

Abstract Submitted
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A new approach to in full potential multiple scattering theory electronic structure calculations¹ G.M. STOCKS, ORNL, YANG WANG, PSC, AURELIAN RUSANU, DON M. NICHOLSON, MARKUS EISENBACH, YEVGENIY PUZYREV, ORNL — Despite the wide use of first principles electronic multiple scattering theory methods there realization as full potential methods has proved problematical with the consequence that atomic relaxation is not typically performed due to the lack of accurate forces. Here we describe some new techniques that facilitate an easy implementation of these full potential methods. In the determination of the scattering path matrix(t-matrix) we eschew the expansion of the shape function and use surface integrals to determine scattering t-matrix. We also use a new method in the treatment of Poisson problem where the charge density is divided in a spherical non-overlapping charge, which is treated using standard methods, and a pseudo charge which is treated by FFT-methods.

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