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High-throughput combinatorial search of novel topological insulators KESONG YANG, WAHYU SETYAWAN, SHIDONG WANG, Department of Mechanical Engineering and Materials Science and Department of Physics, Duke University, JEFFREY MULLLEN, MARCO BUONGIORNO-NARDELLI, Department of Physics, North Carolina State University, STEFANO CURTAROLO, Department of Mechanical Engineering and Materials Science and Department of Physics, Duke University, CURTAROLO GROUP @ DUKE: COMPUTATIONAL MATERIALS SCIENCE TEAM, BUONGIORNO-NARDELLI GROUP @NCSU: ERMES GROUP TEAM — In recent years, topological insulators (TIs) have attracted lots of attentions not only because of their interesting electronic characteristics induced by spin-orbit coupling but also their potential applications. So far, experimentally observed topological insulators mainly include HgTe/CdTe quantum well structure, semiconducting alloy $Bi_{1-x}Sb_x$, and so-called second-generation TI materials, i.e., the family of Bi_2Se_3, Bi_2Te_3, and Sb_2Te_3. Later theoretical simulations predict more TIs such as $TlBiQ_2$ and $TlSbQ_2$ (Q=Te, Se, and S), $LaBiTe_3$ as well as half-Heusler alloys, LuPtSb and ScPtBi. Numerous attempts are being made to look for more TIs. In this presentation, we will introduce our high-throughput combinatorial approach to find novel TI materials based on the AFLOW framework and distributed libraries.

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