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High-throughput computational search for new high mobility transparent (semi)conducting oxides

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Transparent conducting oxides (TCOs) are large band gap materials (to favor transparency) doped with electrons (n-type) or holes (p-type). TCOs are essential to many technologies from solar cell to transparent electronics and there is currently a large effort towards the discovery of new TCOs. I will present the results of a high-throughput computational search for new TCOs especially directed at p-type oxides. Focusing on low effective masses (leading to high mobility), large band gaps and dopability, I will show how thousands of oxides can be screened using various ab initio techniques (from density functional theory to GW) to find new potential high performance TCOs. I will discuss several unsuspected compounds with promising electronic structures and present preliminary experimental results. Beyond the description of those novel TCO candidates, I will chemically rationalize our findings, highlighting several design strategies towards the development of future high mobility TCOs.