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First-principles study of defect properties of zinc blende MgTe JI-HUI YANG, Key Laboratory for Computational Physical Sciences (MOST) and Surface Physics Laboratory, Fudan University, SHIYOU CHEN, HONGJUN XIANG, XINGAO GONG, Key Laboratory for Computational Physical Sciences (MOST) and Surface Physics Laboratory, Fudan University,, SU-HUAI WEI, National Renewable Energy Laboratory, Golden, Colorado 80401, USA — We studied the general chemical trends of defect formation in MgTe using first-principles band structure methods. The formation energies and transition energy levels of intrinsic defects and extrinsic impurities and some defect complexes in zinc blende MgTe were calculated systematically using a new hybrid scheme. The limiting factors for p- and n-type doping in MgTe were investigated. Possible solutions to overcome the doping limitation of MgTe are proposed. The best p-type dopant is suggested to be N with nonequilibrium growth process and the best n-type dopant is suggested to be I with its doping complex $V_{Mg} + 4I_{Te}$.

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