA) coupled with a mapping to the Anderson impurity model to estimate the Coulomb assisted or correlated hybridization between transition metal d-orbitals and ligand sp-orbitals for a number of molecular complexes. We find remarkably high values which can have several physical implications including: (i) renormalization of effective single band or multi-band Hubbard model parameters for the cuprates and, potentially, elemental iron, and (ii) spin polarizing molecular transistors.

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