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An Automatic K-Point Grid Generation Scheme for Enhanced Efficiency and Accuracy in DFT Calculations[1] KYLE MCGILL, TIM MUELLER, Department of Materials Science and Engineering, Johns Hopkins University — We seek to create an automatic k-point grid generation scheme for density functional theory (DFT) calculations that improves the efficiency and accuracy of the calculations and is suitable for use in high-throughput computations. Current automated k-point generation schemes often result in calculations with insufficient k-points, which reduces the reliability of the results, or too many k-points, which can significantly increase computational cost. By controlling a wider range of k-point grid densities for the Brillouin zone based upon factors of conductivity and symmetry, a scalable k-point grid generation scheme can lower calculation runtimes and improve the accuracy of energy convergence.

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