VIBRATIONAL PROPERTIES AND PHOTOIONIZATION OF THE DIAMOND NV CENTER: THEORY AND *AB INITIO* CALCULATIONS

Lukas Razinkovas

Center for Physical Sciences and Technology, Savanoriu Ave. 231, LT-02300 Vilnius, Lithuania
lukas.razinkovas@ftmc.lt

The negatively charged nitrogen-vacancy (NV-) center in diamond has become one of the leading platforms to test and implement various quantum technologies [1]. Most of these applications rely on the optical excitation. However, optical excitation can lead to the photoionization process, whereby NV- is converted to NV0. For many applications this is a detrimental process, but in some cases deliberate ionization of NVs can also be very beneficial [2, 3].

In this talk we will present our recent theoretical work on the NV- center [4, 5]. In the first part, we will discuss the first-principles description of the vibrational broadening of optical emission and absorption lines. In the second part of the talk, we will address the photoionization processes of NV centers. Novel computational techniques to achieve converged photoionization cross sections will be introduced. The main results of our work are summarized in Figure 1.

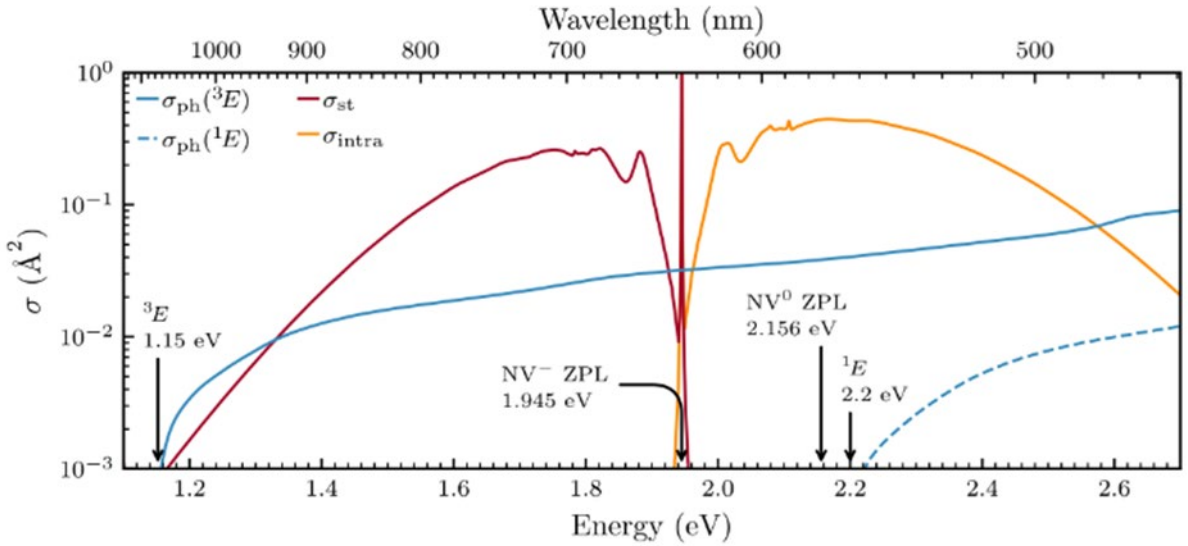

Fig. 1. Calculated cross sections as a function of photon energy. Solid blue: photoionization from the excited state ^{3}E, σ_{ph}; dark red: stimulated emission, σ_{st}; orange: intra-defect absorption, σ_{intra}; dashed blue: photoionization from the singlet state ^{1}E.

In the presentation, the evolution of optical coatings from one-dimensional to tree-dimensional periodic structures will be presented. The focus will be on two topics: i) anisotropic coatings for polarization control [1,2] and ii) the possibility to form the dielectric structures with periodic modulation of optical constants together with the application of angular filtering of light [3,4]. The investigation of different technologies for the single layer and multilayer coating deposition on nanostructured surfaces will be reviewed.

References

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