東京大学グローバルCOEプログラム　機械システム・イノベーション国際拠点

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First-principles modelling of dopants at interfaces in transparent conducting oxides

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要旨

For ZnO and TiO_2 with focus on their use as transparent conducting oxide (TCO) materials, the impact of extended defects in a doped polycrystal on thermodynamic and electronic properties of atomic defects is investigated by first-principles density-functional-theory (DFT) calculations for supercells containing both interfaces and dopants. For host-lattice vacancies, cation dopants substituting Zn or Ti, or anion dopants substituting O, energies of defect formation and interface segregation are determined in the local density approximation (LDA) of DFT. Defect levels in the electronic band structure are analysed in terms of densities of states, which are calculated by means of the LDA with a self-interaction-correction (SIC). The important outcome of this study is detailed microscopic information on how much positions and shapes of electronic defect levels can be altered at grain boundaries with respect to a doped single crystal.

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