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Fermi level pinning in Ti doped PbTe[1] YI-BIN GAO, Dept of Mechanical and Aeronautical Engineering (MAE), Ohio State University (OSU), JAN KOENIG, Fraunhofer Institute for Physical Measurement Techniques, Germany, MICHELE D. NIELSEN, MAE OSU, BARTLOMIEJ WIENDLOCHA, AGH University of Science and Technology, Poland, HARALD BOETTNER, Fraunhofer Institute for Physical Measurement Techniques, Germany, JOSEPH P. HEREMANS, MAE, Dept of Physics, OSU — The doping of PbTe attracts much interest due to the possible improvement of the thermoelectric properties by forming resonant levels. Here we report on doping of PbTe with Ti by molecular beam epitaxy, and back up the results with band structure calculations that show that Ti is a resonant level in the conduction band of PbTe. Ti is found to be a donor, leading to electron concentrations up to $1x10^{19}cm^{-3}$, above which it pins the Fermi level at about 52 meV above the conduction band edge, and further increase of Ti shows no effect. At higher Ti contents the concentration of free electrons starts to rise again. However, Ti doping does not enhance the thermopower above that of similarly-doped PbTe, suggesting that the electrons on Ti are localized. We propose a model for Fermi level pinning due to different ionization states of the donor impurity which is similar to a chemical buffer. Further electronic structure calculations for Ti:PbTe confirm existence of the quasi-localized Ti states in the conduction band of PbTe and predict a local magnetic moment on Ti atom of 1.8 Bohr magnetons.

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