

Abstract Submitted
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Integrated Density of States Lloyd's Formula for Disordered Alloys with Short-Range Order via a KKR-based Dynamical Cluster Approximation¹ D. A. BIAVA, SUBHRADIP GHOSH, W. A. SHELTON, D.

D. JOHNSON, Physics and Materials Science and Engineering, University of Illinois Urbana Champaign — Within Korringa, Kohn and Rostoker (KKR) multiple scattering theory, we have formulated ² a static version of the Dynamic Cluster Approximation (DCA) ³, which is a cluster (or non-local) generalization of the coherent potential approximation (NLCPA) ⁴ that includes environmental effects, including short-range order. Within our KKR-DCA/NL-CPA we present an analytic expression for configurationally-averaged integrated density of states $\langle N(E) \rangle$, or generalized Lloyd's formula. We show also that this Lloyd's formula is stationary with respect to changes in the DCA/NLCPA effective medium, providing a rigorous electronic density functional theory and total-energy formalism for (partially) disordered alloys with(out) short-range order that is exact for infinite sized clusters and reduces to the single-site CPA for a cluster size of one. We show applications to various alloys with(out) short-range order.

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³M. Jarrell and H R Krishnamurthy, Phys. Rev. B 63 125102 (2001)

⁴D.A. Rowlands et al, Phys. Rev. B 67 115109 (2003)

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