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Role of Electronic Structure Calculations in Understanding Superconductors¹ DAVID SINGH, Oak Ridge National Lab — Superconductivity remains one of the most challenging and exciting areas in condensed matter physics. It is a field that often sees surprises. These come in the form of new superconducting materials with unprecedented properties that need explanation. Here we briefly discuss the role that computational electronic structure studies have played in understanding some of these new systems over the years. The materials discussed are high temperature cuprates, borocarbides, Sr_2RuO_4 , MgB_2 , and the iron-based superconductors. Computation has played a key role in understanding properties of these materials and in some but not all cases pointing directly to the mechanism of superconductivity.

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