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**Polymorphism in transition metal compounds: An LDA+Rotationally-invariant slave-boson study** TSUNG-HAN LEE, NICOLA LANATA, Florida State University and National High Magnetic Field Laboratory, YONGXIN YAO, Ames Laboratory and Iowa State University, VLADAN STEVANOVIC, Colorado School of Mines and National Renewable Energy Laboratory, VLADIMIR DOBROSAVLJEVIC, Florida State University and National High Magnetic Field Laboratory — Treating the strong correlation effect in transition metal compounds is a challenging task in first principle simulation, where standard approximations to density functional theory (DFT) usually fail to predict correct ground-state structure and energy ordering among different polymorphs due to the lack of appropriate electron correlation description. In this talk, we show that, within the framework of local density approximation(LDA) plus rotationally-invariant slave-boson(RISB) approach, we are able to recover the correct ground state structure, electronic phases and reasonable equilibrium volumes for 6 transition metal compounds; CrO, MnO, FeO, CoO, CoS, and CoSe, among the rocksalt, zincblende, NiAs, and wurtzite structures. This result demonstrates the potential of LDA+RISB as an accurate and efficient tool for investigating strongly correlated materials and predicting their structures.

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