KKR Electronic Structure Methods: from alloys and correlations to warm dense matter

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Korringa, Kohn, and Rostoker (KKR) multiple-scattering theory within an all-electron Green's function formalism continues to be developed to predict materials behavior in numerous areas from alloying (including atomic short-range order, ASRO) to warm dense matter arising from extreme conditions. Examples of KKR developments and their applications will be discussed, including accurate predictions of alloying from optimal basis sets, ASRO effects from the Dynamical Cluster Approximation to Dynamical Mean-Field Theory, and seamless prediction of warm dense matter, such as Hugoniots, at large pressures and temperatures, e.g., 200,000 K.