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Density functional study of silver defects in telluride thermoelectric materials[1] BYUNGKI RYU, MIN-WOOK OH, SU-DONG PARK, Korea Electrotech Res Inst — Silver impurity in telluride thermoelectric materials forms various defect and impurity structures, such as AgSb rich nanoregion in Ag-Sb-Pb-Te, Ag_2Te and metallic silver in PbTe. To understand the atomic, electronic, energetic, and diffusion properties of silver impurities in telluride systems, we have performed the density functional theory and density functional perturbation theory calculations of silver doped PbTe. Under Te and Ag rich condition, silver telluride impurity phase or Ag-dimer defects are expected to be easily formed. Under Te poor condition, silver point defects are calculated to be easily formed and they are more stable than native point defects of PbTe, implying that silver point defect might be the major dopant responsible for the carrier generation in PbTe. We also calculated the diffusion coefficient and diffusion length of silver point defect in PbTe. Based on the results, we discussed the electrical and thermoelectric properties of silver doped PbTe.

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