Abstract Submitted
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DFT: the lore is wrong[1] JEREMY JORGENSEN, Brigham Young University — Density functional theory (DFT) is the most popular and practical approach to materials simulation, with tens of thousands of articles published on the topic each year over the past decade. DFT codes calculate the charge density that minimizes the total energy via a root finding algorithm. Smoothing methods are supposed to improve the robustness of this algorithm for metals. DFT codes also implement higher order interpolation over tetrahedron and smoothing as a means of improving the computational efficiency of metals. In this talk, we will discuss tests we have performed to quantify the effectiveness of smoothing and tetrahedron methods in achieving these purposes for which they were developed.

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Jeremy Jorgenesne
Brigham Young University

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