

Abstract Submitted
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Speeding up DFT: A faster method for integrating band energy in SCF cycles¹ MATTHEW M. BURBIDGE, JEREMY J. JORGENSEN, CONRAD W. ROSENBROCK, Brigham Young University, DEREK C. THOMAS, University of Texas at Austin, BRET C. HESS, RODNEY W. FORCADE, Brigham Young University, STEFANO CURTAROLO, Duke University Center for Materials Genomics, GUS L. W. HART, Brigham Young University — Typically in SCF cycles, a “rectangle rule” is used on uniformly spaced points (Monk Pack meshes)¹ to integrate the band energy. The use of rectangles is motivated by their fast convergence when used on the fully occupied bands of semiconductors. Unfortunately integration with rectangles is extremely inefficient for metals. This motivates the use of gauss quadrature (or other higher order methods) for integrating the band energy. As we show, however, even in the case of semiconductors where the rectangle convergence is extremely efficient, higher order methods are still *more* efficient. The savings in semiconductors alone are sufficient to motivate the implementation of a higher order method in current DFT codes. Even though higher order quadrature methods were discussed immediately following the original Monkhorst and Pack¹ paper, we revisit the issue in light of modern DFT calculations. [1] H.J. Monkhorst and J.D. Pack, Phys. Rev. B 13, 5188 (1976).

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Matthew M. Burbidge
Department of Physics and Astronomy Brigham Young University

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