Novel two-dimensional materials from high-throughput computational exfoliation of experimentally known compounds

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We search for novel two-dimensional materials that can be easily exfoliated from their parent compounds. Starting from 108423 unique, experimentally known three-dimensional compounds we identify a subset of 5619 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, allow to identify 1844 compounds that are either easily or potentially exfoliable, including all that are commonly exfoliated experimentally. In particular, the subset of 1053 easily exfoliable cases −layered materials held together mostly by dispersion interactions and with binding energies in the range of few tens of meV/A^2 contains several hundreds of entries with few atoms per primitive cell (273 with less than 6 atoms, 606 with less than 12), revealing a wealth of new structural prototypes, simple ternary compounds, and a large portfolio to search for optimal electronic, optical, magnetic, topological, or chemical properties.

References

[1] N. Mounet et al., https://arxiv.org/abs/1611.05234 (2016)

Figures

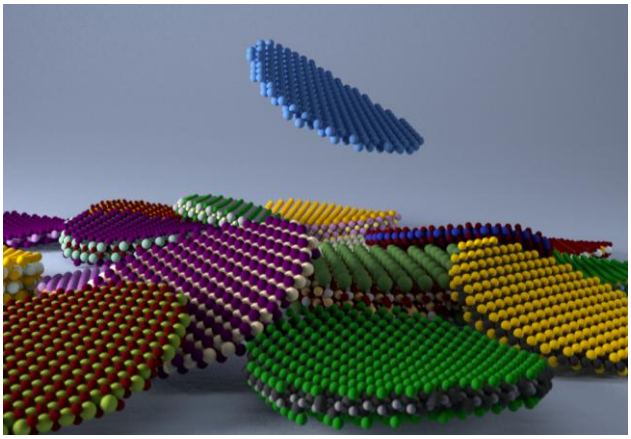

Figure 1: Artist's rendition of the exfoliated layers.

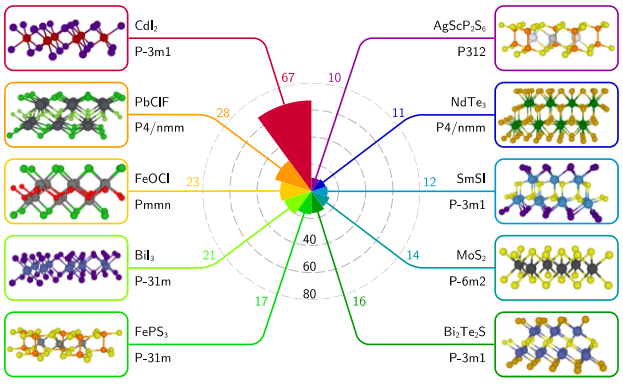

Figure 2: the 10 most common prototypes found; each class includes between 10 and 67 actual crystals.