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The interaction of dopants and native point defects in functional complex oxides[1]

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Oxide semiconductors are often doped with heterovalent substitutional impurities, which modify the Fermi level and lead to the formation of charge-compensating native point defects. Using first-principles calculations, we demonstrate the interplay between doping and native defect formation in complex oxides, highlighting the potential for both positive and detrimental effects. As a first example, we study the proton-conducting complex oxide $SrZrO_3$ (SZO). In undoped SZO, the defect chemistry is dominated by oxygen vacancies (V_O) and strontium vacancies (V_{Sr}) [1], whose concentrations are constrained by charge neutrality. Upon acceptor doping with Sc or Y at the Zr site, the concentration of V_O can be increased, and the concentration of V_{Sr} can be reduced; we discuss how this promotes both proton solubility and diffusion. However, under certain growth conditions, Sc and Y will substitute at the Sr site and act as donors, with detrimental consequences for proton conductivity. The second example is the alkaline-earth stannates ($ASnO_3$; A = Ba, Sr, Ca), which are promising transparent conducting oxides. The stannates can be doped with La donors. High levels of n-type doping can be achieved in $BaSnO_3$; however, the achievable carrier concentrations in (Ba,Sr)SnO3 alloys are much lower [J. Vac. Sci. Technol. A 34, 050601 (2016)]. We investigate the origin of this n-type doping difficulty, finding that the formation energy of A-site cation vacancies becomes very low under n-type conditions; these vacancies act as charge-compensating acceptors, reducing the n-type conductivity. This effect is discussed in light of recent experimental results, and we provide guidelines for engineering the growth environment to achieve higher n-type doping.

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