

## Call for Proposals

No. 42

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### **Priority Programme „Interlinking Catalysts, Mechanisms and Reactor Concepts for the Conversion of Dinitrogen by Electrocatalytic, Photocatalytic and Photoelectrocatalytic Methods (“Nitroconversion”)” (SPP 2370)**

The Senate of the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) has announced the establishment of a new Priority Programme entitled “Interlinking Catalysts, Mechanisms and Reactor Concepts for the Conversion of Dinitrogen by Electrocatalytic, Photocatalytic and Photoelectrocatalytic Methods (“Nitroconversion”)” (SPP 2370). The programme is scheduled to run for six years; the present call invites proposals for the first three-year funding period (2022–2025).

With 945 kJ/mol, the triple bond of the dinitrogen ( $N_2$ ) molecule has one of the highest dissociation enthalpies among covalent bonds. Nowadays, more than 180 million tons of ammonia are produced annually from  $N_2$  world-wide based on the Haber-Bosch process, and the rapid growth of the world’s population would not have been possible without this industrial “artificial  $N_2$  conversion”. Downsides of this technology are however the high energy demand, the large  $CO_2$  emissions associated to this process (for 1 ton of ammonia 20–40 GJ are required and 1.5 tons of  $CO_2$  are produced) and the need of large centralised production sites, impeding decentralisation.

In view of the increasing  $CO_2$  concentration in the atmosphere, ongoing energy transitions, and development of alternative concepts for the activation of small molecules, new approaches for artificial  $N_2$  conversion are in demand. This includes (photo)electrocatalysis or photocatalysis, which can be operated decentralised under less harsh conditions powered by renewable electricity or light. Although intensely researched, the overall energy demand of these approaches for  $N_2$  conversion is still significantly higher, and the space-time yield is far too low to compete with the Haber-Bosch process. Notably, scales of the overall catalytic processes from the nano to the meter level are in most cases investigated isolated from each other, which hampers a disruptive breakthrough.

The Priority Programme focuses on the development of heterogeneous (1) electrocatalytic, (2) photocatalytic and (3) photoelectrochemical  $N_2$  conversion reactions for delocalised and sustainable  $N_2$  conversion pathways with – as a long-term objective – an overall energy consumption and space-time yield comparable to the Haber-Bosch process.

This is to be achieved by establishing insights into structure/activity relationships for catalysts including experimental and theoretical design strategies, along with developing novel electrode and reactor concepts to overcome  $N_2$  mass transfer limitations, and by using novel analytical techniques to investigate the underlying mechanisms to be able to design catalysts rationally, and to develop new reaction pathways. The Priority Programme is explicitly not limited to  $N_2$  conversion processes to ammonia but can also include research on oxidative conversions. Moreover, the respective counter reaction should be analysed in detail as well.

Molecular catalysts and immobilised molecular catalysts on surfaces as well as biological approaches are not part of this Priority Programme. Likewise, plasma-enhanced processes are excluded as well.

The Priority Programme focuses on the development of heterogeneous electrocatalytic, photocatalytic and photoelectrochemical  $N_2$  conversion reactions. Propositions within this programme should use solid materials for artificial dinitrogen conversion. The formation of consortia of multiple principle investigators (preferably 2–3) is envisioned, and joint proposals should cover at least two of the three following areas:

- catalyst synthesis and their physicochemical characterisation
- experimental and/or theoretical investigation of reaction mechanisms
- reaction engineering

Ideas for novel material classes as absorbers or catalysts are welcome as well as model systems to be studied for the understanding of elementary steps at the solid-liquid interface. The submission of proposals interlinking research on electrocatalysis with photoelectrochemistry and/or photocatalysis to identify common design strategies is greatly encouraged. Proposals should pay special emphasis to the interlink with other projects to strengthen the interdisciplinary character of the programme. Here, we encourage possible principle investigators to discuss and connect complementary project ideas already in the submission phase to form topical clusters. The participation of junior research groups and early career researchers 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 2021** via the DFG's electronic submission system "elan". Please go to "Proposal submission – New Project" and select "SPP 2370". 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 investigators) you need to register the new institutional address beforehand. Please make sure that all applicants of your project (in case there is more than one) start their registration at the latest two weeks before the submission deadline.

Please follow the guidelines for project submission in forms 50.05en (part B) and 54.01en. 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 PhD students or postdocs. In the case of joint proposals, the assignment of requested funds to the individual principle investigators 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 online preparation meeting is planned for **26 July 2021**. In order to efficiently plan this meeting, please contact the coordinator until end of June to acknowledge your participation. Participation in this event is not mandatory for proposal submission.

The review colloquium for the Priority Programme will be held in **February 2022** in Bayreuth or as a virtual meeting, depending on the Covid-19 pandemic.

### Further Information

More information on the Priority Programme is available under:

<https://www.spp2370.uni-bayreuth.de/en/index.html>

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](http://www.dfg.de/formulare/50_05)

[www.dfg.de/formulare/54\\_01](http://www.dfg.de/formulare/54_01)

For scientific enquiries, please contact the Priority Programme coordinator:

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