2D Materials: Genome, Discovery and Applications

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Abstract

Given the enormous interest and potential applications of two-dimensional (2D) materials and the importance of discovering new 2D materials, we are developing a genome for 2D materials. An update on the progress of this project will be given. To generate initial structures for the 2D materials database, we have screened three-dimensional (3D) materials in the Materials Project[1] database and identified >2,000 potential layered materials by applying simple rules based on inter-atomic distances and bonded clusters of atoms in the structures. Exfoliation energies of these materials are calculated to identify structures that can be exfoliated into 2D monolayers. High-throughput first-principles calculations are performed to obtain their properties.

High throughput computational screening was carried out to predict 2D hetero-structures with high solar power conversion efficiency (PCE). More than 1,000 hetero-junctions formed by >50 2D materials were considered. Based on the calculated band alignments, close to 100 hetero-junctions were predicted to have PCE higher than 15%, of which 17 have PCE > 20%.

Separately, we found that valley polarization can be achieved by proximity coupling monolayer transition metal dichalcogenides (TMDs), MoS_2, to magnetic insulator substrate, MnO, and the magnitude of valley splitting can be further tuned continually by external strain. Due to the sizeable Berry curvature and time-reversal symmetry breaking in TMDs when placed on magnetic substrate, a spin and valley polarized anomalous Hall current can be obtained in the presence of in-plane electrical field, which provides a mean to detect the valleys by electric measurements and forms the basis for valleytronic device.

References

[1] https://materialsproject.org/
[2] J. J. Linghu, T. Yang, Y. Z. Luo, M. Yang, J. Zhou, L. Shen, Y. P. Feng, submitted.
[3] L. Xu, M. Yang, L. Shen, J. Zhou, T. Zhu, Y. P. Feng, Phys. Rev. B 97 (2018) 041405(R).

Figures

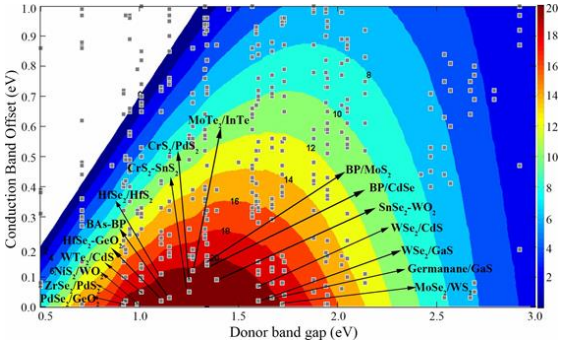

Figure 1: Simulated power conversion efficiency of vertical 2D heterostructure excitonic solar cells.

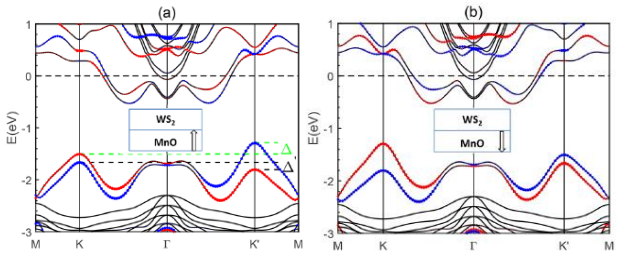

Figure 2: The band structure of the WS2/MnO heterostructure, for surface Mn atoms magnetized upward and downward, respectively.