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Scalable Linear Electronic Structure Method for Free Standing Clusters KAB SEOK KANG, JAMES DAVENPORT, DAVID KEYES, JAMES GLIMM, Brookhaven National Laboratory — We have developed a Scalable Linear Augmented Slater Type Orbital (LASTO) method for electronic-structure calculations on free standing clusters. As with other linear methods we solve the Schrodinger equation using a mixed basis set consisting of numerical functions inside atom centered spheres matched onto tail functions outside. The tail functions are Slater type orbitals which are localized, exponentially decaying functions. To solve the Poisson equation between spheres, we use a finite difference method replacing the rapidly varying charge density inside the spheres with a smoothed density with the same multipole moments. We use multigrid techniques on the mesh which are well-known scalable solvers. This yields the Coulomb potential on the spheres which in turn defines the potential inside via a Dirichlet problem. To solve the linear eigen-problem, we use SCALAPACK, a well-developed package to solve large eigen-problems with dense matrices. We have tested the method on finite clusters of palladium and palladium hydride. Supported by the US Department of Energy under contract DEA02-98CH10886.

James Davenport
Brookhaven National Laboratory

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