

Abstract Submitted  
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**Search and Design of Topological Insulators by High-throughput Method** KESONG YANG, WAHYU SETYAWAN, SHI-DONG WANG, Department of Mechanical Engineering and Materials Science, Duke University, JEFF MULLLEN, MARCO BUONGIORNO-NARDELLI, Department of Physics, North Carolina State University, STEFANO CURTAROLO, Department of Mechanical Engineering and Materials Science, Duke University, DUKE TEAM, NCSU TEAM — Topological insulators (TIs) have attracted enormous interest because of their novel surface conduction effects which are protected by time-reversal symmetry. A high-purity TI with a highly insulating bulk is necessary to realize the potential practical applications of this class of materials. Therefore, numerous attempts are being made to search for TIs with desired properties (e.g., a large band gap and amenability to high-quality crystal growth). In this presentation, we will introduce an effective high-throughput approach to search and design TIs from a vast electronic structure database such as Inorganic Crystal Structure Database (ICSD) and Heusler alloys.

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