Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Optimized basis-set representation for electronic-structure methods: Better Energetics[1] AFTAB ALAM, DUANE JOHNSON, University of Illinois at Urbana Champaign — We derive an analytic expression for an optimal, and rapidly computed, representation for site-centered basis-set expansion (e.g., spherical harmonic). An optimal site-dependent radius are determined from the local saddle-points derived in terms of overlapping atomic charge densities, typically already used for Löwden construction of the starting potentials. These "saddle-point adjusted" sphere radii separate the "spherical" density and potential around an atom from the symmetry-induced, "non-spherical" part in the interstitial, and more properly accounts for charge and size of atoms. These radii also properly determine the weighted Voronoi cells (i.e., power diagram or generalized Wigner-Seitz cells) which are mathematically guaranteed to be convex and space filling. For full-potential and forces, exact integrations over Voronoi interstitials is accomplished easily by isoparametric integration. We implement these ideas in a general Korringa-Kohn-Rostoker coherent potential approximation (KKR-CPA) code within the atomic-sphere-approximation (ASA). For several large-atom/small-atom systems, we show that ASA using saddle-point-adjusted spheres now agrees with formation energies from full-potential calculations and experiments for both chemically ordered and disordered cases, and, hence, predict the stability of the correct phases and its temperature scale.

[1]Department of Energy under BES grants (DE-FG02-03ER4602631) and (LLNL-B573247).

Aftab Alam
University of Illinois at Urbana Champaign

Date submitted: 28 Nov 2008 Electronic form version 1.4