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Accelerating Materials Discovery through Bezier Interpolation of the Electronic Band Structure NATHAN FOULK, JEREMY JORGENSEN, GUS HART, Brigham Young University — To discover the materials that will shape the world of tomorrow, we need to make the materials calculations of today faster. Integrating the electronic band structure is one of the most important parts of these materials calculations. Unfortunately, it is also the slowest part of these materials calculations. We show that interpolating the electronic band structure using Bezier surfaces speeds up this band structure integral, without sacrificing accuracy. We also explore further speedup by using an adaptive mesh refinement in those integration regions which contain the Fermi surface.

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