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High throughput search for thermoelectric materials. Computational stability, transport and doping properties

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Thermoelectric materials can be utilized for an efficient conversion of waste heat to electric power. While thermoelectric properties of known compounds can be rationalized and predicted using only the structure as an input [1], it turns out that a large number of semiconductor structures show potential for favorable thermoelectric properties [2]. This leaves the feasibility of achieving the optimal doping [3] and a low thermal conductivity as key bottlenecks in discovering new thermoelectric materials. In this talk I will discuss simple procedures to screen for these properties and illustrate this by the discovery of an industrially relevant thermoelectric material.

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