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Development and application of accurate analytical models for single active electron potentials[1] MICHELLE MILLER, AGNIESZKA JARON-BECKER, ANDREAS BECKER, JILA and Department of Physics, University of Colorado — The single active electron (SAE) approximation is a theoretical model frequently employed to study scenarios in which inner-shell electrons may productively be treated as frozen spectators to a physical process of interest, and accurate analytical approximations for these potentials are sought as a useful simulation tool. Density function theory is often used to construct a SAE potential, requiring that a further approximation for the exchange correlation functional be enacted. In this study, we employ the Krieger, Li, and Iafrate (KLI) modification to the optimized-effective-potential (OEP) method to reduce the complexity of the problem to the straightforward solution of a system of linear equations through simple arguments regarding the behavior of the exchange-correlation potential in regions where a single orbital dominates. We employ this method for the solution of atomic and molecular potentials, and use the resultant curve to devise a systematic construction for highly accurate and useful analytical approximations for several systems.

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