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Generalized Multiband Typical Medium Dynamical Cluster Approximation: Application to (Ga,Mn)N YI ZHANG, Louisiana State Univ - Baton Rouge, RYKY NELSON, RWTH Aachen University, ELISHA SIDDIQUI, KAMING TAM, Louisiana State Univ - Baton Rouge, UNJONG YU, GIST, Gwangju, Korea, TOM BERLIJN, Oak Ridge National Laboratory, WEI KU, Brookhaven National Laboratory, VIDHYADHIRAJA SUDHINDRA, Jawaharlal Nehru Centre For Advanced Scientific Research, JUANA MORENO, JARRELL MARK, Louisiana State Univ - Baton Rouge — We generalize the multiband typical medium dynamical cluster approximation and the formalism introduced by Blackman, Esterling and Berk so that it can deal with localization in multiband disordered systems with both diagonal and off-diagonal disorder with complicated potentials. We also introduce a new ansatz for the momentum resolved typical density of states that greatly improves the numerical stability of the method, while preserving the independence of scattering events at different frequencies. Starting from the first-principles effective Hamiltonian, we apply this method to the diluted magnetic semiconductor $Ga_{1-x}Mn_xN$, and find the impurity band is completely localized for Mn concentrations $x < 0.03$, while for $0.03 < x < 0.10$ the impurity band has delocalized states but the chemical potential resides at or above the mobility edge. So, the system is always insulating within the experimental compositional limit ($x \approx 0.10$) due to Anderson localization. However, for $0.03 < x < 0.10$, hole doping could make the system metallic allowing double-exchange mediated, or enhanced, ferromagnetism. The developed method is expected to have a large impact on first-principles studies of Anderson localization.

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