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**Non-local first-principles calculations in Cu-Au, Ag-Au and Cu-Ag** YONGSHENG ZHANG, Department of Materials Science & Engineering, Northwestern University, GEORG KRESSE, Faculty of Physics, Center for Computational Materials Science, Universitat Wien, CHRISTOPHER WOLVERTON, Department of Materials Science & Engineering, Northwestern University — Cu-Au is the prototypical alloy system used to exemplify ordering and compound formation, and serves as a testbed for all new alloy theory methods. Yet, despite the importance of this system, conventional density functional theory (DFT) calculations with semi-local approximations (GGA) have two dramatic failures in describing the energies of this system: 1) DFT predicts incorrect ordered ground states for Au-rich compositions, and 2) DFT formation energies of the observed $Cu_3Au$ and CuAu compounds are nearly a factor of two smaller in magnitude than experimental values. Here, we show how modern extensions of DFT based on non-local interactions can rectify both of these failures. Using the self-consistent non-local HSE06 functional, the formation energies of $Cu_3Au$ and CuAu are -71 and -91 meV/atom, respectively, which are in excellent agreement with the experimental measurements. The semi-local GGA predicted $CuAu_2$ is not a stable phase in the HSE06 calculations, and $CuAu_3$ with the $L1_2$ structure is theoretically predicted as a stable phase. For Ag-Au, both semi-local GGA and non-local HSE06 functionals give similar formation energies. The electronic structures are used to explain these different phenomena in Cu-Au and Ag-Au.

Yongsheng Zhang
Department of Materials Science & Engineering,
Northwestern University

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