Symposium Spins in Molecular Systems: Strategies and Effects of Hyperpolarization (SYMS)

jointly organised by
the Thin Films Division (DS),
the Magnetism Division (MA),
the Low Temperature Physics Division (TT), and
the Surface Science Division (O)

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Spin hyperpolarization in molecular systems describes the transient electronic or nuclear spin order that surpasses the Boltzmann distribution. There is an enormously increasing interest in the fundamental aspects of building-up, transport and relaxation of spin hyperpolarization. Strategies that have been tested for building-up spin hyperpolarization include the controlled realization of molecule-based interfaces, spin pumping, spin injection, intersystem crossing or the chiral induced spin selectivity in molecular solids, thin films or devices. On the other hand, significant efforts are being made on the experimental and theoretical side to understand the mechanisms of transport of spin hyperpolarization and the related relaxation processes. This interdisciplinary symposium brings together experts working on various experimental and theoretical aspects of thin films, magnetism, surface science as well as device physics, aiming to identify common mechanisms involved in different hyperpolarization strategies in order to push synergistic advances in this field.

Overview of Invited Talks and Sessions

(Lecture hall H1)

Invited Talks

SYMS 1.1	Wed	15:00–15:30	H1	**Exploring the Non-Perturbative Magnetic Resonance Drive Regime with spin selection rules in a π-Conjugated Polymer** — •Christoph Boehme
SYMS 1.2	Wed	15:30–16:00	H1	**The puzzle of spin and charge transport in the chirality induced spin selectivity effect** — •Bart van Wees
SYMS 1.3	Wed	16:00–16:30	H1	**Nano- and Microscale NMR spectroscopy with spin qubits in diamond** — •Nabeel Aslam
SYMS 1.4	Wed	16:45–17:15	H1	**Spin effects in adsorbed organometallic complexes** — •Richard Berndt
SYMS 1.5	Wed	17:15–17:45	H1	**Quantum Computing with Molecules** — •Mario Ruben

Sessions

SYMS 1.1–1.5	Wed	15:00–17:45	H1	**Spins in Molecular Systems: Strategies and Effects of Hyperpolarization**

SYMS 1: Spins in Molecular Systems: Strategies and Effects of Hyperpolarization

Time: Wednesday 15:00–17:45 Location: H1

Invited Talk SYMS 1.1 Wed 15:00 H1

Exploring the Non-Perturbative Magnetic Resonance Drive Regime with spin selection rules in a π-Conjugated Polymer — •Christoph Boehme — Department of Physics & Astronomy, University of Utah, Salt Lake City, UT 84112, USA

Spin-dependent charge carrier recombination currents in π-conjugated polymers can be governed by radical pair physics, reflecting the spin-permutation symmetry of electron-hole spin-pair states, rather than spin-polarization states. This effect can be used to detect magnetic resonance under conditions unsuitable for conventional spectroscopy, such as low spin polarization or thin-film systems containing small spin ensembles (Frankevich et al., Phys. Rev. B, 1992, 46, 9320; Roundy and Raikh, Phys. Rev. B, 2013, 88, 125206). Recent work has demonstrated this mechanism's utility for studying strong-drive, non-perturbative magnetic resonance, where magnetic radiation amplitudes comparable to the static Zeeman field create hybrid spin-light states. This results in non-linear behaviors like spin-collectivity (Waters et al., Nat. Phys., 2015, 11, 910-914), multi-photon transitions, and fractional g-factor effects (Jamali et al., Nat. Commun., 2021, 12, 465; Jamali et al., Nano Lett., 2017, 17, 4648-4653; Ashton et al., 2020). Experimental confirmations include monochromatic multi-photon transitions, angular dependence of resonance shifts, and hybrid light-matter states, promising advancements in high-fidelity sensing qubits with long coherence times [S. I. Atwood et al., Phys. Rev. B 110, 195304 (2024); S. I. Atwood et al., Phys. Rev. B 110, L060103 (2024)].

Invited Talk SYMS 1.2 Wed 15:30 H1

The puzzle of spin and charge transport in the chirality induced spin selectivity effect — •Bart van Wees — Zernike Institute for Advanced Materials, University of Groningen, The Netherlands

I will present an overview of the current understanding of the chirality induced spin selectivity effect [1], as measured as a magnetoresistance in electronic devices and scanning probe geometries. I will describe the principles of chirality induced coupling of spin and charge currents, and show that this indeed allows to observe the specific chirality in non-linear transport experiments [2,3]. However, experiments at low bias, in the linear transport regime, show that Onsager's reciprocity relations are not obeyed. This, together with the large magnetoresistances which are observed, (sometimes exceeding 90% or more) are not compatible with descriptions in terms of spin (polarized) transport. I will discuss alternative mechanisms, which are based on the modification of the electrostatic potential profile, which depend on the interplay between chirality and magnetisation. These lead to a magnetoresistance due to a modification of the charge transport, not the spin transport. I will point out that open questions remain for these alternative mechanisms, and propose experimental stategies to address these. [1] Evers et al., Advanced Materials 34,13, 2106629 (2022) [2] X.Yang et al., Nano Letters 20, 8,6148 (2020) [3] X.Yang et al., Phys. Rev. B99, 024418 (2019 [4] S.H Tirion, and B.J. van Wees, ACS Nano 18/81, 6028 (2024) [5] Y. Zhao et al., ArXiv2201.03623v3

Invited Talk SYMS 1.3 Wed 16:00 H1

Nano- and Microscale NMR spectroscopy with spin qubits in diamond — •Nabeel Aslam — Leipzig University

Expanding nuclear magnetic resonance (NMR) spectroscopy to the micro- and nanoscale holds significant potential to advance research across disciplines. Potential applications include the chemical analysis of mass-limited samples, single-cell metabolomics for disease diagnostics, and the detection and characterization of individual proteins, such as functional membrane proteins.

In this talk, I will introduce a novel approach to nano- and microscale NMR using nitrogen-vacancy (NV) centers in diamond. These quantum defects can be optically polarized and read out, enabling highly sensitive detection of nuclear spins with exceptional spatial resolution. This capability is further enhanced through hyperpolarization techniques. I will provide an overview of the state-of-the-art in the field, including advancements in detecting nuclear spins on surfaces, integrating NV-based NMR with microfluidic technologies for high-throughput applications, and employing diffusion NMR to study molecular transport at the nanoscale.

Furthermore, I will discuss how nuclear spins in diamond can serve as quantum memories, enhancing the performance and versatility of NV-based sensing. This highly sensitive and versatile method has the potential to uncover new insights into complex systems in chemistry, biology, and material science.

15 min. break

Invited Talk SYMS 1.4 Wed 16:45 H1

Spin effects in adsorbed organometallic complexes — •Richard Berndt — Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel

By adsorbing organometallic complexes onto surfaces, high densities can be achieved and the molecules can be probed individually with a scanning tunneling microscope. This approach has enabled experiments on molecular spin switches and their interactions in artificial arrays. New insights have been gained into spin-crossover molecules, electrostatic interactions and their effect on spin states, and the role of orbital magnetic moments. The talk will highlight some results from this field as well as some of the challenges.

Invited Talk SYMS 1.5 Wed 17:15 H1

Quantum Computing with Molecules — •Mario Ruben — KIT, IQMT, 76344 Leopolshafen-Eggenstein — CESQ, Université Strasbourg, France

Nuclear spin states in molecules act as quantum registers for quantum operations. We report on the implementation of metal complexes into nanometer-sized spintronic devices by a combination of bottom-up self-assembly and top-down lithography techniques. The controlled generation of magnetic molecular nanostructures will be shown and persistence of their magnetic properties under confinement Molecular Quantum Devices will be proven. The Hilbert space spanned by the nuclear spins will be engineered synthetically and addressed both electrically and optically, partially at the single molecule level. Finally, Grovers quantum search algorithm will be implemented on the nuclear spin register of a TbPc2 Qudit.