Advancing the C2DB+ Digital Platform for 2D Materials Science: In-depth Analysis of Point Defects and Bilayers

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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 5,000 2D monolayers [1,2].

Recently, the C2DB has been used as the basis for generating two new and unique databases, namely the Quantum Point Defect Database (QPOD) [3] and the Bilayer Database (BiDB) [4]. While QPOD contains the structures and basic properties of point defects in about 100 different monolayers, BiDB contains homobilayers created by stacking more than 1000 monolayers in all possible configurations. Both of 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 and BiDB, we discuss our ongoing efforts to improve the type, quality, and presentation of the data in the C2DB.

References

[1] Gjerding et al., Recent Progress of the Computational 2D Materials Database (C2DB), 2D Materials 8, 044002 (2021).
[2] Lyngby and Thygesen, Ab initio property characterisation of thousands of previously unknown 2D materials, arXiv:2402.02783.
[3] Bertoldo et al., Quantum point defects in 2D materials - the QPOD database, npj Comput Mater 8, 56 (2022).
[4] S. Pakdel et al., High-throughput computational stacking reveals emergent properties in natural van der Waals bilayers, Nature Communications 15, 932 (2024).