4CF15-2015-000248

Abstract for an Invited Paper
for the 4CF15 Meeting of
the American Physical Society

French Fries or Onions? Improving integration in DFT calculations

GUS HART, Brigham Young Univ - Provo

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. Calculations for metals typically take 100 times longer than calculations for semiconductors. By improving the integration technique can we shrink the"metal deficit"? Conceptually one can attack the problem in the typical "rectangle" fashion (french fries) or by integrating in energy space (onions). The standard approach converges very slowly in the case of metals. 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.