Abstract Submitted
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Systematically exact corrections from multisite configurations on the electronic structure of disordered alloys[1] DOMINIC BIAVA, SUBHRADIP GHOSH, DUANE D. JOHNSON, University of Illinois at Urbana/Champaign, WILLIAM A. SHELTON, A. V. SMIRNOV, Computer Science and Mathematics Division, Oak Ridge National Laboratory — The Korringa-Kohn-Rostoker coherent-potential approximation (KKR-CPA) is widely used to study electronic structure and energy of disordered alloys, but the single-site CPA is missing effects from the local environment, including short-range order. A cluster-based *non-local* CPA (NLCPA) was proposed that recovers the translational-invariance of the medium from reciprocal-space coarse-graining used in the dynamical cluster approximation (DCA), where corrections are casual and systematic as the cluster size increases. We implemented a first-principles KKR-NLCPA/DCA and study the effect of local environment, including short-range order, on the electronic structure of fcc $CuAu$ and bcc $NiAl$.

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