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Self-consistent full-potential relativistic KKR method XIANGLIN LIU, Department of Physics, Carnegie Mellon University, YANG WANG, Pittsburgh Supercomputing Center, Carnegie Mellon University, MARKUS EISENBACH, Center for computational sciences, Oak Ridge National Laboratory, G. MALCOLM STOCKS, Materials science and technology division, Oak Ridge National Laboratory — We implemented the self-consistent full potential relativistic KKR (Korringa-Kohn-Rostoker) method using the sine and cosine matrices formalism. In this scheme no irregular solution is needed, therefore it avoids the pathological behavior of the charge density at small radius. The poles of the single-site Green function are searched to identify the shallow bound states and resonance states, and to facilitate the energy integration of the Green function. As two examples, the bulk properties of noble metals are calculated, and the relativistic effects in polonium are investigated.

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