Title: **A High-Throughput Computational Search for New Transparent Conducting Oxides and New Thermolectrics**

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Abstract:

Many essential materials properties can nowadays be computed using ab initio methods. When coupled with the exponential rise in computational power available to research groups, this predictive power provides the opportunity for large-scale computational searches for new materials. Tens of thousands of novel materials can be generated and screened by their computed properties even before their synthesis, focusing experiments on the most promising candidates and exploring rapidly new chemical spaces. We will present the potential of such high-throughput calculations for searching for new high-performance transparent conducting oxides (TCOs) and thermoelectrics.

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. Combining different ab initio techniques from density functional theory to many-body perturbation theory, we evaluated thousands of oxides in terms of essential TCO properties (e.g., band gap and carrier transport). From these results, we will present interesting new compounds as well as discuss the chemistries likely to form high performance TCOs. We will focus on Ba2BiTaO6 which we proposed as a potential high-mobility, visibly transparent p-type oxide using our high-throughput computational screening and which was synthesized and characterized as such experimentally. Finally, we will discuss the influence of the “second gap” on the transparency of TCOs.

Thermoelectrics are promising for addressing energy issues but their exploitation is still hampered by low efficiencies. So far, much improvement has been achieved by reducing the thermal conductivity but less by maximizing the power factor. The latter imposes apparently conflicting requirements on the band structure: a narrow energy distribution and a low effective mass. We will describe an original approach to fulfill both requirements in bulk semiconductors. It exploits the highly directional character of some orbitals to engineer the band structure and produce a type of low-dimensional transport similar to that targeted in nanostructures, while retaining isotropic properties [6]. We will then present an overview and preliminary analysis of thermoelectric properties computed with the BoltzTraP code for more than 48000 inorganic compounds from the Materials Project. Finally, we will focus on a new group of thermoelectric materials which have been discovered by the high-throughput screening and which were also investigated experimentally.