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Benchmarking Mobility Edge Calculations for a Cluster Typical Medium Theory of Off-diagonal Disordered Systems CONRAD MOORE, KA MING TAM, HANNA TERLETSKA, JUANA MORENO, MARK JARRELL, Louisiana State University — We apply the transfer matrix method and exact diagonalization to electronic lattice systems with substitutional off-diagonal disorder. Established effective medium methods for studying realistic metallic alloy systems have enjoyed much success calculating the properties of disordered systems, but are criticized for inaccurate predictions (for example, of charge transfer and phase evolution) caused by reliance on the Coherent Potential Approximation (CPA) which neglects nonlocal environmental effects. It has been shown that such non-local correlations can be incorporated with the Dynamical Cluster Approximation (DCA). Furthermore, localization effects have been demonstrated with a local order parameter approach that is used to define a typical medium. The validity of the predicted mobility edge from an effective cluster typical medium theory that extends the Blackman, Esterling and Berk formalism to DCA is explored with finite size scaling of transfer matrix data. We demonstrate it as a promising effective medium theory to incorporate into present ab initio methods for realistic disordered systems.

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