Are you a researcher in science, technology, engineering or mathematics with deep technical interest in programming and love for numerical linear algebra? Are you familiar with parallel programming and high-performance computing techniques? Then, you may be interested in our offer. Our Simulation and Data Lab Quantum Materials in the Jülich Supercomputing Centre (JSC) works on algorithmic solution for materials science codes at the largest scales. We develop novel HPC and parallel programming methods to enable the simulation of quantum mechanical systems. We are looking for an experienced researcher with a PhD in applied maths, physics or computer science with experience in numerical linear algebra. At the Jülich Supercomputing Centre (JSC), we operate one of the most powerful supercomputer infrastructures for scientific and engineering applications in Europe and we aim at using these resources to execute large scale simulations.

We are looking to recruit a

**Postdoc - Numerical Linear Algebra in Quantum Physics at Exascale**

**Your Job:**
You will become part of our research team! Simulation and Data Lab Quantum Materials, where you will conduct innovative research to improve scientific software codes—libNEGF, BigDFT, and ChASE—that simulate quantum many-body systems and solve for numerical eigenproblems, respectively. As a member of two pan-European projects, EcoCoE and HANAMI, co-funded by the EU, you will contribute to the advancement of large scale "in silico" simulations applied to quantum materials science.

You will play a crucial role in leading the effort to enhance code scalability on European pre-exascale and future exascale systems like LUMI, LEONARDO, and JUPITER as well as on Japanese supercomputers such as FUGAKU and Oakforest-PACS-II. Additionally, you will closely collaborate with Japanese and European researchers in designing and implementing an Artificial Intelligence methods capable of accelerating the solution of sparse linear systems. You will closely collaborate and co-lead PhD students in this endeavor. You will:

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
• Lead the development of a programming framework handling a variety of data representation from sparse to block sparse to dense
• Support the tasks towards the extension of the MPI cartesian grid to configuration space and phonon bands for the libNEGF code
• Help in designing novel parallel algorithms, ensuring the overall scalability of the codes, and participating in the further development of numerical kernels (e.g., tensor contractions, block recursive linear solves, spectral methods)
• Lead the tasks for the introduction of platform-aware low-level kernels and primitives for improved hardware integration and performance portability
• Work on a novel workflow applying CNN to a large database of sparse eigenproblems with the aim of clustering them based on their spectral properties
• Validate and benchmark calculations on the largest supercomputing clusters in Europe and abroad, and identify workflows and exascale capabilities on specific test-bed structures

Your Profile:
We are looking for a highly motivated postdoctoral researcher who is excited in contributing to international research projects on topics at the interface between numerical linear algebra and application domains. For such an endeavor you have:
• Completed university studies (masters degree) and a doctoral degree in computer science, applied mathematics, computational science (physics, math, chemistry,..) and engineering or a related subject
• Very good knowledge of numerical linear algebra algorithms
• Extensive experience with parallel programming and high-performance computing, in particular with MPI, OpenMP and GPU programming models on large scales
• Strong programming skills, preferably in C++
• Some knowledge of Fortran, Python and Julia is an asset
• Some background knowledge in Machine and deep Learning is an asset
• A self-motivated personality, intellectual independence and the willingness of working towards the solution of challenging problems
• The ability of working on multi-disciplinary topics and in an environment which is team-oriented
• Very good command of written and spoken English

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 support you in your work with:
• A large research campus with green spaces, offering the best possible means for networking with colleagues and pursuing sports alongside work
• Work on frontiers of scientific and technological challenges with access to cutting-edge and unique supercomputing systems including the upcoming first Exascale computer in Europe (JUPITER).
• The opportunity to conduct research in two major European consortia: 1) EoCoE— an European Center of Excellence focused on energy production and storage— and 2) HANAMI—a European consortium dedicated to collaboration with Japanese institutions on themes such as climate, life science and materials.
• The opportunity to attend national and international conferences
• Close support and mentoring from your team leader on a weekly basis
• Comprehensive training courses and individual opportunities for personal and professional further development
• Extensive company health management
• Ideal conditions for balancing work and private life, as well as a family-friendly corporate policy
Flexible work (location) arrangements, e.g. remote work
Flexible working hours in a full-time position with the option of slightly reduced working hours
30 days of annual leave and provision for days off between public holidays and weekends (e.g. between Christmas and New Year)
Targeted services for international employees, e.g. through our International Advisory Service

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

The position is initially for a fixed term of 2 years, with possible long-term prospects. Salary and social benefits will conform to the provisions of the Collective Agreement for the Public Service (TVöD-Bund), pay group 13 -14, depending on the applicant’s qualifications and the precise nature of the tasks assigned to them.

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.