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An investigation of the generalized phase shifts and the integrated density of states for full-potential single site scattering[1] G. MALCOLM STOCKS, Materials Science and Technology Division, Oak Ridge National Laboratory, YANG WANG, Pittsburgh Supercomputing Center, Carnegie Mellon University, J. SAM FAULKNER, Department of Physics, Florida Atlantic University — In the conventional multiple scattering theory approach to *ab initio* electronic structure calculations, the integrated density of states (IDOS) is determined by taking the imaginary part of the Green function integrated along an energy contour. In this presentation, we show a numerically more reliable approach that uses an analytical expression for the IDOS, derived from the Krein's theorem. We compare both approaches, Krein's theorem versus the Green function method, in single site cases (e.g., Cu, Al, Mo). And we discuss the concept of generalized phase shifts, which are the diagonal elements of a unitary transformation of the S-matrix for the full-potential single site scattering, and show their applications in the determination of the IDOS.

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