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KKR-DCA Thermodynamics for Cluster Short-Range Order with Full Charge Self-Consistency DOMINIC A. BIAVA, University of Illinois - Urbana, DUANE D. JOHNSON, Ames Laboratory, Ames, Iowa — The Dynamical Cluster Approximation (DCA) implemented in the Korringa-Kohn-Rostoker (KKR) electronic-structure method gives a systematically exact, *course-grained* theory of the electronic states of substitutionally disordered alloys, including the effects of chemical short-ranged order (SRO). We implement the KKR-DCA within density functional theory (DFT) to calculate directly the charge self-consistent electronic contributions to the alloy grand potential. The KKR-DCA is combined with the chemical entropy from the Cluster Variation Method (CVM), which when minimized predicts the SRO directly. The calculated SRO has been tested in several metallic systems with agreement to measured values. For very large clusters, the KKR-DCA can be sampled, as done within Quantum Monte Carlo, and provides the charge self-consistent thermodynamic grand potential in complex alloys with SRO at finite temperature, at the same level as done for perfect ordered alloys in other electronic-structure methods at zero Kelvin.

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