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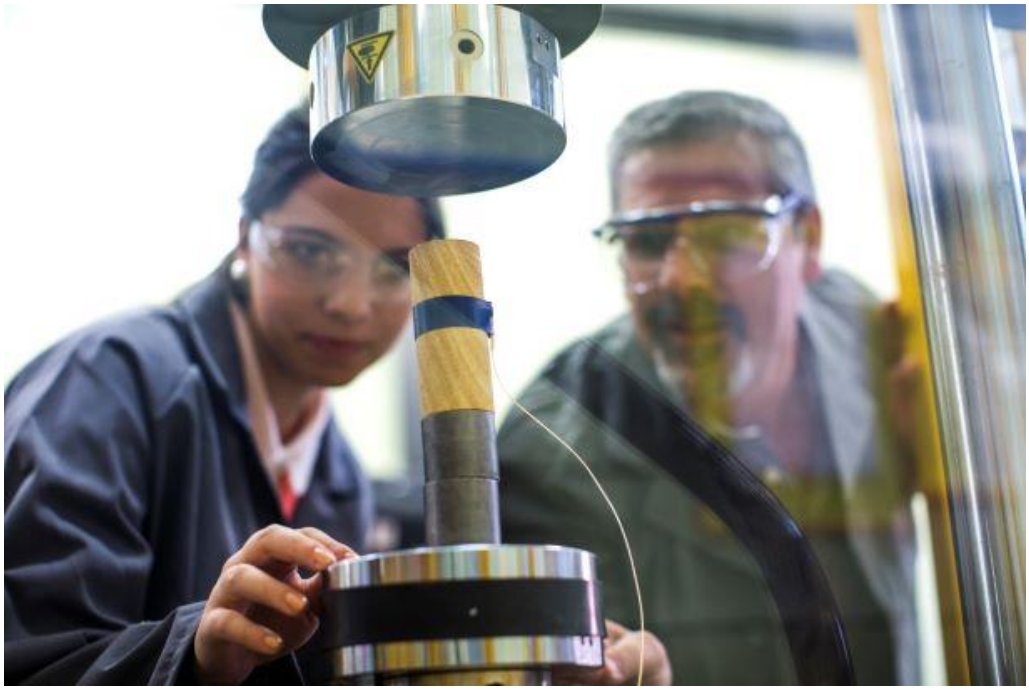

Faculty of Engineering, Computer and Mathematical Sciences

DEVELOP CATALYST MATERIALS FOR FUTURE FUELS BY OPERANDO COMPUTATION

Up for a challenge? Join us to work on a research project with the School of Chemical Engineering & Advanced Materials

At a Glance

Who can apply?

- Australian Citizens
- Permanent Residents
- Onshore Internationals

funding body

- ARC grant funding

Program of Study available

- Doctor of Philosophy (PhD)

Total annual stipend amount

- $28,597pa

Start date

- July 2021.

About the project

This project aims to design catalyst materials for the production of future fuels (green ammonia, hydrocarbon and alcohol). Using carbon and nitrogen as energy carriers, these fuels are generated from renewable sources such as wind or solar; they are safe, reliable, and possess high energy density. The outcomes include advances in computational electrochemistry to the Operando level, electrocatalysts design principles with clearly articulated reaction mechanisms, and candidate materials for experimental validation. Facilitated by advanced computation techniques and reliable catalyst materials design procedure, this project will address the biggest challenge in future fuel generation, which is the lack of efficient catalyst materials.

Dr Yan Jiao's research interest is the Density Functional Theory (DFT) calculation, the development of computational electrochemistry, and

the design of energy materials by computation methods.

The specific methodology Dr Yan Jiao uses to discover and engineer these catalyst materials is molecular modelling on high-performance computers (HPC). She builds atom-by-atom models of these catalyst materials, and investigates the energetics of the reaction pathway for the generation of these fuels. Based on a fundamental understanding of the reaction mechanisms, she designs new catalyst materials that can convert more fuel from the same amount of renewable electricity. Dr. Jiao is also developing computational electrochemistry theory, to more accurately model the energy conversion process, and to design more reliable catalyst materials.

Eligibility criteria

- Applicants with background in computational chemistry or molecular modelling.
- Students with an interest in clean energy, Physical Chemistry, Programming and Computational Chemistry are encouraged to apply.
- Excellent students who hold a Bachelor or Master of Chemical Engineering or an Honours or Masters degree in a related discipline.
- Applicants with well-developed written and verbal communication skills will be considered favourably.
- Students applying for this scholarship should plan for a start around 1/07/2021.

Benefits

- Access to high performance computers
- Work alongside world leading researchers
- Our CaRST program: Free professional development to enhance your employability skills
- Exposure to experts in the field
- No Tuition fees! These are waived for eligible candidates
- Become a field expert and make a real and contribute to solving global challenges
- Publish your contributions and impact our society.

How to apply

- Complete an expression of interest and email together with a copy of your CV and transcripts to Yan Jiao yan.jiao@adelaide.edu.au
- Once your initial eligibility assessment is approved, formally lodge an application for admission and scholarship via the Adelaide Graduate Centre 'How to Apply' link. **Application dates are listed on the website.**

Researcher Profiles

- Use our Researcher Profiles to find out more about potential supervisors.

More about ECMS

The Faculty of Engineering, Computer and Mathematical Sciences is home to world-class research institutes and centres, and internationally renowned academics at the cutting edge of research and discovery.

We are a thriving centre of learning, teaching and research in a vast range of engineering disciplines, computer science, machine learning and high-level mathematics as well as designing Human-centred, sustainable futures in our School of Architecture and Built Environments.

Many of our academic staff are leaders in their fields and graduates are highly regarded by employers.

Learn more about the Faculty of Engineering, Computer and Mathematical Science's Research capabilities at: https://ecms.adelaide.edu.au/research-impact

The University of Adelaide is an Equal Employment Opportunity employer. Women and Aboriginal and Torres Strait Islander people who meet the position requirements are strongly encouraged to apply.

FURTHER INFORMATION

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