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LDA+DMFT Charge self-consistency applied to Yb valence transition ERIK R. YLVISAKER, W. E. PICKETT, UC Davis, A. K. MCMAHAN, LLNL — Ytterbium metal, in a pressure range of 0 to 34 GPa, is known to undergo a gradual transition from a v^2f^{14} state to a v^3f^{13} state where v and f represent valence (spd) and f-orbital occupations, respectively. We present, first, conventional LDA+DMFT studies of this transition using both the Hirsch-Fye QMC and Hubbard I atomic solvers. This application of DMFT to the correlated f-orbitals gives reasonable agreement with the experimental transition. However, the neglect of 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 (transition pressure, energy and equation of state) with and without charge self-consistency for Yb using the Hubbard I impurity solver.

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