

Abstract Submitted
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A High-Throughput Computational Search for New Transparent Conducting Oxides GEOFFROY HAUTIER, ANNA MIGLIO, Universite Catholique de Louvain, GERBRAND CEDER, Massachusetts Institute of Technology, GIAN-MARCO RIGNANESE, XAVIER GONZE, Universite Catholique de Louvain — Transparent conducting oxides (TCOs) are critical to many technologies from solar cells to electronics. However, finding materials that combine the two antagonistic properties of large conductivity and transparency to the visible light can be extremely challenging. In this talk, we will present a high-throughput screening approach aimed at discovering new high-performance TCOs. Combining different *ab initio* techniques from density functional theory to GW, we evaluated thousands of oxides in terms of essential TCO properties (e.g., band gap and carrier transport). From these results, we will present new interesting compounds as well as discuss the chemistries likely to form high performance TCOs.

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