Materials Cloud two-dimensional crystals database (MC2D)

The 2D structures are originating from the computational exfoliation of experimental bulk (3D) materials extracted from the **ICSD** [1], the **COD** [2] and the **MPDS** [3] databases. From the initial database entries, the procedure consisted in:

- cleaning improperly formatted CIF files with **cod-tools**
- filtering out disordered structures, incompletely defined ones and those obviously wrong
- converting CIF files into **AiiDA** structures, using **pymatgen**
- correcting round-off errors in the atomic positions to recover the structure symmetries, thanks to **spglib**
- filtering out duplicate structures
- screening layered materials thanks to a geometrical algorithm based on the identification of chemical bonds from interatomic distances, using van der Waals atomic radii.
- relaxing and computing the binding energies of the layered materials, using the **Quantum ESPRESSO** code with **DFT-PBE** van der Waals functionals (**rVV10** and **DF2-C09**, tested and converged pseudopotentials from the **SSSP)**
- selecting easily exfoliable materials as those for which the binding energy is less than 30 meV/Å^2 (with the DF2-C09 functional) or 35 meV/Å^2 (with rVV10) and potentially exfoliable materials for which the binding energy is less than 120 meV/Å^2
- optimizing the geometry of the monolayers as an isolated system using the PBE functional.

On the subset of 2D easily exfoliable monolayers with less than 6 atoms in the unit cell, found in N. Mounet et al., Nat. Nanotech. doi:10.1038/s41565-017-0035-5 (2018) we also computed (at the PBE level):

- possible ferromagnetic and antiferromagnetic configurations, to obtain the magnetic ground state
- electronic band structure
- phonon dispersion curves.

More details can be found in:

N. Mounet, M. Gibertini, P. Schwaller, D. Campi, A. Merkys, A. Marrazzo, T. Sohier, I. E. Castelli, A. Cepellotti, G. Pizzi & N. Marzari, Two-dimensional materials from high-throughput computational exfoliation of experimentally known compounds, Nat. Nanotech. doi:10.1038/s41565-017-0035-5 **(2018)**

D. Campi, N. Mounet, M. Gibertini, G. Pizzi & N. Marzari, In preparation (2021).

The data archive and AiiDA database of structures and calculations for N. Mounet et al. Nat. Nanotech. doi:10.1038/s41565-017-0035-5 (2018) are available at https://doi.org/10.24435/materialscloud:az-b2.