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Making Sense of the Multitude of Brillouin Zone Integration Methods[1] JEREMY JORGENSEN, GUS HART, Brigham Young University — Over the past 50 years, a host of Brillouin zone (BZ) sampling and integration methods have been proposed. After outlining the principal difficulties associated with BZ integration, we explore the evolution of BZ sampling methods, starting with the mean-value point method, ending with the maximal packing fraction method [1]. We also examine the standard techniques that have been employed in performing BZ integrations, which include various projection methods. Finally, in order to illustrate the complications that arise during BZ integration, we employ an intuitive and realistic toy model, and also use it to investigate band energy convergence with increasing sampling point densities.

Wisesa, Pandu, Kyle A. McGill, and Tim Mueller. "Efficient generation of generalized Monkhorst-Pack grids through the use of informatics." Physical Review B 93.15 (2016): 155109.

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