

Call for Proposals

No. 45

29 May 2024

Priority Programme „Interactive Spin-State Switching (ISS)” (SPP 2491)

The Senate of the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) has announced the establishment of a new Priority Programme entitled “Interactive Spin-State Switching (ISS)” (SPP 2491). The programme is scheduled to run for six years; the present call invites proposals for the first three-year funding period (2025–2028).

Spin-state switching in molecular systems has prospective applications as smart pigment, sensors and in information processing and storage. Furthermore, it is relevant in biological processes and catalysis, where it can alter reactivity pathways. While the switching process itself is of molecular origin, the phenomenon has been mostly studied in bulk or using a top-down approach for the generation of nanostructures. Interactions between adjacent switches are found to be of high importance as they modify the materials’ properties, for instance, leading to cooperative behaviour. While considerable progress has been made in the field, it still lacks an in-depth understanding that would allow us to predict and design systems with desired physical and chemical properties. Similarly, the interaction of molecular spin switches with a matrix or surfaces is insufficiently understood. Recent achievements with microscopy and (ultrafast) electronic spectroscopy and diffraction, combined with the improved theoretical methods to describe such systems, give promise for an in-depth understanding of the switching process and the impact of interactions with the environment in a bottom-up approach. The focus of the Priority Programme “Interactive Spin-State Switching” will be to:

- provide a better understanding of the switching mechanism at the molecular level and of the interactions of the switches with the surroundings or additional functionalities through further development and application of newly emerged ultrafast X-ray methods, spectroscopy, microscopy and theoretical tools;
- develop additional small-scale readouts by exploiting interactions between molecules and with the substrate;
- build up molecular spin switches based on alternative mechanisms, for example, using additional triggers;
- adapting the sensitivity, the energy barrier and the response of the switching in view of device integration, for example, through additional readout options;
- establish unifying concepts between different spin-state switching mechanisms.

The Priority Programme SPP 2491 aims to start at the single molecule level to understand the interaction of switching units with the surrounding and/or with additional properties. The combined efforts of synthesis, sophisticated spectroscopic and high-resolved imaging methods, and

quantum chemistry are needed to develop and refine new fundamental concepts regarding the microscopic switching mechanisms.

Propositions within the Priority Programme 2491 should use a bottom-up approach with a strong focus on understanding microscopic mechanisms and interactions at the atomistic or molecular level. In addition, improved triggers and readouts are an important research target, for example, to investigate switching by electric field or with light as an abundant energy source (impact of photoactive ligand parts). This also includes the detection of spin-state switching by the change of luminescence or conductivity, or improved spin-state switches for device integration (high surface compatibility, improved processability). Furthermore, method developments in the context of exploring spin-state switching with improved spatial and temporal resolutions are welcome. Theory, including method development, is expected to focus on the precise and efficient description of the electronic structure of the molecular units, considering, as needed, the description of environmental effects, ensembles or larger assemblies including interactions with surfaces, or the description of the influence of different triggers (light, fields). Ideas for novel material classes of spin-state switching molecules besides the known phenomena spin crossover (SCO), coordination induced spin state switch (CISSS), valence tautomerism (VT) and electron transfer coupled spin transition (ETCST), as well as combinations thereof, are welcome.

Metal-free spin-state switches and the synthesis of new spin-state switches in bulk without any additional functionalities are not part of this Priority Programme.

The formation of consortia of principal investigators (preferably 2-3) is envisioned, and joint proposals preferably cover two of the three following areas:

- synthesis and characterisation of new multifunctional spin-state switches,
- spectroscopic investigations of ground and excited state properties in different environments,
- theoretical investigations on spin states of molecular systems in static or dynamic settings.

Proposals should emphasise the interlink with other projects to strengthen the interdisciplinary character of the SPP. Here, we encourage possible PIs to discuss and connect complementary project ideas already in the submission phase to form topical clusters. The participation of junior research groups and researchers in early career phases in the consortia is greatly encouraged.

Full proposals for the first three-year funding period must be written in English and submitted no later than **29 October 2024** via the DFG's electronic submission system "elan". Please go to "Proposal submission – New Project" and select "SPP 2491". If you are using the elan system for the first time, please note that you need to register yourself and your institutional address before being able to submit a proposal. Also, if you are planning to move to a different institution (e.g. with a Temporary Position for Principal Investigator), you need to register the new institutional address beforehand. Note that you will be asked to select the appropriate Priority Programme call during both the registration and the proposal process. Please make sure that all applicants of your project (in case there is more than one) start their registration two weeks before the submission deadline at the latest.

Please follow the guidelines for project submission in DFG forms 50.05_en (part B) and 54.01_en. The role and responsibilities assigned to each principal investigator and scientific co-worker

should be evident from the work programme within the proposal, specifically the tasks to be completed by doctoral researchers or postdocs. In the case of joint proposals, the assignment of requested funds to the individual PIs should also be evident.

Please send a copy of the summary of your final proposal by e-mail to the coordinator.

To allow potential participants of this Priority Programme to discuss possible joint proposals, research plans and collaborations, an in-person networking meeting is planned at the FSU Jena for **11 July 2024**. To efficiently plan this meeting, please contact the coordinator by the end of June to acknowledge your participation. Participation in this event is not mandatory for proposal submission.

The review meeting for the Priority Programme will be held in February 2025 in Jena or as a virtual meeting.

Further Information

More information on the Priority Programme is available under:

www.chemgeo.uni-jena.de/spp2491

The elan system can be accessed at:

<https://elan.dfg.de/en>

DFG forms 50.05 and 54.01 can be found at:

www.dfg.de/formulare/50_05

www.dfg.de/formulare/54_01

For scientific inquiries, please contact the Priority Programme coordinator:

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