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High-throughput screening for thermoelectric sulphides by using crystal structure features as descriptors[1] RUIZHI ZHANG, BAOLI DU, KAN CHEN, MIKE REECE, Queen Mary University of London, MATERIALS RESEARCH INSITITUTE TEAM — With the increasing computational power and reliable databases, high-throughput screening is playing a more and more important role in the search of new thermoelectric materials. Rather than the well established density functional theory (DFT) calculation based methods, we propose an alternative approach to screen for new TE materials: using crystal structural features as descriptors. We show that a non-distorted transition metal sulphide polyhedral network can be a good descriptor for high power factor according to crystal filed theory. By using Cu/S containing compounds as an example, 1600+ Cu/S containing entries in the Inorganic Crystal Structure Database (ICSD) were screened, and of those 84 phases are identified as promising thermoelectric materials. The screening results are validated by both electronic structure calculations and experimental results from the literature. We also fabricated some new compounds to test our screening results. Another advantage of using crystal structure features as descriptors is that we can easily establish structural relationships between the identified phases. Based on this, two material design approaches are discussed: 1) High-pressure synthesis of metastable phase; 2) In-situ 2-phase composites with coherent interface.

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