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Signatures of Correlation Effects and Thermopower in FeSi JAN TOMCZAK, KRISTJAN HAULE, GABRIEL KOTLIAR, Department of Physics and Astronomy, Rutgers University, Piscataway, New Jersey 08854, USA — Correlated semiconductors have been studied intensively over the years, because they exhibit an unusual metalization process which is poorly understood. At low temperatures FeSi behaves as an ordinary semiconductor, while at high temperatures the system is a bad metal with a Curie like susceptibility. Analogies with heavy fermion Kondo insulators and mixed valence compounds, and anomalous electron phonon coupling have been invoked to account for this behavior, but lacking quantitative methodologies applied to this problem, a consensus remained elusive to date. Here, we use realistic many-body methods to elucidate the metalization of FeSi. Our methodology accounts for all substantial anomalies observed in FeSi : lack of conservation of spectral weight in optics, Curie susceptibility and an anomalous thermoelectric power. Having quantitatively validated our approach, we propose a new scenario. In correlated insulators such as FeSi the metalization is induced by the emergence of non-quasiparticle incoherent states in the gap. This coherence-incoherence crossover is accompanied by a massive reorganization of the spin excitations. Besides the fundamental interest of our theory, our work is relevant to the design of thermoelectric materials based on correlated insulators.

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