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Two-Step Method for Accelerating DFT Calculations using Pre-Generated Charge Densities HAYDEN OLIVER[1], Brigham Young University — Density Functional Theory packages give us the tools we need to discover new alloys. Unfortunately, the process is very slow. Using a sparse integration grid, we can easily compute the charge density of an alloy, which is then frozen and passed to a much denser grid. By freezing the charge density we hope to accelerate the calculations without sacrificing accuracy by bypassing the more computationally intensive processes of denser grids. We will report on the accuracy/speed trade-offs from using this "frozen charge" method.

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