Engineering and Physical Sciences Research Council

HETSYS MATTERS

NEWS FROM THE EPSRC DOCTORAL TRAINING CENTRE IN THE MODELLING OF HETEROGENEOUS SYSTEMS (HETSYS)

CDT Directors' Update

Welcome to the second edition of ***HetSys Matters***, the newsletter of the HetSys CDT.

It's been a busy summer for HetSys: Our students have been presenting their work at a variety of meetings and international conferences, we hosted our third annual Summer Conference and we are delighted to report that various members of our academic team have been promoted. Students in Cohort 2 have all successfully completed their Post Graduate Diplomas in the Modelling of Heterogeneous Systems. These Diplomas will be formally awarded in Warwick's Winter Graduation Ceremonies in January 2023.

Our external links have only strengthened since the launch of Centre, meaning our students are able to get a strong background exposure to industry through various CDT activities. The growth in our industrial links is certainly a highlight from these first three years of HetSys, one that brings many benefits not only to the CDT, but also to Warwick's Faculty of Science, Engineering and Medicine as a whole.

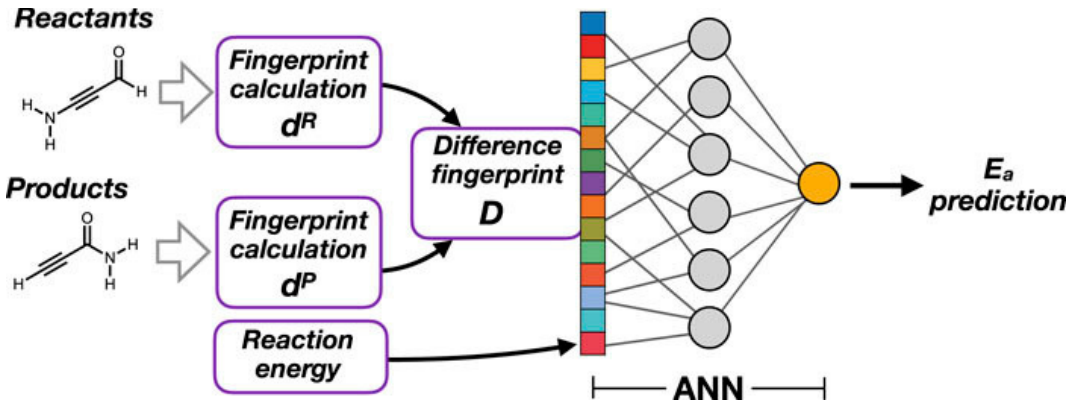
We are now entering our fourth year since our launch in 2019 - we are excited to welcome our latest cohort of students and optimistic about what lies ahead for both our students and the Centre as a whole.

Julie Staunton and James Kermode

INSIDE

How accurate is accurate?

Latest research by Idil Ismail and Scott Habershon examines the impact of uncertainty in machine-learned activation energies on macroscopic observables.



The prediction of the thermodynamic and kinetic properties of chemical reactions is increasingly being addressed by machine-learning (ML) methods, such as artificial neural networks (ANNs). While a number of recent studies have reported success in predicting chemical reaction activation energies, less attention has been focused on how the accuracy of ML predictions filters through to predictions of macroscopic observables. Here, we consider the impact of the uncertainty associated with ML prediction of activation energies on observable properties of chemical reaction networks, as given by microkinetics simulations based on ML-predicted reaction rates. After training an ANN to predict activation energies, given standard molecular descriptors for reactants and products alone, we performed microkinetics simulations of three different prototypical reaction networks: formamide decomposition, aldol reactions, and decomposition of 3-hydroperoxypropanal. We find that the kinetic modeling predictions can be in excellent agreement with corresponding simulations performed with ab initio calculations, but this is dependent on the inherent energetic landscape of the networks. We use these simulations to suggest some guidelines for when ML-based activation energies can be reliable and when one should take more care in applications to kinetics modeling.

This study highlights how using standard "out-of-the-box" fingerprint descriptors and a simple ANN architecture can yield a reliable training model, that can reproduce important macroscopic observables such as rate. Using these methods in conjunction with our existing work on reaction discovery, our ambition is to integrate our reaction discovery schemes with automated generation and microkinetics modeling of chemical reaction networks (CRN). The purpose of this article is to test the extent to which current ML-predicted activation energies are sufficiently accurate to reproduce emergent CRN kinetics.

About the Authors

Idil Ismail is a 4th Year PhD student in the HetSys CDT, **Scott Habershon** is a Professor in Computational\Theoretical Chemistry and a member of the HetSys core team and **Christopher Robinson** is a Post-Doctoral Researcher at Heriot-Watt University.

Publication Details:

I Ismail, C Robertson and S Habershon

"Successes and challenges in using machine-learned activation energies in kinetic simulations"

J. Chem. Phys. 157, 014109 (2022); *Editors Pick* https://doi.org/10.1063/5.0096027

Molecules of Interest

How Steven Tseng and Gabriele Sosso are using machine learning to improve drug design

Machine learning can be used to do and/or improve upon several things – almost anything if one believes the Internet. In the context of drug design and discovery, however, machine learning techniques can be harnessed to predict the functional properties (such as the toxicity, the physical stability, or the bioavailability) of new drugs – without the need for our experimental colleagues to synthesise these new molecules in the lab (a costly and time-consuming process). Crucial to this endeavour is the choice of a good "descriptor", that is, a mathematical object that encodes as much information as possible about the structure of the molecules of interest.

Steven Tseng (3rd year HetSys PhD student/Sosso Group) has recently been working in conjunction with Trent Barnard (Warwick Chemistry/Sosso Group), Albert Bartok-Partay (HetSys), James Darby (Warwick Engineering) and Anders Broo (AstraZeneca) to systematically improve the accuracy and ultimately the predictive power of a descriptor that has been gaining lot of traction within the last few years. This is achieved by using genetic algorithms to explore the many possible combinations of hyperparameters that enter the definition of this particular descriptor – the Smooth Overlap of Atomic Positions (or SOAP) descriptor.

To find out more, an article has been published in the latest edition of Molecular Systems Design & Engineering (MSDE) - an interdisciplinary journal reporting cutting-edge molecular engineering research, and details are below.

This work represents a small but significant step forward in that it will allow the community to obtain "better" descriptor by leveraging the code – associated with this paper - that has been made available to the general public via GitHub.

Publication Details:

Trent Barnard, Steven Tseng, James P. Darby, Albert P. Bartók, Anders Broo and Gabriele C. Sosso

Leveraging genetic algorithms to maximise the predictive capabilities of the SOAP descriptor

Mol. Syst. Des. Eng., 2022, Advance Article DOI: https://doi.org/10.1039/D2ME00149G

Follow the Sosso Group on Twitter @SossoGroup

HetSys Presents...

After almost two years of online conferences and workshops, we are delighted to see our students and colleagues presenting their work on international stages. Some highlights from the last few months include:

HetSys Takeover at the 2022 Psi-K Conference

A group from HetSys travelled to Lausanne to take part in the long-overdue 6th general conference for the worldwide Psi-K Community. This major conference - the largest worldwide in electronic-structure – brings together the community of over 1000 members and is a key event in the field.

Our students featured throughout the conference programme with **Chris Woodgate** and **Joe Gilkes** both giving talks, and work from **Omar Adesida, Connor Allen, Carlo Maino, Idil Ismail** and **Lakshmi Shenoy** showcased in the poster sessions. Carlo's poster was awarded a commendation prize, and that wasn't the only achievement that he was celebrating from the event – Carlo set himself the challenge to cycle all the way from Coventry to Lausanne to take part in the conference – over 2300km! His motivation was a combination of environmental sustainability and also that cycling is a lot more fun than standing in an airport security queue...

MMM10 Baltimore

Lakshmi Shenoy, **Iain Best** and **Omar Adesida** were selected to give talks at the 10th International Multiscale Materials Modelling Conference (MMM10) - the world's largest theoretical and computational forum on multiscale materials modelling.

Lakshmi presented: "Developing a Gaussian Approximation Potential for Simulation of Fracture in Irradiated alpha-Iron", Iain presented "Uncertainty Quantification in Atomistic Simulations using Interatomic Potentials" and Omar presented "Exploring the Phase Behaviour of Hard-Sphere Dimers with Nested Sampling." They were joined by HetSys Co-Director James Kermode who is a member of the forum's International Advisory Board.

Presentation Prizes and Awards

Several of our students were awarded prizes for their talks and posters at conferences over the summer, including a presentation prize for **Adam Fisher** for his presentation " Using Kinetic Activation-Relaxation Technique to Investigate Crystal Growth in NiAl Superalloys" which he gave at the NSIR Conference in July 2022. **Lakshmi Shenoy** was awarded the prize for best poster at the Computer Simulation of Irradiation Effects in Solids (COSIRES) Conference for her work on developing a machine learning interatomic potential for simulation of fracture in alpha-iron and **Joe Gilkes** won the poster prize at the the Sulis HPC Showcase event in Birmingham.

A group of HetSys students also did very well at the recent Midlands Computational Chemistry Meeting 2022. **Joe Gilkes** was awarded first poster prize for "Stacking the odds: Distribution-biased generative deep learning for targeted design of organic electronics"; **Omar Adesida** (Cohort 2) was awarded second poster prize for "Exploring the Phase Space of Hard Sphere Dimers Using Nested Sampling", and **Idil Ismail** (Cohort 1) was awarded second prize for her talk "High throughput screening of mechanistic hypotheses using machine learning and multi criteria decision making".

Staff promotions

We are delighted to announce that several members of the HetSys Core Team have received promotions this year.

James Kermode (HetSys Co-Director) and Nicholas Hine (Director of Studies) have both been promoted to Professor along with Reinhard Maurer (Chemistry and HetSys Core Team).

Other Core Team members and project supervisors Livia Bartok-Partay (Chemistry), Susana Gomes (Mathematics) Tim Sullivan (Mathematics) and Radu Cimpeanu (Mathematics) have been promoted to the position of Associate Professor.

HetSys Summer Conference 2022

In July 2022 HetSys hosted its third annual conference, which focussed on different areas of Computational Materials Modelling. Participants included the current HetSys students, URSS project students, some of our incoming students as well as staff, friends and associates from across the faculty and our industry partnerships.

We enjoyed keynote talks from **Professor Catherine Powell** (Manchester) on Uncertainty Quantification and **Professor Keith Butler** (STFC) on Machine Learning Models as well as excellent talks, posters and flash presentations from our students.

This annual conference is an important event in the HetSys calendar. It communicates results and potential impact from PhD projects to a wide multidisciplinary audience which enables our students to gain valuable experience and feedback. Furthermore it builds and enhances new and existing collaborations with partners both within Warwick and externally.

The year's conference was the Centre's first annual conference to be an in-person event. It was a great success, thoroughly enjoyed by all.
HetSys Director, Professor Julie Staunton commented:

> *The quality of all the contributions was really impressive as was the range and depth of engagement and discussion throughout the conference. We all also appreciated the air-conditioned environment at Scarman during the peak of the heatwave!"*

We were delighted to award several prizes during the proceedings. **Joe Gilkes** was awarded the prize for the best talk and poster from Cohort 2, and **Arre Rajkumar** was awarded the prize for best talk and poster from Cohort 1. Other performance prizes were awarded including the 2022 Outreach Prize to **Idil Ismail** for her outstanding work in organising the Computational Toolkit Seminar Series, along with Excellence in HetSys training to **Andrew Angus** and **Peter Lewin-Jones**.

PhD Projects for 2023 entry

We are delighted to announce that recruitment for the fifth cohort of HetSys Students is now open. We are looking to recruit enthusiastic students from across the Physical Sciences who enjoy using their mathematical skills and thinking flexibly to solve complex problems. HetSys students benefit from a specially designed, integrated training programme, designed to enable them to become high-quality computational scientists and a supportive environment with plenty of opportunities for skills development and network-building.

HetSys studentships include a stipend to cover living costs, university fees and a generous research support training grant. Funding is open to both UK and a small number of International Students on a competitive basis.

For full details of the available projects for 2023 entry, along with the admissions and recruitment process, please visit the HetSys website.

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