Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Speeding up DFT: A new approach to k-point integration JEREMY J. JORGENSEN, Brigham Young University, DEREK C. THOMAS, University of Texas at Austin, MATTHEW M. BURBIDGE, Brigham Young University, IAN H. SLOAN, The University of New South Wales, CONRAD W. ROSENBROCK, RODNEY W. FORCADE, BRET C. HESS, GUS L.W. HART, Brigham Young University — The bottleneck for high throughput material prediction is computational speed. Increasing the convergence rate of the band energy integration will decrease computation time. Band energy, despite its small contribution to the total energy, plays a large role in the calculation of formation enthalpies, where energy differences and not magnitudes are of greater importance. Current DFT codes generally choose k-points using the Monkhorst-Pack scheme, and then integrate the energy bands using the rectangle method. Instead, we interpolate the energy bands with splines, create a spline representation of the Fermi surface, and analytically integrate the energy bands beneath the Fermi surface to find the band energy. Our conservative estimate is a tenfold increase in computational efficiency for the band energy calculation.

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Date submitted: 13 Nov 2014 Electronic form version 1.4