Building a digital 2D materials discovery platform

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The ever-increasing computer power in combination with accurate ab initio modelling codes and automated workflow engines has ushered in a new era of materials researches where computer experiments are used to guide and accelerate the discovery of new materials. Today, there are numerous databases containing a myriad of computed materials structures and properties. Among these, the Computational 2D Materials Database (C2DB) provides open access to a wide range of computed properties for more than 17,000 2D monolayers [1, 2].

Recently, the C2DB has been used as the basis for generating numerous new and unique databases, such as the Quantum Point Defect Database (QPOD) [3], the Bilayer Database (BiDB) [4], and 2D-alloy DB [5] and the van der Waals heterostructure database HetDB (to-be published), among others. While QPOD contains the structures and basic properties of point defects in about 100 different monolayers, BiDB contains homobilayers created by stacking more than 1,000 monolayers in all possible configurations. The 2D-Alloys database contains almost 1,000 transition metal dichalcogenide (TMDC) alloys including high entropy alloys, and HetDB contains several hundred van der Waals heterobilayers. All these databases are seamlessly connected to the C2DB and accessible via a standard web portal.

Here we report on the most recent advances of the C2DB+ digital platform. In addition to the QPOD, 2D-alloy DB, and BiDB, we discuss our ongoing efforts to improve the type, quality, and presentation of the data in the C2DB.

References

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