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An investigation of the internal sum convergence in the full potential multiple scattering theory[1] YANG WANG, Pittsburgh Supercomputing Center, AURELIAN RUSANU, G. MALCOLM STOCKS, Oak Ridge National Laboratory, J. SAM FAULKNER, Department of Physics, Florida Atlantic University — The ab initio methods based on multiple scattering theory (MST) have proved to be a very powerful technique for the electronic structure calculation for solids. The latest advances in the implementation of full potential MST have allowed us to investigate dislocations, point defects, and radiation damage effects on the physical properties of structural materials. In the conventional formulation of full potential MST, the single site wavefunctions $\phi_{l,m}$ are expanded in terms of spherical harmonics with angular momentum l up to a cutoff value ϕ-$l_{\max}$. This cutoff value defines the extension of the internal sum and is usually taken to be the same as KKR-$l_{\max}$, the cutoff value for the Bloch wave expansion (in terms of $\phi_{l,m}$) so that the single site sine and cosine scattering matrices used for calculating the t-matrix and the Green function are square matrices. In this presentation, we show a technique that allows for ϕ-$l_{\max}$ to be greater than KKR-$l_{\max}$, so to allow for converging the internal sum, while keeping the calculation of the t-matrix and the Green function tractable. We compare the results obtained from different ϕ-$l_{\max}$ values and discuss the implications of the internal sum convergence.

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