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Integrability constraints for atomic-orbital integrals with applications to semi-empirical modeling of multi-element systems[1] C. LEAHY, A. TCHERNATINSKY, M. YU, C.S. JAYANTHI, S.Y. WU, University of Louisville —
Semi-empirical modeling of atomic-scale systems is often plagued by several issues related to atomic-orbital integrals. There are typically several sets of parameters which give similar results, suggesting that some combinations of parameters are redundant. The energy eigenvalues are not guaranteed to be real, which can and do result in systems that do not have a calculable energy. The use of *d*- orbitals results in an unreasonable increase in the number of parameters, making it difficult to model the transition metals. And the extraction of parameters for multi-element systems from those of single-element systems is not well-understood. We have improved these issues by accounting for the constraints which arise from the fact that the elements of the Hamiltonian and overlap matrix are specific integrals of specific atomic orbitals. These constraints are implemented using convolution and deconvolution between the two-center integrals and the radial parts of the orbitals. The result is a 50% decrease in the relevant number of parameters for *s* and *p* orbitals, and a 83% decrease for the *d* orbitals. The eigenvalues are now always real. And the parameters for multi- element systems can be obtained using a convolution of the single-element orbitals, eliminating the need for artificial averaging or re-fitting techniques.

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