

CPP 25: Molecular Electronics and Photonics (joint session TT/CPP)

Time: Tuesday 12:00–13:00

Location: HSZ 201

CPP 25.1 Tue 12:00 HSZ 201

Single photon emitters in hBN via ultra-low energy helium ion implantation — ●RENU RANI¹, MIHN BUI^{1,2}, CHENFENG LU^{1,2}, BILAL MALIK^{1,2}, FELIX JUNGE³, THORSTEN BRAZDA¹, DETLEV GRÜTZMACHER^{1,2}, HANS HÖFSÄSS³, and BEATA KARDYNAL^{1,2} — ¹Peter Grünberg Institut-9, Forschungszentrum Jülich, Jülich — ²Department of Physics, RWTH Aachen, Aachen — ³II. Institute of Physics, University of Göttingen, 37077 Göttingen

A discovery of quantum emitters in hexagonal boron nitride (hBN) has recently incited immense interest for quantum technologies. It offers a platform for fundamental science but is also of interest for applications in quantum photonics owing to its robust single photon emission at room temperature. Recent studies have suggested that these SPEs are associated with intrinsic defects, which led to efforts to engineer the SPE in hBN by various methods such as plasma treatment, annealing, laser, e-beam and ion irradiation methods. Despite these efforts, the origin of single photon emission and the correlation of emission with particular defects still need to be scrutinized. Here we use ultra-low energy ion implantation to introduce defects in hBN. We show that helium ions with energies as low as 50 eV are extremely efficient in introducing single photon emitters in hBN. We also show that low temperature annealing increases the density of the emitters. We consider the possible defects that helium ions at the implantation energy can generate in hBN and use statistical data on single photon emitters to discuss the possible origin of the emission. Finally, we discuss the viability of creating emitters in pre-selected locations.

CPP 25.2 Tue 12:15 HSZ 201

Mechanosensitive single-molecule junctions — ●FABIAN PAULY — University of Augsburg, Augsburg, Germany

Quantum interference of electron waves passing through a single-molecule junction provides a powerful way to influence its electrical properties. By distorting a molecule, showing a destructive quantum interference, small changes of electrode distance can lead to huge changes of electrical conductance. This mechanosensitivity is a desirable feature for highly sensitive stress sensors. Here, I will discuss recent combined experimental and theoretical studies of mechanosensitive molecular wires based on paracyclophanes and porphyrins [1-4]. Experimental findings are interpreted in terms of quantum interference effects between molecular frontier orbitals by theoretical calculations based on density functional theory and the Landauer scattering formalism.

- [1] D. Stefani et al., *Nano Lett.* 18, 5981 (2018)
- [2] K. Reznikova et al., *J. Am. Chem. Soc.* 143, 13944 (2021)
- [3] W. M. Schosser et al., *Nanoscale* 14, 984 (2022)
- [4] C. Hsu et al., *Chem. Sci.* 13, 8017 (2022)

CPP 25.3 Tue 12:30 HSZ 201

Designing mechanosensitive molecules: A genetic algorithm-based approach — ●MATTHIAS BLASCHKE and FABIAN PAULY — Institute of Physics, University of Augsburg, D-86159 Augsburg, Germany

Single molecules can be used as miniaturized functional electronic components, when connected to metallic electrodes. Mechanosensitivity describes a change of conductance for a certain change of electrode separation and is a desirable feature for applications such as ultrasensitive stress sensors [1-4]. We combine methods of artificial intelligence with high-level simulations based on electronic structure theory to design optimized mechanosensitive molecules from predefined building blocks. In this way we overcome time-consuming, inefficient trial and error cycles in molecular design. We unveil the black-box machinery usually connected to methods of artificial intelligence by presenting all important evolutionary processes. In addition, we identify general features that characterize well-performing molecules. Our genetic algorithm provides a systematic and powerful way to search chemical space and to identify the most promising molecular candidates.

- [1] D. Stefani et al., *Nano Lett.* 18, 5981 (2018)
- [2] K. Reznikova et al., *J. Am. Chem. Soc.* 143, 13944 (2021)
- [3] W. M. Schosser et al., *Nanoscale* 14, 984 (2022)
- [4] C. Hsu et al., *Chem. Sci.* 13, 8017 (2022)

CPP 25.4 Tue 12:45 HSZ 201

Towards cavity-mediated molecule-molecule coupling — ●ANDRÉ PSCHERER¹, JAHANGIR NOBAKHT¹, TOBIAS UTIKAL¹, STEPHAN GÖTZINGER^{2,1,3}, and VAHID SANDOGHDAR^{1,2} — ¹Max Planck Institute for the Science of Light, Erlangen, Germany — ²Department of Physics, Friedrich-Alexander University Erlangen-Nürnberg (FAU), Erlangen, Germany — ³Graduate School in Advanced Optical Technologies (SAOT), Friedrich-Alexander University Erlangen-Nürnberg, Erlangen, Germany

We recently demonstrated that a single molecule coupled to a Fabry-Pérot cavity reacts nonlinearly to light at the single-photon level. This was shown in four-wave mixing, optical switching and photon number sorting experiments [1]. We aim to exploit this level of control to couple two molecules to each other via the cavity mode and to explore two-photon transitions that become possible in such a system. We gain access to the excited state population through spectrally tailored cavity mirrors which transmit red-shifted fluorescence. In this contribution, we will report on our progress, challenges, and intermediate results.

- [1] A. Pscherer et al., *Phys. Rev. Lett.* **127**, 133603 (2021)