

Abstract Submitted  
for the 4CS20 Meeting of  
The American Physical Society

**Useful Predictions of Materials Begin with Accurate Band Integration**<sup>1</sup> JEREMY JORGENSEN, TOM SEDERBERG, GUS HART, Brigham Young University — Technologies are often limited by the properties of available materials, and so discovering materials with superior properties will advance technology. We are able to simulate many possible materials and predict their properties with computers and scientific software. The properties of materials are obtained by integrating the material's electronic band structure. The electronic band structure is qualitatively a collection of intersecting sheets. Efforts have been made to separate the sheets to simplify calculations of properties of materials. We mathematically describe the electronic band structure, answer the question: “Are the electronic energy sheets separable?”, and study the role intersecting sheets play in the calculations of properties of materials.

<sup>1</sup>ONR (MURI N00014-13-1-0635)

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Date submitted: 25 Sep 2020

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