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Data-driven discovery of new Dirac semimetal materials QIMIN YAN, Department of Physics, UC Berkeley; Molecular Foundry, LBNL; Department of Physics, Temple University, RU CHEN, Department of Physics, UC Berkeley; Molecular Foundry, LBNL, JEFFREY NEATON, Department of Physics, UC Berkeley; Molecular Foundry, LBNL; Kavli Energy NanoSciences Institute at Berkeley — In recent years, a significant amount of materials property data from high-throughput computations based on density functional theory (DFT) and the application of database technologies have enabled the rise of data-driven materials discovery. In this work, we initiate the extension of the data-driven materials discovery framework to the realm of topological semimetal materials and to accelerate the discovery of novel Dirac semimetals. We implement current available and develop new workflows to data-mine the Materials Project database for novel Dirac semimetals with desirable band structures and symmetry protected topological properties. This data-driven effort relies on the successful development of several automatic data generation and analysis tools, including a workflow for the automatic identification of topological invariants and pattern recognition techniques to find specific features in a massive number of computed band structures. Utilizing this approach, we successfully identified more than 15 novel Dirac point and Dirac nodal line systems that have not been theoretically predicted or experimentally identified. This work is supported by the Materials Project Predictive Modeling Center through the U.S. Department of Energy, Office of Basic Energy Sciences, Materials Sciences and Engineering Division, under Contract No. DE-AC02-05CH11231.

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