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**Impurity clustering and impurity-induced bands in PbTe-based bulk thermoelectrics**[1] S.D. MAHANTI, Michigan State University, KHANG HOANG, University of Califonia, Santa Babara, M.G. KANATZIDIS, Northwestern University — Complex multicomponent systems based on PbTe are of great current interest for high-temperature thermoelectric applications. A deeper understanding of the atomic and electronic structures of these materials is crucial for explaining, predicting, and optimizing their properties, and to suggest new materials for better performance. In this talk, we present our first-principles studies of the energy bands associated with monovalent (Ag) and trivalent (Sb, Bi) impurities and impurity clusters in PbTe. We find that monovalent and trivalent impurity atoms attract one another and tend to form impurity-rich clusters. The electronic structure of the host material is strongly perturbed by these impurities. Based on the calculated band structures, we suggest how to tailor the band gap and band structure near the band gap (hence transport properties) by choosing the type of impurity and its concentration or tuning the monovalent/trivalent ratio [1]. We are also able to explain qualitatively the measured transport properties of a large class of PbTe-based bulk thermoelectrics. [1] K. Hoang, S. D. Mahanti, and M. G. Kanatzidis, arXiv:0911.2685.

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