Exploring the features of $E_n(\mathbf{k})$ ANDREW SUPKA, Department of Physics and Science of Advanced Materials Program, Central Michigan University, NICHOLAS MECHOLSKY, Department of Physics and Vitreous State Laboratory, The Catholic University of America, CORMAC TOHER, STEFANO CURTAROLO, Materials Science, Electrical Engineering, Physics and Chemistry, Duke University, MARCO BUONGIORNO NARDELLI, Department of Physics and Department of Chemistry, University of North Texas, MARCO FORNARI, Department of Physics and Science of Advanced Materials Program, Central Michigan University — The full dispersions, $E_n(\mathbf{k})$, are conventionally represented on specific high-symmetry paths or integrated to determine the density of states. Novel methodologies, developed within the AFLOW consortium, allow analysis of the full energy dispersion efficiently in order to seek for valleys with optimized properties. We discuss results from high-throughput calculations performed with AFLOWπ to illustrate the importance of the full band structure in the optimization of the electronic transport coefficients. We will focus our discussion on binary chalcogenides.

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