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Discovery of Novel Oxides Using Machine Learning and First-Principles Calculations ANTOINE EMERY, LOGAN WARD, CHRIS WOLVERTON, Northwestern Univ — Oxide materials are used for a variety of technologically relevant applications such as solid oxide fuel cell, water splitting and transparent conductors. Up until now, mostly binary and simple ternary oxides have been carefully synthesized and characterized. As a result, there are opportunities to discover new, more complex and more efficient materials for numerous applications. As the number of possible compounds is prohibitively large to explore entirely experimentally or via first-principles calculations, we use machine learning to reduce the number of compositions to be calculated via more costly methods such as density functional theory (DFT). We show that this approach reduces significantly the time spent calculating unstable compounds, allowing the exploration of larger structures and wider chemical spaces. The machine learning-aided DFT approach presented in this work also showcases a reliable framework enabling the acceleration of materials discovery.

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