DFT search for point defects in semiconductors for quantum devices

IGOR ABRIKOSOV[1]

[1]*Linköping University, Campus Valla, Linköping, Sweden*
igor.abrikosov@liu.se

ABSTRACT

Defects in semiconductors, such as NV centers in diamond, have shown excellent properties suitable for room temperature qubits. Thus, identification of new point defects in wide band gap semiconductors that can implement qubits and single photon emitters accelerates a transition towards the next generation quantum technology. We present a DFT-based strategy for a systematic exploration of the vast area of point defects with high potential for quantum applications. First, accuracy and efficiency aspects of DFT methods relevant for the studies are discussed [1]. Next, Automatic Defect Analysis and Qualification (ADAQ) package developed for high-throughput simulations of magneto-optical properties of point defects in semiconductors is introduced [2]. Data for tens of thousands of point defects in diamond and SiC is collected in the ADAQ database [3]. Upon exploring this database, we identify a collection of color centers of particular interest. Presenting one case, the ClV center in SiC [4] we demonstrate through high-accuracy DFT calculations that the center is similar to the NV center in diamond in its local structure and shares many qualitative and quantitative features in the electronic structure and spin properties. In contrast to the NV center, however, the ClV center in SiC exhibits emission in the telecom range near the C band. We conclude that it is possible to theoretically identify promising new color centers and discuss opportunities to implement theoretical predictions in experiments.

References

[1] V. Ivády, I. A. Abrikosov, and Adam Gali, First principles calculation of spin related quantities for point defect qubit research. *Npj Comp. Mater.* **2018**, 4, 76.

[2] J. Davidsson, V. Ivády, R. Armiento, and I. A. Abrikosov, Adaq: Automatic workflows for magnetooptical properties of point defects in semiconductors. *Comput. Phys. Commun* **2021**, 269, 108091.

[3] J. Davidsson, W. Stenlund, A. S. Parackal, R. Armiento, I. A. Abrikosov, Na in Diamond: High Spin Defects Revealed by the ADAQ High-Throughput Computational Database. *arXiv:2306.11116*; https://defects.anyterial.se/

[4] O. Bulancea-Lindvall, J. Davidsson, R. Armiento, I. A. Abrikosov, Chlorine vacancy in 4H-SiC: An NV-like defect with telecom-wavelength emission. *Phys. Rev. B* **2023**, 108, 224106.