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Dynamical Mean Field Treatment of the Valence Transition in Yb ERIK YLVISAKER, UC Davis, ANDREW MCMAHAN, LLNL, WARREN PICKETT, UC Davis — At ambient pressure, Yb metal is a divalent rare-earth with configuration $f^{14}v^2$ where v represents the valence (s, p, d) occupation. When pressure is applied it undergoes a gradual transition to a trivalent configuration ($f^{13}v^3$), completing by 34 GPa. We investigate this valence transition using the all-electron DMFT(HI) method (which includes 6s, 6p, 5d and 4f in the basis) with the Hubbard I atomic solver. Experimental evidence suggests that this transition involves a linear combination of these two many-body states ($\alpha f^{13} + \beta f^{14}$) with α increasing as pressure is applied. We present evidence that DMFT can appropriately model this type of wavefunction, and that this is necessary to capture the gradual nature of the valence transition in Yb. The DMFT(HI) results are sensitive to the parameter chosen for the $4f$ energy level and its volume dependence; however, a good description of the valence transition can be achieved with reasonable adjustments in this function. We also compare and contrast DMFT results with LDA+U, which seems to have fundamental difficulties in modeling this transition. The equation of state provided by the DMFT(HI) method is significantly more accurate than the LDA or LDA+U methods give. More rigorous DMFT (QMC) calculations are currently underway to establish what the accuracy of the HI approximation is.

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