



Trinity College Dublin

Coláiste na Tríonóide, Baile Átha Cliath

The University of Dublin

Five-year Postdoctoral Researcher Position in Computational Chemistry (Electronic Structure and Density Functional Theory)

Salary: €41,025 - €67,890 (+ pension) per annum, depending on experience.

Commencement before June 2021 (but negotiable, remote working by negotiation).

Application will be reviewed as received.

A five-year Postdoctoral Research position is available in the research team of **Prof. Stephen Dooley** at the **School of Physics, Trinity College Dublin**.

Project: A Computational Chemist is sought to work on a **European Research Council Consolidator Grant** entitled Mod-L-T: Models for Lignocellulose Thermochemical Conversion. Mod-L-T creates the first detailed, elementary, mass- and energy-conserved chemical reaction kinetic model for lignocellulose pyrolysis. Pyrolysis is a promising method to produce valuable products from lignocellulose and the basic fundamental process of more complex thermochemical technologies, such as catalysis. **Mod-L-T** deciphers the elementary reaction mechanism and kinetics of lignocellulose pyrolysis by elucidating the mysterious molecular-level details of the reaction kinetics of hemicellulose and lignin structures.

The mechanism and kinetics of the pyrolysis reaction of hemicellulose and lignin functionalities will be rigorously and systematically determined by the study of model molecules of incrementally increasing structural complexity by a combination of experimental and theoretical means. Potential Energy Surfaces in the gas and solution phase will be determined by the M06-2X/6-311++G(d, p) or similar methodology with implicit and explicit solution modelling. This new fundamental knowledge is then assimilated for applications by the construction of detailed reaction kinetic models for hemicellulose, lignin and lignocellulose pyrolysis.

Role: working in a friendly and collaborative team, the primary duties of the postdoctoral researcher are:

- Calculate potential energy surfaces corresponding to gas phase (principally) and solution phase C/H/O and C/H/O + metal systems by the application of electronic structure and density functional theory codes.
- Contribute to the assimilation of the outputs of these calculations into reaction kinetic models.
- Lead the writing of research findings in peer-reviewed publications and contributions to collaborative book chapters.
- Lead the presentation of the team's findings at international conferences and stakeholder events.
- Contribute to the engagement of scientific collaborators, industry and other stakeholders.
- Contribute to the preparation of research proposals.

Research Environment: You will join the research group of Prof. Stephen Dooley who work on various science aspects of the low-carbon energy transition. Established in 2014, and hosted in the School of Physics, the group will grow to approximately twenty researchers in 2022 and is funded by a portfolio of government and industry actors including *the European Research Council, Science Foundation Ireland, the Sustainable Energy Authority of Ireland, Siemens Energy and Ryanair DAC*. You will have opportunities to interact with other research groups within Trinity, where Sustainable Energy is an identified research thrust. You will have the opportunity to travel to disseminate your research and to interact with several collaborating institutions in the United States and Europe.

Working in a very supportive research environment, you will be mentored, encouraged and trained in the skills needed to achieve your career objectives.

Essential Requirements: The successful candidate will have:

- A PhD in a chemistry or physics or a closely related area.
- A good record of high quality peer-reviewed publications commensurate with experience.
- Demonstrated competence in the application and/or development of Electronic Structure and Density Functional Theories.
- Experience of Electronic Structure and Density Functional Theory codes, such as Gaussian.
- Demonstrated capacity to learn new numerical modelling methods.
- Willingness to interface with information from experiment to guide modelling efforts.
- Excellent communication skills.
- Demonstrated ability to manage time independently and to manage project delivery.
- Ability to learn new skills and to teach others.
- Experience in report writing, presentation writing and delivery, or proposal writing.
- A passion for science, sustainability or pursuit of enterprise.

Application: Prospective candidates should send a two page CV containing names and contact details of two referees and a 1-page letter outlining your interest in the position and relevant experience to Prof. Stephen Dooley at dooley.recruitment@tcd.ie. Please quote the entire job title in the subject line of your email. Applications will be evaluated as received and candidates of all demographics, educational backgrounds and genders that show a good record of academic achievements will be considered.



Trinity College Dublin
School of Physics

IOP | Institute of Physics
Juno Practitioner

