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Searching for new Thermoelectric Materials from Theory[1]

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Thermoelectric (TE) materials is a type of energy materials that can be applied to directly convert waste heat into electricity. Research on advanced TE materials has been a world-wide focus in recent years. By employing density functional *ab initio* methods, we are trying to find new compounds with promising TE performance. In this talk, the following topics will be mainly covered. 1) General discussion on the directions of searching for new TE compounds with good performance; 2) Filling fraction limits (FFLs) for filler impurities in $CoSb_3$. By combining *ab initio* calculations and thermodynamic consideration, we explained the FFLs, revealed the underlined physical mechanism behind FFLs, and found a simple rule for selecting new filler atoms. A few new filled skutterudites with ultra high filling fractions of impurities were predicted theoretically and synthesized experimentally, and they do show promising thermoelectric performance. 3) Rare-earth-related Half-Heusler compounds are used as model systems to discuss the effect of localized electronic states on thermoelectric performance. By that, we will partially discuss the possibility of going beyond narrow-gap materials for thermoelectrics.

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