Semiconductor Nanostructures “Momentum” Research Group:

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In 2024, our research group has made further substantial steps towards developing elementary hardware elements for quantum information processing. These elements are solid-state quantum bits, in most cases point defects which show magneto-optical behavior which can be harnessed to store and process quantum information. A proper investigation of such systems include their precise physical description, as for both their actual molecular structure and electronic system properties, as well as proposing a set of so-called quantum protocols which make them really usable as quantum bits, and finally validating their fundamental chemical and engineering properties for the usage in real quantum information processing environments. In almost every case, these systems are also promising candidates for nanometrology (nanosensing, biosensing) applications, as the physics of these two fields are closely related. We executed *ab initio* calculations on modeling the qubits by KIFÜ high-performance computing units as well as our local high performance computation cluster.

Defect qubits in solids. The most important methodological developments are related to the dynamic properties of nuclei, how to calculate spin resonance parameters such as hyperfine tensors and expected values of quadruple moments in dynamic Jahn-Teller systems, and how to derive, for example, the nuclear spin relaxation rate of nitrogen-vacancy center in diamonds (NV) the relaxation [1]. Furthermore, we found that mixed hydrogen and fluorine termination of (100) diamond surface is preferential to host shallow NV quantum sensors [2]. We also explained the microscopic mechanism of spin polarization of NV center under high magnetic fields [3]. We studied defect qubits in other materials too. We highlight two additional results. We identified a new color center in silicon that was engineered via epitaxy [4]. In the two-dimensional hexagonal boron nitride we characterized ultraviolet emitters when the stacking sequences are modified including moiré lattices. We found that the shape of the photoluminescence spectra can strongly vary in these host materials [5].

Development of experimental setups and materials. In the optically detected magnetic resonance laboratory (ODMR), we started to combine fluorescence lifetime imaging and electron spin resonance techniques in a user friendly design. This project is carried out in cooperation with R&D Ultrafast Lasers Ltd, University of Ulm and qutools GmbH in the framework of EUREKA program. We also develop materials showing persistent luminescence upon X-ray excitation, the so-called XEOL process. We designed a table top experimental setup to observe the XEOL process that we apply in a Horizon Europe Pathfinder project (PERSEUS).

References

[1] Resonant Versus Non-resonant Spin Readout of a Nitrogen-Vacancy Center in Diamond Under Cryogenic Conditions

[2] Diamond surface functionalization via visible light-driven C-H activation for nanoscale quantum sensing

[3] Terahertz emission from diamond nitrogen-vacancy centers

[4] All-Epitaxial Self-Assembly of Silicon Color Centers Confined Within Sub-Nanometer Thin Layers Using Ultra-Low Temperature Epitaxy

[5] Exceptionally strong coupling of defect emission in hexagonal boron nitride to stacking sequences