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Accurate electronic structure calculations of lead chalcogenides by QSGW method SERGEY FALEEV, OLEG MRYASOV, Seagate Technology — Enhancement of the energy conversion efficiency of thermoelectric materials has been a long goal of materials physics. Recent experiments show that distortion of the electronic structure of PbTe by adding small amount of impurities results in enhancement of the Seebeck coefficient and doubling of the ZT factor [Heremans et al., Science 321, 554 (2008)]. This enhancement is thought to be due to the impurity-induced increase of the energy dependence of density of states near the Fermi level. The reliable theoretical prediction of the energy states of impurities in host matrix (which often very difficult to measure experimentally) are required in order to explain the experiments and predict and optimize properties of new materials. Accurate calculations for bulk system is a first necessary step required for further study of systems with impurities. Here we report results for bulk lead chalcogenides obtained with recently developed QSGW method [Faleev et al., PRL 93, 126406 (2004)]. We found that electronic structure of lead chalcogenides and, in particular, the band gaps and effective masses are predicted with much higher accuracy within the QSGW approach than within most commonly used DFT theory. This result opens way for predictive search of novel thermoelectric materials.

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