The Computational 2D Database: Using high throughput calculations and data mining to find high-mobility semiconductors

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After the discovery of graphene, the hunt has been on for novel 2D materials with unique properties. Many layered structures have already been added to the arsenal, including hexagonal boron nitride, black phosphorus, the transition metal dichalcogenides and many more. Recently, there has been a push for computational discovery and description of 2D materials.

The Computational 2D Materials Database (C2DB) is a new database of predicted 2D materials, and organises organises a variety of structural, elastic, electronic, magnetic, dielectric, and optical properties. More than 1500 2D materials are currently included. All material properties are systematically calculated by state-of-the art density functional theory and many-body perturbation theory (GW and the Bethe-Salpeter Equation). Tight numerical settings and strict convergence criteria are employed throughout the workflow to ensure the highest numerical data quality.

The availability and quality of of the large amounts data, make for natural application of data mining techniques. In particular, using the data present in the database, one can estimate the mobility of the semiconductors, using the deformation potentials[1] and the takagi formalism[2]. At the same time, interesting trends and correlations in the mobilities can be investigated.

We will give an overview of the capabilities of the database, in the context of the specific example of searching for high-mobility 2D semiconductors.

References

[1] J. Bardeen and W. Shockley, Phys Rev, 1950 (80) 72
[2] S. Takagi *et al, IEEE* transactions on electron devices, 1994 (41) 2357

Figures

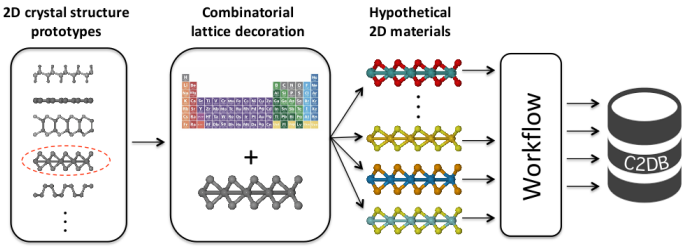

Figure 1: The workflow used to generate the C2DB

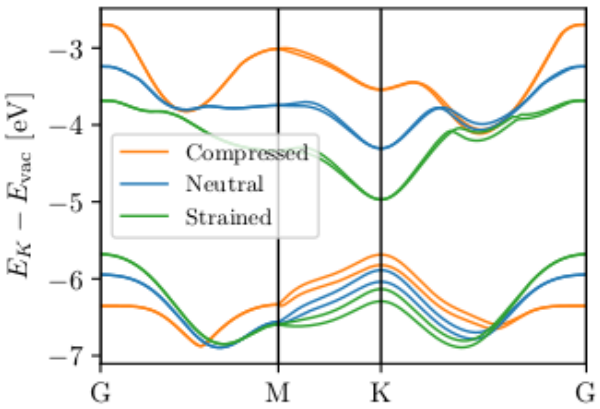

Figure 2: The lowest conduction band and highest valence band of MoS2 under different strains.