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High-throughput search for improved transparent conducting oxides

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High-throughput methodologies are a very useful computational tool to explore the space of binary and ternary oxides. We use these methods to search for new and improved transparent conducting oxides (TCOs). TCOs exhibit both visible transparency and good carrier mobility and underpin many energy and electronic applications (e.g. photovoltaics, transparent transistors). We find several potential new n-type and p-type TCOs with a low effective mass. Combining different ab initio approaches, we characterize candidate oxides by their effective mass (mobility), band gap (transparency) and dopability. We present several compounds, not considered previously as TCOs, and discuss the chemical rationale for their promising properties. This analysis is useful to formulate design strategies for future high mobility oxides and has led to follow-up studies including preliminary experimental characterization of a p-type TCO candidate with unexpected chemistry. G. Hautier, A. Miglio, D. Waroquiers, G.-M. Rignanese, and X. Gonze, How Does Chemistry Influence Electron Effective Mass in Oxides? A High-Throughput Computational Analysis, Chem. Mater. 26, 5447 (2014). G. Hautier, A. Miglio, G. Ceder, G.-M. Rignanese, and X. Gonze, Identification and design principles of low hole effective mass p-type transparent conducting oxides, Nature Commun. 4, 2292 (2013).