University of Birmingham

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About

Paul graduated from Glamorgan University with an undergraduate degree in Forensic Science. He then attended Cardiff University and attained a masters in Molecular Modelling. Following this, Paul came to the University of Birmingham to start his PhD in the integrated study of hydrogen and fuel cell applications.

Paul's PhD within the Doctoral Training Centre, which is funded by EPSRC, focuses on theoretical studies of the electrocatalyst (EC) for applications in Proton Exchange Membrane Fuel Cells (PEMFCs).

Density Functional Theory (DFT) calculations have been performed on a number of bimetallic systems with an aim of reducing Pt loading while improving properties of the electrocatalyst.

Qualifications

- BSc (Hons, 2:1) Forensic Science
- MSc Molecular Modelling

Biography

Paul graduated from Glamorgan University with a degree in Forensic Science (2008). He then studied at Cardiff University where he attained a masters in Molecular Modelling (2009). Wishing to continue with theoretical studies, he then started his PhD at the University of Birmingham combining knowledge gained from his undergradute and masters degrees on a theory based project split between the schools of Chemical Engineering, Chemistry and Biosciences.

Paul's research spans the fields of nanoclusters and interactions of nanoparticles and biological molecules. Focusing on structural prediction, reaction kinetics, and interactions of small biological molecules with either metallic atoms or small metallic clusters. During Paul's PhD he has presented numerous posters at conferences, workshops and events within the UK and internationally. Select oral presentations include:

- Modelling of Advanced Functional Materials using Terascale Computing - March 2012
- RSC Theoretical Chemistry Group Graduate Student Meeting - May 2012
- Midlands Electrochemistry Group Meeting 2012 - July 2012
- 3rd BEAR Postgraduate Conference 2012 - July 2012

Paul is also a member of the American Chemical Society and an Associate Member of the Royal Society of Chemistry.

Research

Supervisors: Prof. Roy Johnston (/staff/profiles/chemistry/johnston-roy.aspx) & Prof. Lynne Macaskie (/staff/profiles/biosciences/macaskie-lynne.aspx)

The expensive platinum catalysts in the electrode are said to attribute 33-50% of the cost of the PEMFC. Furthermore, these catalysts are prone to poisoning and degradation, leading to a reduction in the cell performance over time. To try and tackle these problems research is focused on two areas, the reduction in cost of electrocatalysts and the improvement of catalytic properties such as reaction kinetics and durability. To study nanoalloys simulations are performed on Pt based clusters of varying compositions alloyed with early transition metals in order to study catalytic activity.

Structural Searches

Structural searches have been performed the Birmingham Cluster Genetic Algorithm coupled with emperical potentials as well as using the novel Genetic Algorithm coupled with DFT (GA-DFT) method. The range of sizes being studies is between a few to a few hundred atoms. This allows the study of size effects as well as compositional effects.

Reaction Kinetics

This research is focused on looking at stable structures and compositions of bimetallic clusters for improved catalytic properties. In order to study catalytic activity, adsorption of small molecules onto cluster surfaces is being simulated to study adsorption energies comparing to density of states characteristics. Following on from this, the Nugded Elastic Band method is used to compute reaction barriers.

Other activities

Outreach activities include:

- Answered questions about fuel cell technology at the centres stand at Sustainability Live 2010/11.

- Lecture to school children on the need and state of hydrogen and fuel cell technologies as a future energy source 2010.
- Demonstrating fuel cell technology to school children for an RSC "Chemsitry At Work" event 2011.
- Presentation to school children giving an overview of climate change, renewable energy and the hydrogen economy at Sci-Tech 2012.

Other responsibilities include:

- Fuel cell website editor.
- 2nd BEAR Post Graduate Conference 2011 Organising Committee.
- 2nd BEAR Post Graduate Conference 2011 Session Chair.

Outside of his studies Paul has a keen interest in doing more science.

Publications

- Jennings, P. C.; Aleksandrov, H. A.; Neyman, K. M.; Johnston, R. L. *Nanoscale*, **2014**, 6, 1153-1165 - **Link (http://pubs.rsc.org/en/content/articlelanding/2014/nr/c3nr04750d)**
- Jennings, P. C.; Johnston, R. L. *Comp. Theor. Chem.* **2013**, *1021*, 91-100 - **Link (http://dx.doi.org/10.1016/j.comptc.2013.06.033)**
- Jennings, P. C.; Pollet, B. G.; Johnston, R. L. *J. Phys. Chem. C*, **2012**, *116*, 15241-15250 - **Link (http://dx.doi.org/10.1021/jp303577t)**
- Jennings, P. C.; Pollet, B. G.; Johnston, R. L. *Phys. Chem. Chem. Phys.* **2012**, *14*, 3134-3139 - **Link (http://pubs.rsc.org/en/content/articlelanding/2012/cp/c2cp23430k)**