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Dopants and defects in conductive oxide spinels[1] ANDRIY ZAKUTAYEV, JOHN PERKINS, PHILLIP PARILLA, TULA PAUDEL, STAPHAN LANY, DAVID GINELY, ALEX ZUNGER, National Renewable Energy Laboratory — We will discuss the effects of extrinsic and intrinsic imperfections (dopants and defects) in a group of conductive oxide materials related to Co3O4. Co3O4 is a spinel with Co2+ and Co3+ on tetrahedral and octahedral sites, respectively. Doping of Co3O4 with Zn and Ni represent two limiting cases: Zn2+ ions have a preference to occupy tetrahedral (Co2+) sites and are predicted to be unable to dope effectively; Ni2+ ions have a preference to occupy octahedral (Co3+) sites, so these atoms are expected to be efficient dopants. We found that substitution of Co3O4 spinel with up to 33 percent of Zn and Ni results in formation of ZnCo2O4 normal spinel and NiCo2O4 inverse spinel, and causes 100-fold and 1000-fold increases in conductivity, respectively, matching the predicted trend. Increase in Zn and Ni concentraion up to 40 percent cause phase separation of ZnO and NiO and leveling out of the conductivity. The conductivity decreases sharply above 50-60 percent Zn and Ni substitution level. Small differences with the theoretical predictions may be explained by non-equilibrium character of the thin film deposition process.

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Andriy Zakutayev
National Renewable Energy Laboratory

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