Morten Gjerding
Sten Haastrup, Mikkel Strange, Mohnish Pandey, Thorsten Deilmann, Per S. Schmidt, Nicki F. Hinsche, Morten N. Gjerding, Daniele Torelli, Peter M. Larsen, Anders C. Riis-Jensen, Jakob Gath, Karsten W. Jacobsen, Jens Jørgen Mortensen, Thomas Olsen, Kristian S. Thygesen
CAMD, Department of Physics and Center for Nanostructured Graphene (CNG), Technical University of Denmark, 2800 Kgs. Lyngby

mogje@fysik.dtu.dk

The Computational 2D Materials Database: High-throughput modeling and discovery of atomically thin crystals

Here we present the Computational 2D Materials Database[1] (C2DB), a comprehensive open-access database of around 2000 two-dimensional materials which organizes a large variety of structural, thermodynamic, elastic, electronic, magnetic, and optical properties. The material properties have been systematically calculated by state-of-the-art density functional theory and many-body perturbation theory (G_0W_0 and the Bethe–Salpeter equation for ~250 materials) following a semi-automated workflow for maximal consistency and transparency. The C2DB is fully open and can be browsed online (http://c2db.fysik.dtu.dk) or downloaded in its entirety and is constantly expanding by including new crystal prototypes following our lattice decoration approach (Fig. 1). Applications of the database will be presented, identifying a large number of new potentially synthesizable 2D materials for applications within plasmonics, spintronics and (opto-)electronics. The C2DB offers a comprehensive and easily accessible overview of the rapidly expanding family of 2D materials and forms an ideal platform for computational modeling and design of new 2D materials and van der Waals heterostructures.

References

[1] Haastrup et al., 2D Materials, 5 (2018) 042002

Figures

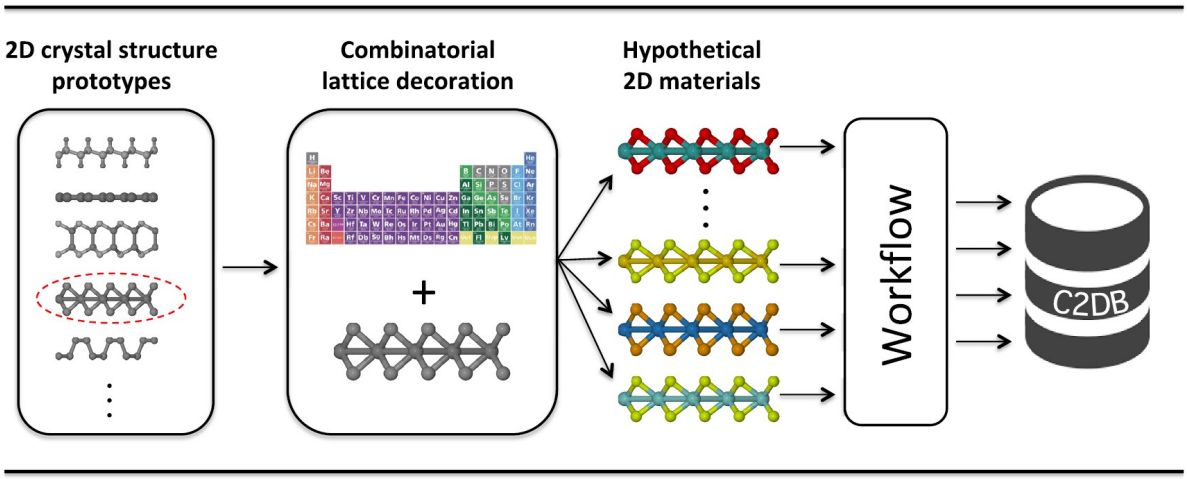

Figure 1: The materials in the C2DB are initially generated by decorating an experimentally known crystal structure prototype with atoms chosen from a (chemically reasonable) subset of the periodic table.