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LDA+DMFT Charge Self-consistency Applied to Yb Valence Transition ERIK YLVISAKER, WARREN PICKETT, UC Davis, ANDREW MCMAHAN, LLNL, JAN KUNES, University of Augsburg — Elemental ytterbium metal is known to undergo a gradual transition from a divalent spd^2f^{14} state to a trivalent spd^3f^{13} state in a pressure range of 0 to 34 GPa. We present LDA+DMFT studies of this transition, comparing three impurity solvers (Hirsch-Fye QMC, continuous time QMC and Hubbard I) with each other and with experimental data. All Yb states of interest are kept; no downfolding to a minimum basis is done. This application of DMFT (especially the QMC solvers) to the correlated f-orbitals gives reasonable agreement with the experimental transition. However, the neglect charge self-consistency is questionable for a valence transition where the concentration of valence electrons changes. Therefore we generalize the procedure and compare and contrast LDA+DMFT results with and without charge self-consistency for Yb using the Hubbard I impurity solver.

Erik Ylvisaker
UC Davis

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