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Ab-initio Total Energy Calculation for Full-potential Multiple Scattering Theory Methods[1] YANG WANG, Pittsburgh Supercomputing Center, Carnegie Mellon University, AURELIAN RUSANU, MALCOLM STOCKS, DON NICHOLSON, MARKUS EISENBACH, Oak Ridge National Laboratory — The *ab initio* methods (e.g., KKR, KKR-CPA, LSMS) based on multiple scattering theory have the clear advantage of being able to calculate the Green function in a straightforward manner, which has important implications in the application of electronic structure calculations. But these methods have mostly been implemented within muffin-tin approximations. Recent advances in the numerical implementation of full- potential multiple scattering theory and, in particular, the development of an innovative Poisson equation solver have made carrying out the fully self-consistent full-potential calculation possible. In this presentation, we discuss various implementations of the full-potential total energy calculation, and we investigate the convergence of the total energy with respect to the angular momentum expansion cutoff for scattering matrices. Finally, we compare the full-potential total energy with the muffin-tin approximation results.

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