Computational Design of Quantum Defects in Low-Dimensional Semiconductors

Fabian Bertoldo
Simone Manti, Sajid Ali, Kristian Thygesen
Technical University of Denmark, DK-2800 Kgs. Lyngby
fafb@dtu.dk

2D materials are known to host intriguing electronic properties and thus offer a fascinating platform for quantum photonics. In particular, 2D materials have been shown to host single-photon emitters (SPE). It is therefore vital to investigate the influence of defects within different host materials which are much easier to create and control in monolayers compared to bulk systems. Based on the computational 2D materials database (C2DB) [1] we first perform a computational screening for intrinsic point defects of stable theoretically predicted and experimentally known low-dimensional semiconductors. We will present a tool within the atomic simulation environment (ASE) [2] to automatically identify intrinsic point defects for given structures and calculate properties like formation energies, charge transition levels, and more to pave the way towards creating a database of intrinsic defects in 2D semiconductors.

References

[1] The Computational 2D Materials Database: High-throughput modeling and discovery of atomically thin crystals, S. Haastrup et al. 2D Materials 5, 042002 (2018)
[2] The atomic simulation environment - a Python library for work-ing with atoms, A. Larsen et al. Journal of Physics: Condensed Matter, 29(27): 273002, 2017

Figures

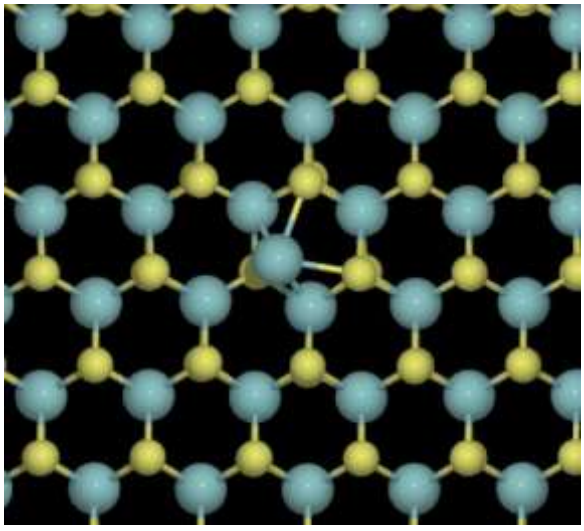

Figure 1: Mo substitutional defect in 2H-MoS_2 monolayer