

Abstract Submitted
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High-throughput discovering half-metals from materials magnetic properties database JUNKAI XUE, SHIDONG WANG, KESONG YANG, Department of Mechanical Engineering and Materials Science, Duke University, CHAITANYA DAS PEMMARAJU, STEFANO SANVITOS, School of Physics and CRANN, Trinity College, Dublin-2, Ireland, STEFANO CURTAROLO, Department of Mechanical Engineering and Materials Science, Duke University — Half-metal materials have been found by investigating their magnetism data, such as band gap and spin polarization around the Fermi level. An efficient algorithm has been implemented to create a database to aid discovering materials magnetism properties. With this tool, a series of new half-metals has been obtained. We present this magnetism data as well as how the online database is used.

Junkai Xue
Dept of Mechanical Engineering and Materials Science, Duke University

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