Computational Exfoliation of All Known Inorganic Materials

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Abstract We use extensive, high-throughput first-principles calculations to identify novel 2D materials that can be exfoliated from known parent compounds. Starting from 480,000 non-unique structures harvested from experimental databases of crystal structures (ICSD [1] and COD [2]), we identify first 6400 unique inorganic materials that appear layered according to simple geometric and bonding criteria. Then, quantum simulation based on van-der-Waals-corrected density-functional theory are used to assess the metallic, insulating or magnetic character of the 3D parents and of the individual 2D layers, together with their binding energies, leading to the identification of a 2D portfolio of 1800 candidate structures that are layered and weakly, van-der-Waals bound. Full phonon dispersions are computed to assess mechanical or charge-density wave instabilities. This large portfolio of prospective materials can now be explored for optimal properties and performance, or to observe the emergence of exciting physical properties; such work is made possible and straightforward by the development within the Swiss MARVEL NCCR of the AiiDA materials' informatics platform [3] for computational science – exploiting in this case its automated-workflows engine, database structure, sharing capabilities, and pipelines to and from crystallographic repositories.

Work done in collaboration with Nicolas Mounet, Philippe Schwaller, Andrea Cepellotti, Andrius Merkys, Ivano Eligio Castelli, Marco Gibertini, and Giovanni Pizzi.

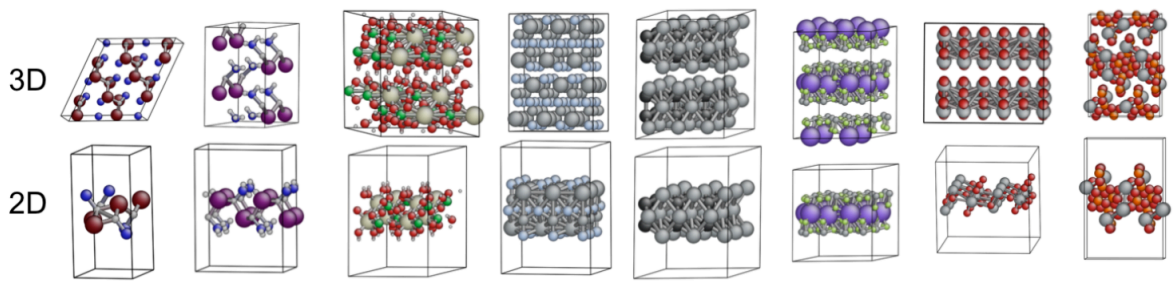
References

[1] http://www.fizkarlsruhe.com/icsd.htm

[2] S. Grazulis et al, Nucleic Acids Research, 40, D420 (2012).

[3] G. Pizzi, A. Cepellotti, R. Sabatini, N. Marzari and B. Kozinsky, Comp. Mat. Sci. 111, 218 (2016).

Figures



A few 3D layered materials, and their 2D counterparts, identified with high-throughput first-principles simulations.