



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!

The Institute for Advanced Simulations – Materials Data Science and Informatics (IAS-9) focuses on data-driven methods tailored to challenges in the physical sciences and engineering. The research group "Knowledge Engineering for Materials Science" focuses on applying semantic technologies to improve data interoperability, reuse, and reasoning in materials research. Our work focuses on using ontologies and knowledge graphs to structure materials data and embed physical meaning into datasets, while leveraging techniques such as Large Language Models (LLMs) to improve semantic enrichment. We also contribute to the development of domain ontologies, metadata standards, and software tools that enable FAIR data practices across scientific workflows. Our work aligns with Helmholtz-wide and national data initiatives including NFDI-MatWerk, and contributes to shaping a sustainable, AI-ready research data infrastructure.

We are offering a

PhD position – Large Language Models and Semantic AI for Data-Driven Materials Science and Physics

Your Job:

Join an interdisciplinary team that brings state-of-the-art AI research together with cutting-edge materials science and physics. Depending on your background you will work collaboratively on the following tasks with either with a stronger model-development or application focus:

- Design knowledge-graph-augmented transformers and retrieval-augmented generation (RAG) pipelines that enable semantic querying and reasoning over materials-science/physics corpora
- Developing pipelines for semantic enrichment of unstructured data, including entity recognition, relation extraction, and automatic ontology alignment in physics and materials domains
- Build and maintain ontologies, OWL/RDF knowledge graphs, SPARQL endpoints,

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

and open benchmarking suites to guarantee FAIR, reusable research data

- Mine and link structure-property relationships from DFT, MD, phase-field, TEM/SEM, and other multimodal datasets from simulation and experiment
- Develop benchmarking protocols and toolkits to evaluate AI models on materials science tasks as well as integrate your semantic-AI services into high-throughput GPU/HPC workflows, contributing to data management, metadata structuring, and semantic annotation
- Collaborate with experimentalists and theorists to validate extracted knowledge via in-situ spectroscopy, synchrotron work, and high-throughput synthesis—and present your results at leading AI and materials conferences

Your Profile:

- A completed university degree (Master's or equivalent) with excellent grades in computer science, materials science, physics, or a related discipline
- Practical experience in data science, including the application of machine learning (ML) methods or large language models (LLMs)
- Proficiency in Python programming and confident use of Unix/Linux environments; ideally experience with version control systems (e.g., Git)
- Interest in or experience with semantic web technologies, including metadata schemas, ontologies, or knowledge graphs
- Excellent command of written and spoken English
- Strong communication and teamwork skills, and the ability to work effectively in an interdisciplinary and collaborative research environment

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 dynamic, interdisciplinary research environment at the forefront of materials informatics
- Comprehensive training courses and individual opportunities for personal and professional further development. 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>
- The opportunity to attend national and international conferences
- Optimal conditions for work-life balance, including a family-friendly corporate policy, flexible working hours, the option for home office days, and 30 vacation days per year
- A creative work environment at a leading research facility, located on an attractive research campus at the TZA Aachen <https://tza-aachen.de> and the Forschungszentrum Jülich
- Flexible working hours in a full-time position with the option of slightly reduced working hours (<https://go.fzj.de/near-full-time>)
- Targeted services for international employees, e.g. through our International Advisory Service

Neben spannenden Aufgaben und einem kollegialen Miteinander bieten wir Ihnen noch viel mehr: <https://go.fzj.de/Benefits>

Place of employment: Jülich/Aachen

The position is for a fixed term of 4 years. Pay in line with 80% of pay group 13 of the

Collective Agreement for the Public Service (TVöD-Bund) and additionally 60 % of a monthly salary as special payment („Christmas bonus“). Pay higher than the basic pay may be possible. The monthly salaries in euro can be found on the BMI website: <https://go.fzj.de/bmi.tvod.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 are looking forward to your application including a CV, university degree certificates, grade transcripts, two references and/or letters of recommendation (e.g. by a previous supervisor), and a motivation letter. Please ensure that relevant experience is clearly demonstrated and briefly highlighted in your motivation letter.

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>