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Ab initio emission lineshape modeling of color centers in semiconductors

Rokas Silkinis and Lukas Razinkovas

Department of Fundamental Research, Center for Physical Sciences and Technology (FTMC), Saulėtekio al. 3, LT-10257, Vilnius, Lithuania

Email: rokas.silkinis@ftmc.lt

Deep-level point defects in semiconductors have emerged as versatile platforms for quantum sensing, communication, and information processing. Identifying and characterizing these centers requires reliable theoretical methods to determine their electronic and optical signatures. In this work, we present high-resolution calculations of the emission lineshapes for a handful of technologically relevant color centers using a force-constant embedding methodology [1]. This approach exploits the short-range nature of interatomic forces to describe the vibrational structure and electron–phonon coupling, enabling the simulation of defects in the dilute limit entirely from first principles.

However, standard density functional theory (DFT) often struggles with defects exhibiting complex electronic structures or non-adiabatic vibronic interactions. By combining the embedding methodology with specialized computational strategies, we demonstrate that it is possible to accurately reproduce experimental spectral fingerprints that fall outside the reach of standard adiabatic frameworks. Our results underscore the need for new methodologies to advance predictive modeling and the discovery of quantum point defects in semiconductor materials.

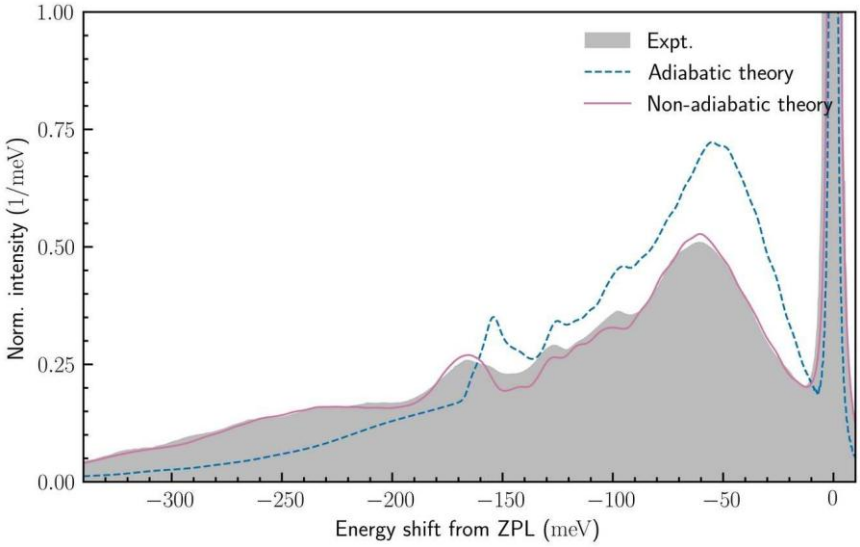

Figure 1. Calculated emission lineshapes of the NiV center in diamond obtained using adiabatic and non-adiabatic theories. Experimental lowtemperature data are taken from [2].

REFERENCES

[1] L. Razinkovas, M. W. Doherty, N. B. Manson, C. G. Van de Walle, and A. Alkauskas, Vibrational and vibronic structure of isolated point defects: The nitrogen-vacancy center in diamond, Phys. Rev. B 104 (2021) pp. 045303. [2] A. T. Collins and P. M. Spear, The 1.40 eV and 2.56 eV centres in synthetic diamond, J. Phys. C: Solid State Phys. 16 (1983) pp. 963-973.