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Development of a relativistic impurity embedding code based on the KKR Green function method DAVID BAUER, PASCAL KORDT, PHIVOS MAVROPOULOS, RUDOLF ZELLER, STEFAN BLÜGEL, Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany — We present a new implementation of the KKR Green function method for electronic structure calculations of impurity atoms embedded in a crystalline host. Our code is able to treat impurity atoms not necessarily positioned at host sites. This became possible by a two step approach: For large deviations of the impurity from the host position a virtual atom method is used where the host Green function is expanded around the new impurity position. Then, small displacements are treated by an expansion of the Green function. In addition, we include in our code a newly developed accurate method to directly solve the coupled Lippmann-Schwinger equations for non-spherical potentials via a system of algebraic equations. When spin-orbit effects are included in the presence of spin polarization, this is especially important for the irregular solutions because of the coupling of different angular momenta up to the origin. We apply the method to solve the Schrödinger, the scalar-relativistic as well as the Dirac equation by using appropriate source terms.

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