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Electron correlation, spin-orbit coupling, intersite effects and the metal-insulator transition in pyrochlore iridates[1] RUNZHI WANG, ARA GO, ANDREW MILLIS, Columbia University — We perform density functional theory (DFT) plus single-site and cluster dynamical mean-field theory (DMFT/CDMFT) calculations to study the metal-insulator transition in the pyrochlore iridates $Lu_2Ir_2O_7$, $Y_2Ir_2O_7$ and $Eu_2Ir_2O_7$. The calculations include spin-orbit coupling. Single-site DMFT calculations indicate that the Lu compound is much more insulating than the Y or Eu materials but predict that the critical interaction strength is almost exactly the same for the Eu and Y compounds, although experimentally the metal-insulator transition temperatures are quite different. We further carry out the cluster DMFT (CDMFT) and observe much larger differences, consistent with experiments, demonstrating the crucial role played by spatial correlations.

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