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Ten-fold speed up of DFT: Improving k-point integration GUS HART, Brigham Young University, DEREK C. THOMAS, University of Texas at Austin, JEREMY J. JORGENSEN, MATTHEW M. BURBIDGE, BRET C. HESS, CONRAD W. ROSENBROCK, Brigham Young University, IAN H. SLOAN, University of New South Wales, RODNEY W. FORCADE, Brigham Young University, STEFANO CURTAROLO, Duke University — The amount of recent cpu time ($>$ 100 mega cpu hours) spent in our group on high-throughput materials prediction led us to re-examine convergence issues in standard DFT calculations. For total energy calculations, k-point convergence can be increased two-fold and ten-fold for semiconductor and metals, respectively. For semiconductors, the popular "rectangle approximation method" using Monkhorst-Pack grids convergences much faster than expected (for reasons that will be explained), which explains why it gained popularity in the early development of DFT codes. (Its simplicity is also a likely factor.) However, it is not possible to adapt the method to the case of partially-occupied bands in metals while preserving the rapid convergence of semiconductors. Using a rectangle rule for metals, irrespective of any smearing method, leads to the well-known problem that convergence rates are 100s times worse than for semiconductors. Revisiting the k-point integration issue in light of modern DFT practice, we demonstrate that this "metal deficit" can be reduced to only a factor of 5–10 worse than semiconductors. The further complication of integrating inside the Fermi surface for metals is solved with our approach without the need for smearing and its associated ad hoc parameters.

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