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POS-31 Exploration of 2D materials for high-efficiency thermoelectric conversion

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Thermoelectric materials can be used to construct solid-state devices that convert excess heat into electrical power. Because roughly half of all energy generated is lost as waste heat, efficient thermoelectric devices represent an opportunity to significantly reduce global energy production. However, predicting whether a material will exhibit efficient thermoelectric conversion is a highly nontrivial task due to the complicated interdependence of the relevant material properties, namely electrical conductivity, thermal conductivity and Seebeck coefficient. This makes ab initio methods for calculating thermoelectric properties extremely valuable, as they allow for the identification of novel materials/structures with excellent thermoelectric characteristics, without the need for expensive and time-consuming experimental trial-and-error.

By combining density functional theory calculations of electronic structure with rigorous transport theory, our group is able to calculate the thermoelectric properties of materials entirely from first-principles. This poster will present our investigations of a class of 2D materials (for example bismuth telluride) that have been suggested to possess desirable properties for efficient thermoelectric conversion not shared by their bulk counterparts, making them a promising candidate for use in next-generation thermoelectric devices.

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