TWO-DIMENSIONAL MATERIALS FROM HIGH-THROUGHPUT COMPUTATIONAL EXFOLIATION OF EXPERIMENTALLY KNOWN COMPOUNDS

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Two-dimensional (2D) materials have emerged as promising candidates for next-generation electronic and optoelectronic applications. Yet, only a few dozen 2D materials have been successfully synthesized or exfoliated.
Here, we search for 2D materials that can be easily exfoliated from their parent compounds. Starting from 108,423 unique, experimentally known 3D compounds, we identify a subset of 5,619 compounds that appear layered according to robust geometric and bonding criteria.
High-throughput calculations using van der Waals density functional theory, validated against experimental structural data and calculated random phase approximation binding energies, further allowed the identification of 1,825 compounds that are either easily or potentially exfoliable.
In particular, the subset of 1,036 easily exfoliable cases provides novel structural prototypes and simple ternary compounds as well as a large portfolio of materials to search from for optimal properties. For a subset of 258 compounds, we explore vibrational, electronic, magnetic and topological properties, identifying 56 ferromagnetic and antiferromagnetic systems, including half-metals and half-semiconductors.