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An Automated Application Framework to Model Disordered Materials Based on a High Throughput First Principles Approach COREY OSES, Duke Univ, KESONG YANG, UC San Diego, STEFANO CURTAROLO, Duke Univ, DUKE UNIV COLLABORATION, UC SAN DIEGO COLLABORATION — Predicting material properties of disordered systems remains a long-standing and formidable challenge in rational materials design. To address this issue, we introduce an automated software framework capable of modeling partial occupation within disordered materials using a high-throughput (HT) first principles approach. At the heart of the approach is the construction of supercells containing a virtually equivalent stoichiometry to the disordered material. All unique supercell permutations are enumerated and material properties of each are determined via HT electronic structure calculations. In accordance with a canonical ensemble of supercell states, the framework evaluates ensemble average properties of the system as a function of temperature. As proof of concept, we examine the framework's final calculated properties of a zinc chalcogenide ($ZnS_{1-x}Se_x$), a wide-gap oxide semiconductor ($Mg_xZn_{1-x}O$), and an iron alloy ($Fe_{1-x}Cu_x$) at various stoichiometries.

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