Fully relativistic ab initio calculations using multiple scattering theory for non-spherical space filling potentials

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The Kohn-Korringa-Rostocker multiple scattering method for solving the Kohn-Sham equation that arises in Density Functional theory has been one of the important approaches for the computational investigation of solid state systems. It has proven itself for all electron calculations in magnetic systems and, in combination with the coherent potential approximation, for the study of disordered alloy systems. Real space formulations of multiple scattering theory have demonstrated excellent linear scalability on current supercomputing architectures. Yet, treatment of non-spherical scattering potentials presented significant numerical challenges, that have only been solved in recent years. A combination of these full potential techniques with the solution of the Dirac equation will allow the investigation of the influence of relativistic effects, such as spin orbit-coupling, on the crystal structure of heavy elements and the coupling of atom position and magnetic order. Here we present our new formulation for the solution of the Dirac equation of the relativistic scattering problem for non spherical scatterers [J. Phys.: Cond. Matt. 28, 355501 (2016)] that solves the differential equation for the expansion parameters ("Sine" and "Cosine" matrices) which relate the free space spherical solution to the scattering wave functions. We verfy our method and demonstrate the increasing change in the electron distribution for two sets of elements of increasing atomic number. (Cu – Ag - Au and V – Nb – Ta). Finally, we combine this single scatterer formalism with our MST code to calculate bulk properties of condensed matter systems. We will demonstrate the capability of our new formalism by applying it to the calculation of the ground state of simple cubic Polonium.