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Pressemitteilung

Helmholtz-Zentrum Dresden-Rossendorf
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12.02.2025
http://idw-online.de/de/news847371

Forschungsprojekte
Chemie, Energie, Informationstechnik, Physik / Astronomie, Werkstoffwissenschaften
überregional

New catalysts for more sustainability: CASUS scientist receives 1.8 million euros from BMBF "Quantum Future" program

The German Federal Ministry of Education and Research (BMBF) funds research into controlled quantum states of individual or coupled systems with its ongoing emerging talent program "Quantum Future". Among the first selected projects, which kicked off in January 2025, is "qHPC-GREEN", proposed by junior research group leader Dr. Werner Dobrautz. The computational chemist aims to model quantum mechanical systems at the heart of certain biochemical and physical phenomena that are relevant to environmental and energy challenges. The project running until the end of 2029 will combine quantum and high-performance computing to achieve this goal.

The project to be tackled with the grant Dobrautz received is tightly connected to catalysts. They increase the rate of chemical reactions without being altered in this process themselves. A vast majority of today's chemical and biochemical products rely on catalysts during production but their potential for even more innovation is huge. With his newly established junior research group "AI4Quantum" Werner Dobrautz is, among other topics, trying to understand how certain biocatalysts, a group of catalysts based on molecules that constitute life, work. "With this understanding, we could try to develop new industrial catalysts that can convey chemical reactions needed for more sustainable production processes", he says.

In his research proposal "Quantum-enhanced high-performance computing for the green energy transition" (qHPC-GREEN), successful in the BMBF's emerging research talent program "Quantum Future", Dobrautz picked a relevant use case: "Ammonium-based fertilizers raised agricultural productivity to a completely new level after their introduction over 100 years ago. But their industrial production needs a huge amount of energy. A technical process based on biological nitrogen fixation facilitated by the enzyme nitrogenase and its iron-molybdenum cofactor is a very promising alternative." However, this biocatalytic conversion of hydrogen and nitrogen into ammonium is not fully understood so far.

Divide-and-conquer strategy

A classic approach to lift the roadblock is to model the processes of the reaction. But it turned out that even today's high-performance computers (HPC) are not capable to unravel the complexity of the quantum mechanical mechanisms at the core of this nitrogen fixation route. "What we deal with here is what we call a small quantum system with less than 100 electrons and nuclei, typically represented by a few atoms or molecules", explains Dobrautz. "Additionally, the behavior of electrons in this system is highly interdependent due to their mutual repulsion and quantum mechanical interactions. This is what we call a quantum system with strong electronic correlation. Unfortunately, standard approximations used in quantum chemistry to model systems do not capture the true nature of systems with strong electronic correlation."

With no good approximations or other shortcuts available, the only solution is to let computers do all the calculations. As even classic HPC are not powerful enough, the qHPC-GREEN project aims to involve quantum computers (QC). The hybrid algorithmic framework suggested by the applicant directs calculations for weakly correlated regions of the quantum mechanical system under scrutiny to HPC – and calculations for strongly correlated regions to QC. "My approach combines the strengths of both classical and novel quantum computing hardware. While many hybrid systems are in development, our divide-and-conquer approach ensures resource efficiency even with the current constraints of quantum hardware", explains Dobrautz.

The HPC calculations for this project will be done both in-house, on HPC infrastructure of CASUS that is currently being installed at HZDR's new data center as well as at the JUWELS supercomputing cluster at Forschungszentrum Jülich. On the quantum computing side, the project benefits from collaborations with IBM Research Zurich in Switzerland, the Wallenberg Centre for Quantum Technology in Sweden, Finnish software company Algorithmiq, and Jülich Supercomputing Centre's JUNIQ (Jülich UNified Infrastructure for Quantum computing). As most quantum computing resources are still in the ramp-up phase and interest in using them is overwhelming, Dobrautz points out the – in comparison – modest qubits requirements of his approach, making his implementation viable on near-term quantum devices, which is a critical differentiator compared to more resource-intensive approaches tackling the problem of understanding strongly correlated quantum systems.

Success for Saxony's AI strategy

CASUS Director Prof. Thomas D. Kühne points out that postdoctoral researchers looking for their next career step currently have many options when they are an expert in artificial intelligence (AI) and quantum computing – and even more when they come with self-acquired funding: "I am therefore extremely pleased that Werner Dobrautz has decided to set up his first own research group with us. CASUS, the HZDR and Saxony's research landscape are thus once again proving that their concepts and the overall framework are at the forefront of the current competition for the most talented minds."

The 1.8 million euros awarded to him, Dobrautz will spent on hiring scientific personnel and on business travels. The third round of the emerging talent program "Quantum Future" runs from 2023 to 2026. Together with qHPC-GREEN, projects at the University of Hamburg (IonLinQ, 4.8 million euros) and at the University of Augsburg (HoliQC2, 1.3 million euros) kicked-off in January 2025. Further projects will likely be announced in the course of the year. Two times ten junior research groups have already been funded and established as part of the first two competitions in 2017 and 2021 with the majority of the selected group leaders by now already appointed to professorships.

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The Helmholtz-Zentrum Dresden-Rossendorf (HZDR) performs – as an independent German research center – research in the fields of energy, health, and matter. We focus on answering the following questions:
- How can energy and resources be utilized in an efficient, safe, and sustainable way?
- How can malignant tumors be more precisely visualized, characterized, and more effectively treated?
- How do matter and materials behave under the influence of strong fields and in smallest dimensions?

To help answer these research questions, HZDR operates large-scale facilities, which are also used by visiting researchers: the Ion Beam Center, the Dresden High Magnetic Field Laboratory and the ELBE Center for High-Power Radiation Sources.
HZDR is a member of the Helmholtz Association and has six sites (Dresden, Freiberg, Görlitz, Grenoble, Leipzig, Schenefeld near Hamburg) with almost 1,500 members of staff, of whom about 680 are scientists, including 200 Ph.D. candidates.

About the Center for Advanced Systems Understanding
CASUS was founded 2019 in Görlitz/Germany and pursues data-intensive interdisciplinary systems research in such diverse disciplines as earth systems research, systems biology or materials research. The goal of CASUS is to create digital images of complex systems of unprecedented fidelity to reality with innovative methods from mathematics, theoretical systems research, simulations as well as data and computer science to give answers to urgent societal questions. The founding partners of CASUS are the Helmholtz-Zentrum Dresden-Rossendorf (HZDR), the Helmholtz Centre for Environmental Research in Leipzig (UFZ), the Max Planck Institute of Molecular Cell Biology and Genetics in Dresden (MPI-CBG), the Technical University of Dresden (TUD) and the University of Wrocław (UWr). CASUS, managed as an institute of the HZDR, is funded by the German Federal Ministry of Education and Research (BMBF) and the Saxon State Ministry for Science, Culture and Tourism (SMWK). www.casus.science/

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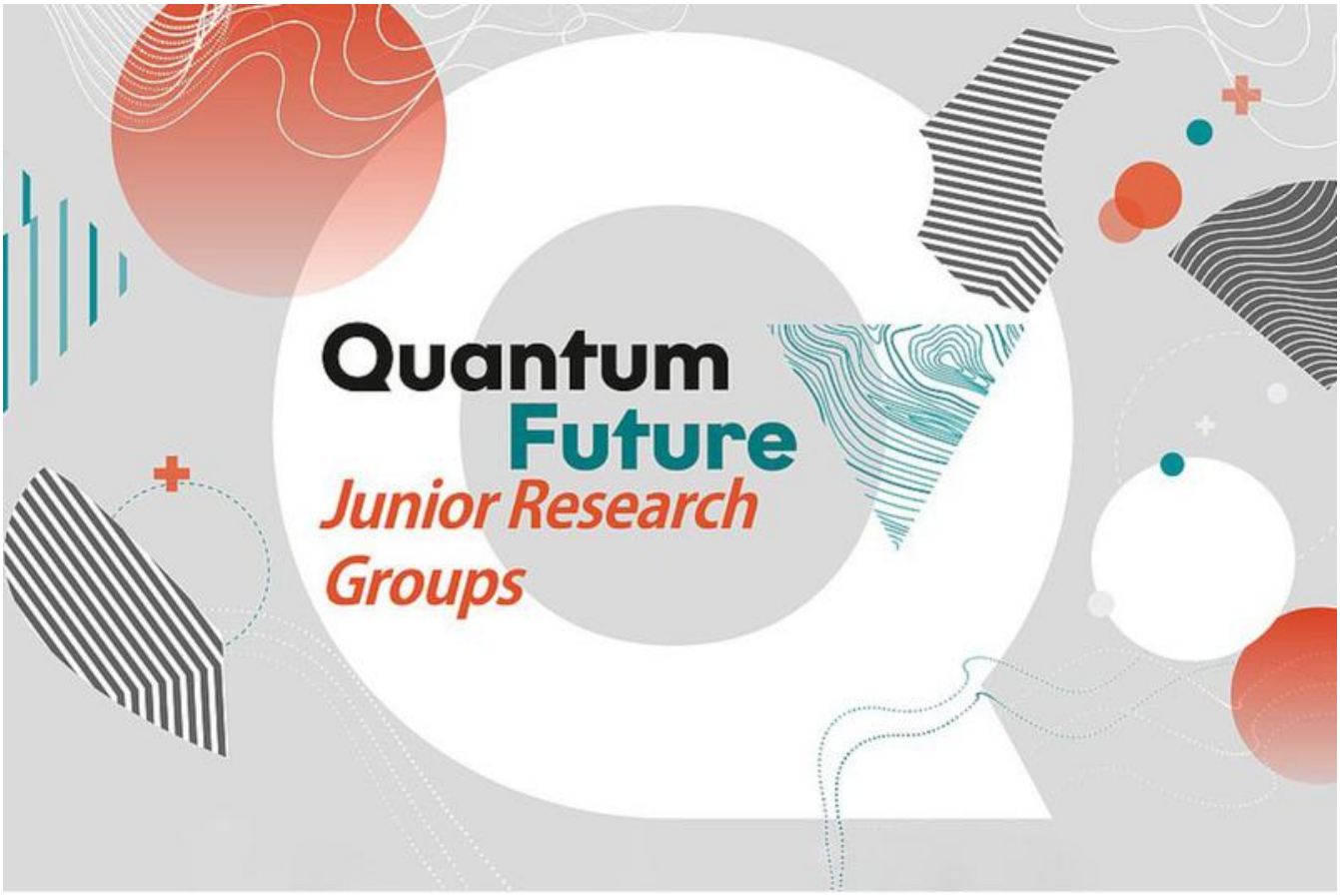

With the Quantum Future competition for emerging talent, the BMBF is helping to improve the framework conditions, particularly for scientists in an early career phase, and to increase Germany's attractiveness as a research location.
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