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A convergence test of the full potential KKR method[1] G.M. STOCKS, Oak Ridge National Laboratory, YANG WANG, Pittsburgh Supercomputing Center, Carnegie Mellon University — The full-potential Korringa-Kohn-Rostoker (KKR) method is a powerful tool for the ab initio study of the electronic structure of solids. In this method, the expansion of crystal wavefunctions, the LDA potential, and the charge density are determined by three angular momentum parameters respectively. Essentially, these three angular momentum parameters are an important key for controlling the convergence of an electronic structure calculation. In this presentation, we demonstrate the convergence character of the full potential KKR method by running the electronic structure calculation for a set of transition metals. We will discuss the implication of the results, and show the optimal choice of the angular momentum parameters, which are the one that requires the least computational cost for the desired accuracy for the total energy.

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Yang Wang
Pittsburgh Supercomputing Center, Carnegie Mellon University

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