Research Fellow (Computational Materials Modelling)
Nanyang Technological University

Job Title	Research Fellow (Computational Materials Modelling)
Department	Energy Research Institute @ NTU
Institution	Nanyang Technological University Singapore, , Singapore
Date Posted	Apr. 30, 2025
Application Deadline	Open untill filled
Position Start Date	Available Immediately
Job Categories	Research Scientist/Associate
Academic Field(s)	Chemistry - General Physics - General Materials Sciences/Polymer Sciences
Job Website	https://ntu.wd3.myworkdayjobs.com/Careers/job/NTU-Main-Campus-Singapore/Research-Fellow--Computational-Materials-Modelling-_R00020582
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Apply By Email	

Job Description

Established in 2010, the Energy Research Institute @ NTU (ERI@N) is a pan-university research institute that focuses on systems-level research for tropical megacities. It performs translational research that covers the energy value chain from generation to innovative end-use solutions, motivated by industrialisation and deployment. ERI@N has multiple Interdisciplinary Research Programmes

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which focus on translational Research, Development & Deployment which focus on specific area of the energy value chain, and a number of Living labs and Testbeds which facilitate large scale technology deployment enabling validation and demonstration of real-world applications.

For more details, please view https://www.ntu.edu.sg/erian

We are looking for a Research Fellow to perform advanced theoretical and computational simulations in the area of density functional theory (DFT). The role will focus on understanding and predicting the properties of novel functional materials, including surfaces and interfaces, that are relevant to catalysis, energy storage, and low-carbon energy systems.

Key Responsibilities:

- Conduct DFT simulations to investigate catalytic reaction mechanisms and electronic structures of materials
- Develop and validate computational models related to energy applications
- Interface closely with experimental collaborators to guide synthesis and characterization
- Contribute to drafting publications and presenting research findings
- Maintain documentation of computational workflows and results
- Train junior researchers and assist in proposal development
- Support the lab’s ongoing projects in low-carbon energy research

Job Requirements:

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PhD in Physics, Chemistry, Materials Science, or a closely related field

- Demonstrated expertise in DFT using packages such as VASP, Quantum ESPRESSO, or similar
- Experience in high-performance computing environments
- Track record of publications in peer-reviewed journals
- Ability to work independently and collaboratively in multidisciplinary teams
- Strong written and verbal communication skills
- Willingness and ability to train and advise graduate students on relevant procedures
- Consistent reporting and meticulous documentation of work

A candidate with a strong foundation in theoretical condensed matter physics, quantum chemistry, and materials modelling is needed. This position will contribute to cutting-edge research in density functional theory (DFT)-based simulations for materials discovery and energy applications. The role involves investigating the electronic structure and surface properties of energy-related materials, with a focus on catalytic interfaces, adsorption processes, and structure–activity relationships. Providing technical expertise to the research team, the successful candidate will also be expected to design and implement simulation workflows and, depending on experience, may lead independent theoretical projects in collaboration with experimental teams.

The ideal candidate holds a PhD in Physics, Chemistry, Materials Science, or a related field, with demonstrated experience in first-principles simulations such as DFT. The candidate should be proficient in using DFT software packages (e.g., VASP, Quantum ESPRESSO), high-performance computing, and Python-based workflow scripting. They should be capable of working independently or as part of a collaborative research team, publishing scientific results, maintaining clear and reproducible documentation, and contributing actively to interdisciplinary discussions. Additionally, a strong publication record and prior involvement in energy materials or catalysis modelling is highly

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desirable.

We regret to inform that only shortlisted candidates will be notified.

Contact Information

Please reference Academickeys in your cover letter when applying for or inquiring about this job announcement.

Contact

Singapore