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Improving Band Interpolation and Band Integration in DFT^1 JEREMY JORGENSEN, MATT BURBIDGE, SPENCER HART, CONRAD ROSENBROCK, Brigham Young Univ - Provo, CRISTOPH ORTNER, University of Warwick, DEREK THOMAS, University of Texas, IAN SLOAN, University of New South Wales, GUS HART, Brigham Young Univ - Provo — A multitude of energy band interpolation and integration methods have been developed as a means to improve the accuracy and reduce computer run times of material's properties calculations. Each method adjusts one or more of the following parameters: the location of the sampling points, the interpolation basis functions, the conditions imposed on the interpolation and the integration technique employed. Common problems encountered when interpolating energy bands include handling band crossings, band kissings, and cusps. Our approach fits the energy bands with splines, finds the Fermi level with "adaptive cubes", integrates the bands using Gaussian quadrature, employing various smoothings at the Fermi level, and extrapolates the smoothed integrals of the spline representation to the band integral. We attempted to fix band crossings and kissings with band character decomposition; however, the resolution it provided was insufficient to distinguish one band from another in all cases. We discuss the potential of the tight-binding pseudo-atomic orbitals (PAO) basis to resolve band crossing and kissing issues.

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