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Relativistic single-site Green's function for full potential scattering XIANGLIN LIU, Department of Physics, Carnegie Mellon University, YANG WANG, Pittsburgh Supercomputing Center, Carnegie Mellon University, MARKUS EISENBACH, G.MALCOLM STOCKS, Material Science and Technology Division, Oak Ridge National Lbaboratory — The Green's function of an electron scattered by a single potential is essential for a multiple-scattering theory (MST) based electronic structure calculation. Robust solver for this single site Green's function has been developed for non-relativistic system, as well as for spherical potential relativistic system, but works on a relativistic full potential (FP) solver are still unsatisfactory. Here a new method to obtain this relativistic-FP Green's function in analogy with the non-relativistic MST has been implemented using the so called phase integral technique. Compared to the previous relativistic-FP method, no matching on the boundary is needed and the coupling of partial waves is not limited to $\Delta l = 0$ in this method. As an example, the density of states (DOS) of copper has been calculated using both integral of the Green's function and the Krein theorem and the agreement is shown. This work will be the basis for developing a MST based relativistic ab initio electronic structure calculation method.

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