

We invite applications for

two PhD student (m/f/d) positions in Germany,

one in the Theoretical Molecular Spintronics group of Prof. Dr. Carmen Herrmann (University of Hamburg, tinyurl.com/herrmann-group), and one in the Computational Materials Design group of Prof. Dr. Jonny Proppe (TU Braunschweig, tinyurl.com/proppe-group).

The earliest starting date is April 1, 2023.

The focus of both PhD projects will be on the computational design of nanostructured systems with promising applications such as catalysis, biomedicine, thermoelectrics, batteries, and sensing. Magnetic metal-organic frameworks and single-molecule junctions in electronic components will constitute the core systems of the investigations, which will build on our recent joint publication and preprint on machine learning magnetic properties (<https://doi.org/10.1021/acs.jpca.0c05983>) and molecular conductance (<https://doi.org/10.26434/chemrxiv-2022-95ssc-v2>).

Our groups combine long-standing expertise on data-driven approaches in computational chemistry (Proppe group) and in theoretical molecular electronics and spintronics (Herrmann group). Both PhD projects will be located at the interface between quantum chemistry and machine learning, providing opportunities to acquire a broad range of skills.

Project 1 (Herrmann group): The main focus is on developing problem-tailored descriptors for machine-learning structure–property relationships, and for extracting insight from such calculations. The underlying data will be generated by molecular dynamics simulations and quantum chemistry.

Project 2 (Proppe group): The main goal of this project is to accelerate the discovery of novel nanostructured systems. To this end, data-economic algorithms (active learning) inspired by physical principles will be developed to replace prohibitively expensive quantum chemical calculations with machine-learned predictions.

Applicants should have a strong interest in theoretical chemistry/nanoscience and data science, a (prospective) master's degree or equivalent in one of these fields or a related subject, and a solid command of programming languages (in particular Python). Good basic knowledge of theoretical chemistry and condensed matter physics is preferable, as well as hands-on experience in machine learning. Solid English skills (both written and oral) are mandatory, knowledge of (or the willingness to learn) German is a plus.

The positions have guaranteed funding for 36 months. Salary will be paid at the TV-L E13 67% level, which corresponds to a regular work contract with healthcare, social security, paid parental leave and paid vacation. Guaranteed funds are available to attend yearly conferences.

Both PhD positions are part of a DFG-funded collaboration between our

groups. Regular meetings in Braunschweig and Hamburg will be a critical component of the PhD program. Braunschweig is a modern city with a rich past and only a stone's throw away from the headquarters of Volkswagen AG. The Proppe group is located at the charming Oker river, which encloses the medieval town center. Hamburg is a vibrant city in the north of Germany, with a long-standing history of being open to the world. The Herrmann group is located on the DESY campus, and we are part of the cluster "AIM: Centre for Ultrafast Imaging" within the national Excellence Initiative.

Please send your application documents via e-mail to Prof. Dr. Carmen Herrmann (carmen.herrmann[at]chemie.uni-hamburg.de) or Prof. Dr. Jonny Proppe (j.proppe[at]tu-braunschweig.de).

The application deadline is January 6, 2023.

Severely disabled persons are preferred in case of equal aptitude. Proof of disability must be enclosed. Our universities strive to reduce under-representation in all areas and positions. Therefore, applications from women are particularly welcome.

Personal data is stored for the purpose of carrying out the application process. Application costs cannot be reimbursed.

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