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Theory of Band Warping and its Effects on Thermoelectronic Transport Properties[1] NICHOLAS MECHOLSKY, LORENZO RESCA, IAN PEGG, VSL/Catholic University of America, MARCO FORNARI, Central Michigan University — Transport properties of materials depend upon features of band structures near extrema in the BZ. Such features are generally described in terms of quadratic expansions and effective masses. Such expansions, however, are permissible only under strict conditions that are sometimes violated by materials. Suggestive terms such as "band warping" have been used to refer to such situations and ad hoc methods have been developed to treat them. We develop a generally applicable theory, based on radial expansions, and a corresponding definition of angular effective mass which also accounts for effects of band non-parabolicity and anisotropy. Further, we develop precise procedures to evaluate band warping quantitatively and as an example we analyze the warping features of valence bands in silicon using first-principles calculations and we compare those with semi-empirical models. We use our theory to generalize derivations of transport coefficients for cases of either single or multiple electronic bands, with either quadratically expansible or warped energy surfaces. We introduce the transport-equivalent ellipsoid and illustrate the drastic effects that band warping can induce on thermoelectric properties using multi-band models.

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