Anti-Site Defects in p-Type Co$_2$ZnO$_4$: Better than Perfect

Scientific Achievement
The Center for Inverse Design (CID) demonstrates that intrinsic anti-site defects actually improve electrical properties of Doping Type II spinels, in agreement with prior CID prediction.

Significance and Impact
This work confirms a fundamental hole-generating process in Co$_2$ZnO$_4$, thereby enabling increased p-type conductivity via intentional non-equilibrium growth.

Research Details
• p-type (hole-carrier) transparent conducting oxides are highly desired for photovoltaics and displays. However, to date, no high-performance materials are known.
• The CID previously predicted via theory that anti-site defects should be a net hole producer for a special class of III-II Normal spinels typified by Co$_2$ZnO$_4$ and denoted Doping Type II.
• Resonant (variable beam energy) elastic X-ray diffraction (REXD) measurements done on as-deposited and annealed epitaxial Co$_2$ZnO$_4$ films confirm this prediction.
• For Inverse spinel Co$_2$NiO$_4$, spin-dependent electronic structure calculations predict Co$_2$NiO$_4$ to be a spin-polarized semi-metal.
• Consequentially, for Co$_2$NiO$_4$, decreasing defects through annealing is predicted to increase conductivity—just the opposite of the predicted effect for Doping Type II Co$_2$ZnO$_4$. This is also confirmed by REXD measurements.
• These new insights into the role of anti-site disorder underpin a new Design Principle whereby non-equilibrium growth is used to create beneficial disorder.