Theoretical Modeling of Vibrationally Resolved Optical Lineshapes of Semiconductor Deep-Level Defects

Lukas Razinkovas
Department of Fundamental Research, FTMC, Saulėtekio al. 3, Vilnius, Lithuania

Optically active semiconductor deep-level defects have emerged as essential building blocks for various quantum technologies, including quantum computing, quantum sensing, and quantum communication. Theoretical modeling and characterization of their optical properties are pivotal in chemical identification, understanding their fundamental properties, and harnessing their potential for quantum applications.

This talk aims to explore the theoretical modeling techniques employed to unravel the vibrationally resolved optical signatures of deep-level defects. The presentation will begin by overviewing the established theory for optical transitions between two non-degenerate electronic states. Practical computational methodologies to obtain high-resolution optical emission and absorption lineshapes will be presented with examples of defects in diamond, silicon, and silicon carbide.

Next, the talk will explore the theoretical modeling approaches employed to simulate and interpret optical spectra associated with transitions involving degenerate electronic states. Such electronic degeneracy commonly gives rise to the dynamical Jahn-Teller effect, which emerges from the intricate coupling between electronic and vibrational degrees of freedom. The presentation will explore practical computational methodologies that enable the analysis of multimode Jahn-Teller coupling and its impact on optical lineshapes.