Enabling Practical p-Type Doping in Oxide Spinels

The Center for Inverse Design has identified a class of metal oxide spinels—typified by Co_2ZnO_4—that have no intrinsic hole-killers and hence enable unopposed p-type doping in easily grown materials.

- A unified team of theorists and experimentalists from NREL, CU, Northwestern, and SLAC addressed the challenge of creating effective and practical hole-doped (p-type) oxides needed for contacts in photovoltaics (PV).
- To enable high levels of p-type doping, the potential compensating hole-killing oxygen vacancies endemic to many oxides must be avoided.
  - *Theory predicted A_2BO_4 spinels will have low oxygen vacancy concentration.*
- Four distinct electronic structure doping types (DT1–DT4) predicted for spinels.
  - *DT2 is special, having no significant hole killers, not even cation defects.*
  - *Co_2ZnO_4 is a prototype for this materials class.*
- The predicted site-occupancy and doping physics were confirmed by energy-dependent X-ray diffraction experiments at SLAC.
- Li, Mg, and Ni were predicted to be the best extrinsic dopants (Fig. 1), and this was confirmed by experiments (Fig. 2).
- Successful materials have been transferred to PV device testing.

Reference: J.D. Perkins, T.R. Paudel, A. Zakutayev, P.F. Ndione, P.A. Parilla, D.L. Young, S. Lany, D.S. Ginley, A. Zunger, N.H. Perry, Y. Tang, M. Grayson, T.O. Mason, J.S. Bettinger, Y. Z. Shi, and M.F. Toney, *Phys. Rev. B*, 10.1103/PhysRevB.84.205207 (2011).

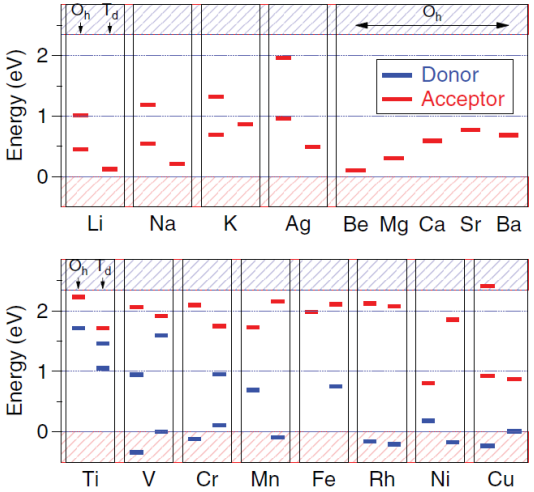

Fig. 1: Theoretical screening of 17 dopants. Li, Mg, and Ni are the best.

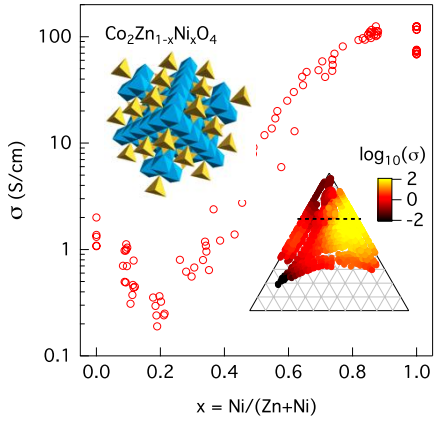

Fig. 2: Replacing Zn with Ni improves conductivity by 100x.