Conducting research for a changing society: This is what drives us at Forschungszentrum Jülich. As a member of the Helmholtz Association, we aim to tackle the grand societal challenges of our time and conduct research into the possibilities of a digitized society, a climate-friendly energy system, and a resource-efficient economy. Work together with around 7,500 employees in one of Europe's biggest research centres and help us to shape change!

Are you eager to pursue a four-year doctoral project that bridges scientific disciplines? Are you excited by complex societal challenges that demand interdisciplinary solutions? Then the Program for Collaborative Doctoral Projects is the perfect opportunity for you. Many of today's most pressing problems can only be tackled through interdisciplinary collaboration. That's why our projects are designed specifically to connect diverse scientific fields and foster cross-institutional collaboration, enabling you to benefit from the combined expertise and supervision of experienced researchers from multiple institutes at Forschungszentrum Jülich. As one of Europe's largest and most multidisciplinary research centres, Forschungszentrum Jülich offers access to state-of-the-art infrastructure and a vibrant scientific community.
Join us in developing solutions for a rapidly changing world and help shape the future by working in an international environment. For more information about the Program for Collaborative Doctoral Projects please visit: https://go.fzj.de/Collaborative-Doctoral-Projects

We are offering an interesting

Collaborative Doctoral Project (PhD Position) - Quantum-Classical Co-Simulation Framework Development for Neurobiological Systems

Your Job:
The overarching goal is to implement a code for multiscale quantum mechanics / molecular mechanics (QM/MM) molecular dynamics simulations using a Quantum Centric Supercomputing (QSC) approach [1,2] for the QM problem. This will be integrated within the in-house MiMiC framework [3] and applied to study proton transport in H+-coupled transporters. The project will be carried out in collaboration with a team of experts at FZJ (INM-9: Institute of Neuroscience and Medicine - Computational

The job will be advertised until the position has been successfully filled. You should therefore submit your application as soon as possible. We look forward to receiving your application via our **Online-Recruitment-System!**

Questions about the vacancy?
Get in touch with us by using **our contact form.**
Please note that for technical reasons we cannot accept applications via email.
www.fz-juelich.de

Biomedicine, IBI-1: Institute of Biological Information Processing - Molecular and Cellular Physiology; JSC: Jülich Supercomputing Centre) and from the US (IBM Research and Michigan State University).

Specific tasks include:

- Implement the classical components of the Sample-Based Quantum Diagonalization [1] method within the MiMiC multiscale simulation framework
- Develop and integrate a communication interface between quantum computers (via Qiskit) and classical HPC resources
- Validate the QCS-MiMiC implementation on IBM's ibm_cleveland quantum computer by reproducing recently published benchmark QM/MM simulations [2]
- Apply the developed code to simulate proton transport in vesicular glutamate transporters
- Collaborate closely with an interdisciplinary team across quantum computing, molecular simulation, and neurobiology
- Participation in conferences in Germany and abroad (incl. presenting your research results)
- Exchange with internal and external as well as national and international project partners
- Preparing scientific publications and project reports

[1] Kaliakin, D., Shajan, A., Moreno, J. R., Li, Z., Mitra, A., Motta, M., Johnson, C., Saki, A. A., Das, S., Sitdikov, I., Mezzacapo, A., & Merz, K. M. (2024). Accurate quantum-centric simulations of supramolecular interactions. http://arxiv.org/abs/2410.09209
[2] Bazayeva, M., Li, Z., Kaliakin, D., Liang, F., Shajan, A., Das, S., & Merz, K. M. (2025). Quantum-Centric Alchemical Free Energy Calculations. Mm, 1–35. http://arxiv.org/abs/2506.20825
[3] mimic-project.com

Your Profile:

- University degree (Master) in Physics, Chemistry, Computer Science, or related fields, with an overall grade of at least "gut" (or equivalent, e.g. cum laude)
- Expertise in quantum mechanics; Experience with HPC, programming (e.g., Python, C/C++), and/or scientific computing is a plus
- Strong interest in quantum computing and molecular simulations
- Willingness to work in an interdisciplinary, international team
- Fluent command of written and spoken English
- High degree of independence and commitment
- Very reliable and conscientious style of working

Please feel free to apply for the position even if you do not have all the required skills and knowledge. We may be able to teach you missing skills during your induction.

Our Offer:

We work on the very latest issues that impact our society and are offering you the chance to actively help in shaping the change! We offer ideal conditions for you to complete your doctoral degree:

- A large research campus in a green setting, offering excellent opportunities for networking with colleagues and for sports and recreation alongside your work
- Excellent scientific and technical infrastructure
- Opportunity to participate in (international) conferences and project meetings

- Continuous professional support from your scientific supervisors
- 30 days of annual leave
- The option of flexible working arrangements
- Targeted services for international employees, e.g. through our International Advisory Service
- Further development of your personal strengths, e.g. through an extensive range of training courses; a structured program of continuing education and networking opportunities specifically for doctoral researchers via JuDocS, the Jülich Center for Doctoral Researchers and Supervisors: https://www.fz-juelich.de/en/judocs

In addition to exciting tasks and a collaborative working atmosphere at Jülich, we have a lot more to offer: https://go.fzj.de/benefits

We offer a 4-year PhD position. Salary and social benefits in conformity with the provisions of the Collective Agreement for the Civil Service (TVöD). Depending on your qualifications and the precise nature of the tasks, salary grade 13 TVöD-Bund (up to 100%) and additionally 60 % of a monthly salary as special payment („Christmas bonus“). The monthly salaries in euro can be found on the BMI website: https://go.fzj.de/bmi.tvoed.entgelt

Further information on doctoral degrees at Forschungszentrum Jülich (including its various branch offices) is available at https://www.fz-juelich.de/en/careers/phd

We welcome applications from people with diverse backgrounds, e.g. in terms of age, gender, disability, sexual orientation / identity, and social, ethnic and religious origin. A diverse and inclusive working environment with equal opportunities in which everyone can realize their potential is important to us.

Further information on diversity and equal opportunities: https://go.fzj.de/equality