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Issues related to Convergence Properties of First Principles Full Potential Multiple Scattering Electronic Structure Calculations[1] AURELIAN RUSANU, G. MALCOLM STOCKS, MARKUS EISENBACH, DON M. NICHOLSON, Oak Ridge National Laboratory, YANG WANG, Pittsburgh Supercomputer Center — Despite some clear advantages for specific problems, the implementation of full potential electronic structure methods based on the use of multiple scattering theory (MST) (KKR derived approaches) has received much less investment than alternate electronic structure methods. Here we describe some new techniques that facilitate an easy and accurate implementation of first principles full potential MST methods. The method consists of solving: (1) the full-potential single site scattering problem, where we avoid the usage of the shape function by surface integrals methods to determine the scattering matrices, and (2) the Poisson problem, where the site centered full-potential is constructed from a sphere bounded non-overlapping charge density and a smooth space-filling charge density. Specifically, we discuss issues related to accuracy and convergence properties of these techniques within the context of the order-N Locally Self-consistent Multiple Scattering (LSMS) method.

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