Abstract Submitted
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Gadolinium Doping in ZnTe[1] Z.X. MA, Lawrence Berkeley National Lab., LEI LIU, LBNL, UCB, KIN MAN YU, WLADEK WALUKIEWICZ, DALE PERRY, LBNL, PETER YU, LBNL, UCB, SAM MAO, LBNL, UCB — We have investigated, experimentally and theoretically, the effects of Gd doping on the structural and optical properties of ZnTe films grown by pulsed laser deposition. A few % of Gd doping was found to *reduce* the ZnTe lattice constant with *no change* in the fundamental band gap. When the doping level is increased to >7%, the lattice constant becomes more or less constant, but the band gap increases abruptly by as much as 50 meV. First principle calculations based on density functional theory using the linearized augmented plane wave method were performed using ZnTe supercells containing either isolated defects or defect complexes. The reduced lattice constant on Gd doping can be attributed to the presence of defect complexes involving substitutional Gd ions and neighboring vacancies. The insensitivity of the band gap at lower Gd concentration can be explained by self-compensation of these defects. The increase in the band gap energy at higher concentration is attributed to band-filling effect.

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