PhD Advert Template

Project title: Understanding the changing nature of electrolyser catalysts

Accept all year-round applications

Funding information: Self-funded students only

Project description:

Proton exchange membrane wate electrolysers (PEWEs) will play a critical role in the net-zero economy by enably the storage of excess renewable energy in the form of a chemical fuel, such as hydrogen. The hydrogen could then be used either to produce heat in industrial applications or in hydrogen fuel cell electric vehicles (FCEVs). PEWEs have demonstrated excellent performance and durability; however, their use of scarce and expensive precious metal catalysts, such as iridium, make their cost excessive. Prof. Secanell’s research group has demonstrated the loading of iridium can be substantially reduced to less than 0.1 mg/cm2; however, this also reduces the durability of the device as iridium is oxidised and also dissolved during operation. Therefore, it is critical to understand how to predict the changing nature of the iridium catalsyst in order to reduce its degradation and develop PEWEs that achieve a trade-off between the amount of catalyst used and degradataion. Prof. Secanell’s research team has been developing an open-source software for the computer-aided design of proton exchange membrane electrolysers for several years. The finite-element based framework, which is [available online](http://www.openfcst.org), simulates the transient, multi-phase mass, heat and charge transport, as well as electrochemical reactions taking place inside an electrolyser. Thus far, however, the computational models have not accounted for degradation during operation. The aim of this project is to extend the modelling capabilities to account for catalyst oxidation and degradation, in order to include end of life performance as part fo the design cycle. The PhD student involved in this project will be in charge of extending the current software capabilities by developing advanced micro-kinetic models that aim at predicting catalyst oxidation and dissolution. Funding for conference travel and internships will be provided.

The PhD student would work under the supervision of Prof. Marc Secanell, a leading researcher in the field of mathematical modeling of electrochemical energy systems, fabrication and characterization of polymer electrolyte fuel cells and electrolysers, and design and optimisation. His laboratory has experimental equipment for validating all numerical models developed. He has received over 5,000 citations, has an h-index of 41 (see <https://bit.ly/2NrH9zq>), has been invited to speak at prestigious conferences (e.g., the Electrochemical Society Meetings and the Gordon Research Conference in Fuel Cells), and was co-chair of the 2022 Gordon Research Conference in Fuel Cells. Graduates under his supervision have been able to secure industry jobs at leading companies such as Johnson Matthey (UK), Siemens (US), Ballard Power Systems (Canada), Altair Engineering (Spain/US), and Circle Cardiovascular Imaging Inc. (Canada); postdoctoral fellowships at Lawrence Berkeley National Laboratory (US) and Paul Scherrer Institute (Switzerland); and faculty positions at the Indian Institute of Technology (IIT) and University of Calgary (Canada).

Applicants are expected to have the following qualifications:

**Basic qualifications**

1. A B.Sc, M.Sc., or equivalent degree in Chemical Engineering, Mechanical Engineering, Applied Mathematics, or Applied Physics.
2. Programming experience in any language (C/C++, Python, Fortran, Matlab, or others).
3. Strong communication and teamwork skills.
4. Strong desire to learn mathematical modeling of electrochemical systems and numerical methods.

**Preferred qualifications (these qualifications are a plus)**

1. Programming experience in an object-oriented language, preferably C++ and/or Python.
2. Experience in and understanding of numerical methods, in particular, the finite element method and its implementation in libraries such as deal.ii.
3. Experience in and understanding of electrochemical systems.
4. At least one scientific journal or conference publication.

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Application enquires: Prof. Marc Secanell marc.secanell@ncl.ac.uk

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[ ]  agricultural sciences

[ ]  agricultural technology

[ ]  arable farming

[ ]  livestock farming

[ ]  forestry & arboriculture

[ ]  other

Anthropology

[ ]  biological anthropology

[ ]  social anthropology

[ ]  other

Architecture, Building & Planning

[ ]  architecture

[ ]  built environment

[ ]  construction management

[ ]  landscape architecture

[ ]  rural planning

[ ]  surveying

[ ]  urban planning

[ ]  other

Biological Sciences

[ ]  bacteriology

[ ]  behavioural biology

[ ]  biochemistry

[ ]  biodiversity

[ ]  bioinformatics

[ ]  biophysics

[ ]  biotechnology

[ ]  cancer biology

[ ]  cell biology

[ ]  developmental biology

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[ ]  ecotoxicology

[ ]  entomology

[ ]  environmental biology

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[ ]  marine biology

[ ]  microbiology

[ ]  molecular biology

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[ ]  plant biology

[ ]  plant cell biology

[ ]  reproductive biology

[ ]  structural biology

[ ]  systematic biology

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[ ]  zoology

[ ]  other

Business & Management

[ ]  accounting

[ ]  business

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[ ]  event management

[ ]  hospitality

[ ]  human resource management

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[ ]  project management

[ ]  sport management

[ ]  tourism

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Chemistry

[ ]  analytical chemistry

[x]  applied chemistry

[x]  computational chemistry

[ ]  environmental chemistry

[ ]  industrial chemistry

[x]  inorganic chemistry

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[ ]  petrochemical chemistry

[ ]  pharmaceutical chemistry

[x]  physical chemistry

[ ]  polymer chemistry

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Communication & Media Studies

[ ]  broadcast media

[ ]  digital media

[ ]  journalism

[ ]  print media

[ ]  production

[ ]  public relations

[ ]  publishing

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Computer Science

[ ]  artificial intelligence

[ ]  computer architectures

[ ]  computer vision

[ ]  computer graphics

[ ]  cyber security

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[ ]  human computer interaction

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Creative Arts & Design

[ ]  animation

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[ ]  film studies

[ ]  fine art

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[ ]  theatre studies

[ ]  other

Economics

[ ]  econometrics

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Education

[ ]  further education

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Engineering

[ ]  acoustics engineering

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[ ]  atomic engineering

[ ]  automotive engineering

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[ ]  structural mechanics

[ ]  systems engineering

[ ]  thermodynamics

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Environmental Sciences

[ ]  climate science

[ ]  hydrology

[ ]  marine sciences

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[ ]  pollution

[ ]  soil science

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Finance

[ ]  actuarial science

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[ ]  insurance

[ ]  investment

[ ]  taxation

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Food Sciences

[ ]  food hygiene

[ ]  food production

[ ]  other

Forensic and Archaeological Sciences

[ ]  archaeological science

[ ]  forensic science

[ ]  other

Geography

[ ]  agricultural geography

[ ]  cultural geography

[ ]  economic geography

[ ]  environmental geography

[ ]  geographical information systems gis

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[ ]  marine geography

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[ ]  political geography

[ ]  remote sensing

[ ]  social geography

[ ]  transport geography

[ ]  urban geography

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Geology

[ ]  applied geology

[ ]  geochemistry

[ ]  geophysics

[ ]  geoscience

[ ]  geotechnology

[ ]  hydrogeology

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[ ]  palaeontology

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[ ]  other

History & Archaeology

[ ]  african history

[ ]  american history

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[ ]  archaeology

[ ]  asian history

[ ]  australasian history

[ ]  british and irish history

[ ]  economic history

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[ ]  heritage studies

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[ ]  history of art

[ ]  history of religions

[ ]  history of science

[ ]  medieval history

[ ]  military history

[ ]  modern history

[ ]  russian history

[ ]  social history

[ ]  world history

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Information Services

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[ ]  information systems

[ ]  librarianship

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Languages, Literature & Culture

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[ ]  asian studies

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[ ]  chinese

[ ]  danish

[ ]  dutch

[ ]  english language

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[ ]  japanese

[ ]  middle eastern studies

[ ]  norwegian

[ ]  portuguese

[ ]  russian

[ ]  spanish

[ ]  swedish

[ ]  other

Law

[ ]  criminal law

[ ]  commercial law

[ ]  contract law

[ ]  property law

[ ]  other

Linguistics & Classics

[ ]  ancient greek

[ ]  celtic studies

[ ]  classics

[ ]  latin

[ ]  linguistics

[ ]  other

Materials Science

[ ]  ceramics

[ ]  glass

[ ]  metallurgy

[ ]  polymers

[ ]  textiles

[x]  other

Mathematics

[ ]  applied mathematics

[ ]  applied statistics

[ ]  computational mathematics

[ ]  data analysis

[x]  engineering mathematics

[x]  mathematical modelling

[ ]  medical statistics

[ ]  operational research

[ ]  probability

[ ]  pure mathematics

[ ]  statistics

[ ]  stochastic processes

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Medicine

[ ]  anatomy

[ ]  audiology

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[ ]  complementary medicine

[ ]  dentistry

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[ ]  toxicology

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Nursing & Health

[ ]  adult nursing

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[ ]  mental health nursing

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Philosophy

[ ]  ethics

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Physics

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Politics & Government

[ ]  development studies

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[ ]  international relations

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Psychology

[ ]  child psychology

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[ ]  criminology

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[ ]  social work

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[ ]  sport coaching

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[ ]  sport performance

[ ]  sport technology

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Theology & Religious Studies

[ ]  divinity

[ ]  religious studies

[ ]  theology

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Veterinary Sciences

[ ]  animal welfare

[ ]  veterinary dentistry

[ ]  veterinary medicine

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[ ]  veterinary nutrition

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[ ]  other