From Detrimental to Useful Point Defects in 2D Semiconductors: Introducing the QuPoD Database

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Point defects are unavoidable entities in any crystal structure and their presence has an impact on applications in semiconducting materials. On the one hand, defects can be detrimental to performance for example in photovoltaic applications [1]. On the other hand, one can make use of a point defect's unique properties to form the basis for novel applications in spintronics [2] and quantum computing [3], as can be seen with the realization of single photon emitters (SPEs) in 2D materials [4]. Based on the computational 2D materials database (C2DB) [5] we perform a systematic study of intrinsic point defects among numerous host materials to find new and interesting defect candidates for potential future applications, as well as identifying defect tolerant materials. We find general trends in the formation of defects in 2D semiconductors and present a tool within the atomic simulation recipes (ASR) [6] and atomic simulation environment (ASE) [7] to facilitate automatic high-throughput calculations of defects. The publicly available and easily browsable defect database (QuPoD) is presented featuring over 500 defect systems with a wide range of defect properties included. These properties range from thermodynamic defect energetics, electronic and structural defect symmetries, transition dipole moments, hyperfine coupling parameters. QuPoD aims to help understanding the physics of point defects better and to assist driving the transition towards new defect mediated applications in 2D materials.

References

[1] Polman, et al., Science, 532 (2016)
[2] Awschalom, et al., Science, 330 (2013) 1174
[3] Eckstein, et al., MRS Bulletin 38 (2013) 783
[4] Chakraborty, et al., Nature Nanotechnology 10 (2015) 507
[5] Gjerding, et al., 2D Materials, 8 (2021) 044002
[6] Gjerding, et al., Comp. Mat. Science, 199 (2021) 110731
[7] Larsen, et al., Journal of Physics: Condensed Matter, 29 (2017) 273002

Figures

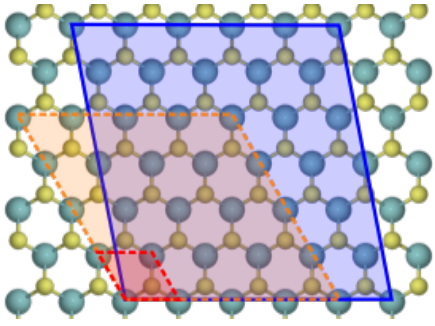

Figure 1: Setup of defect supercells with the ASR defect framework.