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Relativistic Green's Functions in Full-Potential Multiple-Scattering Theory XIANGLIN LIU, Department of Physics, Carnegie Mellon University, YANG WANG, Pittsburgh Supercomputing Center, Carnegie Mellon University, MARKUS EISENBACH, G.MALCOLM STOCKS, Materials Science and Technology Division, Oak Ridge National Laboratory — The Greens functions play a central role in MST based KKR method. Obtaining the Greens functions by solving the Dirac equation is appealing since it naturally incorporated the electron spin and the spin-orbit coupling effects. Here we implemented the full-potential relativistic KKR method using a technique called the sine and cosine matrices formalism. The charge density and the density of states of some pure element crystals have been calculated. Different expressions of the Greens functions have been investigated for numerical benefits.

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