

# HetSys Matters

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

## CDT Directors' Update

Welcome to the fourth edition of HetSys Matters! It has been a busy year for the HetSys Centre for Doctoral Training and we have lots of exciting news to report. Since the last edition, our second cohort of students have completed their studies and moved into a range of academic and non-academic roles. We are proud to report that two students in cohort 2, Lakshmi Shenoy and Joe Gilkes, were winners of the Faculty of Science, Engineering and Medicine thesis prize. Peter Lewin-Jones also won the Faculty of Mathematics thesis prize and both Peter and Lakshmi Shenoy were also awarded IAS Early Career fellowships to stay on at Warwick after the end of their PhD work.

Cohort 3 are now busy writing their theses this summer, while Cohort 4 have successfully completed and been awarded their Postgraduate Diplomas in Modelling of Heterogeneous Systems. More and more of our students are doing HetSys proud presenting their work at a variety of national and international conferences, which you can read more about on page 2 and published a growing number of outstanding publications on page 3.

This year we welcomed the first cohort funded by the HetSys II grant, Cohort 6 (picture below), which comprises 12 students who are just coming to the end of the core part of the revised HetSys training programme. With the start of the new grant we have updated our training to place an increased emphasis on the use of AI and machine learning in scientific research, while keeping our strong focus on robust software engineering and quantifying uncertainties in modelling.

HetSys is fortunate to have an excellent administrative team who are an essential part of the successful delivery of our programme of activities. Sarah Jarratt has been promoted to the role of Centre Manager and we are very pleased to welcome Jin Kang as our CDT Administrative Officer. Jin has hit the ground running making an expanded range of development and training events available to our students, including a new more-interactive format for our research theme discussion day, training in pitching research projects and succeeding in interviews and expanded responsible research and innovation training.

**HetSys Director, James Kermode and Deputy Directors, Livia Bartók-Pártay and Nicholas Hine**

**Cohort 6:** L:R - Sean Wu, Luca Gasparro, Rumesh Sudhakaran, Keyi Wei, Luca Seaford, Swathi Mahashetti, James Gulliford, Maks Diakiewicz, George McKay, Facundo Costa, David Bewicke and George Simmons



## INSIDE

- [HetSys Updates](#)
- [HetSys Publications](#)
- [Life after the PhD - Alumni Updates](#)
- [Prizes & Presentations](#)

“ My time on the CDT has been amazing. It allowed me to delve into quantum chemistry and machine learning, develop my programming and analytical skills, and travel internationally. Thank you especially to my supervisor, and to all the friends I've made along the way, I couldn't have done it without you!

Connor Allen, Alumnus ”

## HetSys Community

A warm welcome to the following colleagues who will be bringing their specific expertise to our HetSys Community:

Bryn Davies, Maths - supervisor;  
Ellen Luckins, Maths - supervisor;  
Svenja Janke, Senior Research Software Engineer, RTP;  
Christopher Patrick, Physics;  
Jin Kang, CDT Administrative Officer.



**It's been a busy and exciting time for the HetSys community, with a wide range of activities supporting our students' development.**

In February, we relaunched our Student-Staff Liaison Committee (SSLC), led by Thomas Hudson, Director of Studies with support from Jin Kang, CDT Administrative Officer, and welcomed Chantal Baer (cohort 3) as Chair. This initiative ensures that student voices remain central to our continuous improvement efforts. Later that month we had a strong presence at PG Live events in Edinburgh, Birmingham, Liverpool and London as we promoted our studentships for 25/26 entry.

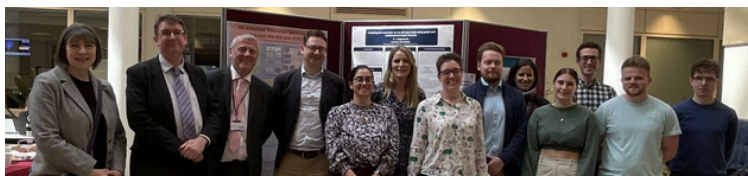
March saw our annual research afternoon, providing students with a supportive platform to share their progress, exchange ideas and receive valuable feedback from peers. As part of our seminar series HetSys Happenings, we sponsored 'Polymers & Composites for Hydrogen Economy' an event organised by the International Institute for Nanocomposites Manufacturing (IINM). This unique event brought together a mixture of excellent speakers from academia and industry who provided their perspective on both fundamental and applied aspects in this emerging field, including materials modelling.

In April, we were pleased to host a visit from the EPSRC Executive Chair, Professor Charlotte Deane – more details on that below, and during May, students took part in two dedicated sessions focused on enhancing their presentation and interview skills, equipping them with practical techniques and the confidence required for presenting at conferences, attending interviews and taking part in academic discussions.

June featured a training session on Responsible Research and Innovation, empowering students to consider ethical and societal impacts, engage stakeholders effectively, and enhance the transparency and relevance of their work. This aligns with our strategic goal of strengthening research quality and meeting evolving funding and policy expectations. Several HetSys members represented the programme at the International Conference for Undergraduate Research (ICUR), an annual interdisciplinary academic conference that showcases the best in undergraduate research from around the world, sharing their work with a wide audience of final-year undergraduates and promoting the opportunities and training available through the HetSys CDT.

Looking ahead to July, we're excited for our annual BBQ and the highlight of the HetSys events calendar—our Annual Summer Conference. This event brings together students, academics, and industry partners to celebrate research achievements, with keynote speakers offering insights into their fields of expertise. Later this year, we'll be planning a range of student-led events, including a weekly coffee club to encourage cross-cohort networking and support, as well as preparing to welcome cohort 7. Our regular activities—weekly drop-in sessions, WCPM Seminars, and HetSys Happenings—will continue to enrich our vibrant and supportive research community. We're hoping to expand our network by welcoming international visiting students and academics, further strengthening the global reach of HetSys.

As always, we're incredibly proud of the energy, creativity, and commitment shown by our students and staff whose contributions continue to shape a dynamic and inspiring environment for research and collaboration.



**HetSys extends a warm welcome to the EPSRC**

In April we welcomed the EPSRC Executive Chair, Professor Charlotte Deane, and Deputy Chair Jon Rowe to meet with our talented HetSys CDT PhD students. It was a privilege to showcase the cutting-edge, interdisciplinary research happening across HetSys – made possible through EPSRC's continued support.

Despite tight schedules, the EPSRC team engaged directly with our students across career stages and research areas, gaining first-hand insight into the breadth of innovation here at Warwick. They especially appreciated hearing from our PhD students – a group whose work truly demonstrates the impact of strategic funding.

**HetSys Representatives at the GAP/(M)ACE Users and Developers Workshop**

Last September, HetSys Director James Kermode and HetSys Supervisor Albert Bartók-Pártay, participated in the GAP/(M)ACE Users and Developers Workshop held in Berlin, accompanied by a strong group from Warwick.



Highlights included engaging presentations from HetSys PhD students Fraser Birks, Chantal Baer, Vincent Fletcher. Additionally, congratulations to Valdas Vitartas for winning one of the best poster awards.

Pictured (L-R): Vincent Fletcher (cohort 4), Fraser Birks (cohort 4), Tom Rocke (cohort 3), James Kermode, Valdas Vitartas (cohort 5), Albert Bartók-Pártay, Connor Allen (cohort 2), Chantal Baer (cohort 4).



**HetSys Hits Lausanne**

Earlier this year, HetSys made a strong showing at the CECAM workshop "Fulfilling the Multiscale Promise in Materials" in beautiful Lausanne – and what a week it was!

**Reflections on the APS Global Physics Summit March 2025**

Our students and staff contributed to the programme with presentations that showcased the breadth and innovation of HetSys research, including Machine Learned Potentials for Two-Dimensional Materials, High-Entropy Alloys and Excited-State Dynamics at Surfaces.

These contributions not only highlighted the high-quality research being conducted within HetSys but also served as catalysts for engaging discussions and new collaborative ideas. We were delighted to see the HetSys community playing an active role in shaping the future of materials modelling and look forward to continued participation in future APS conferences.



Pictured (L-R): Anas Siddiqui (cohort 3), Adam Fisher (cohort 2), Nicholas Hine (HetSys Deputy Director), Reinhard Maurer, Chris Woodgate (cohort 1, now at Bristol) and Nils Hertl.

Brilliant talks from Geraldine Anis (cohort 3), Vincent Fletcher (cohort 4), Lakshmi Shenoy (cohort 2, now postdoc at Sheffield), and Livia Bartók-Pártay (HetSys Deputy Director) sparked loads of lively discussions and great feedback.

Chantal Baer (cohort 4) and Fraser Birks (cohort 4) kept the poster session engaging with their presentations and across the board, our HetSys students brought curiosity, energy, and sharp insights to the discussions throughout the workshop.

The event was co-organised by HetSys Director James Kermode, along with collaborators from Max Planck, Fraunhofer IWM, CNRS, and more.

The workshop looked back at what the multiscale materials community has achieved – and forward to the big challenges ahead. We're excited to see HetSys students right at the heart of that journey.

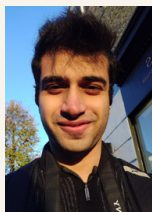
Pictured: (L-R) Fraser Birks (cohort 4), Vincent Fletcher (cohort 4), Livia Bartók-Pártay, James Kermode, Geraldine Anis (cohort 3), Lakshmi Shenoy (cohort 2) and Chantal Baer, (cohort 4)

HetSys students have continued to push the boundaries of computational science with several exciting new publications.

Geraldine Anis (cohort 3), working alongside Thomas Hudson and Peter Brommer, published new research in Physical Review Materials on dislocation dynamics in nickel. The paper presents a novel method for parameterizing dislocation motion from atomistic simulations, enabling uncertainty propagation through continuum-scale models – a valuable advance in materials modelling.

Kat Blow (cohort 2), published research looking at how seeded molecular dynamics represent an increasingly popular approach to investigate crystal nucleation via computer simulations and Oscar Holroyd (cohort 3) alongside his supervisor Radu Cimpanu, proposed a method to stabilise a solution to equations describing the interface of thin liquid films falling under gravity with a finite number of actuators and restricted observations.

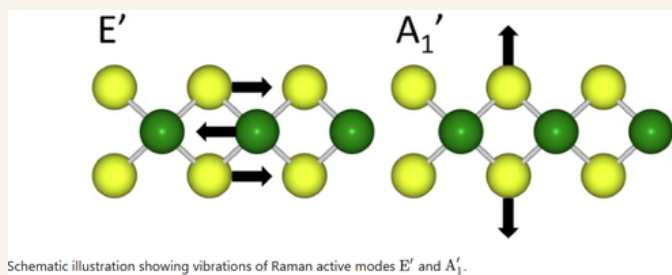
Peter Lewin-Jones (cohort 2) and Duncan Lockerby investigated whether colliding liquid drops will bounce or merge and the complex physics behind it and lastly, Arielle Fitkin (cohort 4) contributed computational insights to a collaborative paper on zinc-based electrodes for solar cells., published with support from supervisors Gabriele Sosso and Ross Hatton, this work adds a valuable perspective to the development of next-generation photovoltaic materials.



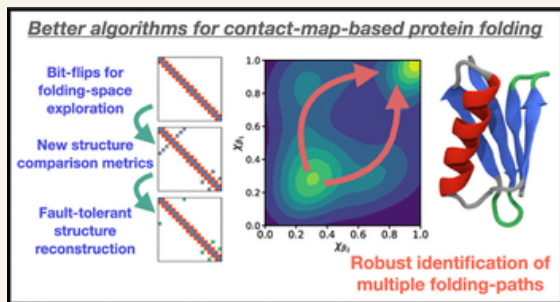
Cohort 3 student Anas Siddiqui's research focuses on the development of Machine Learned Interatomic Potentials tailored for 2D Materials, encompassing their alloys and twisted bilayers. He is deeply committed to leveraging AI to drive progress in science and technology, aiming to forge connections between state-of-the-art AI research and real-world applications.

This paper entitled Machine-learned interatomic potentials for transition metal dichalcogenide  $Mo_{1-x}W_xS_{2-2y}Se_{2y}$  alloys written by Anas Siddiqui and HetSys Deputy Director Nicholas Hine, was included in NPJ Computational Materials 10, article number 169 doi.org/10.1038/s41524-024-01357-9.

Machine Learned Interatomic Potentials (MLIPs) combine the predictive power of Density Functional Theory (DFT) with the speed and scaling of interatomic potentials, enabling theoretical spectroscopy to be applied to larger and more complex systems than is possible with DFT. In this work, they trained an MLIP for quaternary Transition Metal Dichalcogenide (TMD) alloy systems of the form  $Mo_{1-x}W_xS_{2-2y}Se_{2y}$ , using the equivariant Neural Network (NN) MACE. By demonstrating the ability of this potential to calculate vibrational properties of alloy TMDs including phonon spectra for pure monolayers, and Vibrational Density of States (VDOS) and first-order Raman spectra for alloys across the range of x and y they showed that they retained DFT level accuracy while greatly extending feasible system size and extent of sampling over alloy configurations. They were able to characterise the first-order Raman active modes across the whole range of concentration, particularly for the "disorder-induced" modes.



Cohort 3 student Ziad Fakhoury's PhD project is entitled "Protein origami: New computational methods to predict protein folding ensembles" and builds on previous work undertaken by the Habershon group on reaction pathway discovery by encoding protein folding events as a sequence of discretized graph hops. Pathways can then be generated through an (adjacency matrix)-space search. Ziad will study the thermodynamic and kinetic properties of the generated discretized folding ensembles to identify most likely folding mechanisms. This publication Contact-Map-Driven Exploration of Heterogeneous Protein-Folding Paths written alongside HetSys Supervisors Gabriele Sosso and Scott Habershon appeared in the Journal of Chemical Theory and Computation Vol 20, Issue 18 doi.org/10.1021/acs.jctc.4c00878.



After showing physically realisable protein-folding pathways can be generated using directed walks in the space of inter-residue contact-maps; combined with a back-transformation to move from protein contact-maps to Cartesian coordinates, it was demonstrated how this approach can generate protein-folding trajectory ensembles without recourse to molecular dynamics. In this article, they demonstrate that this framework can be used to study a challenging protein-folding problem that is known to exhibit two different folding paths which were previously identified through molecular dynamics simulation at several different temperatures. From the viewpoint of protein-folding mechanism prediction, this particular problem is extremely challenging to address, specifically involving folding to an identical nontrivial compact native structure along distinct pathways defined by heterogeneous secondary structural elements.

The paper shows how the previously reported contact-map-based protein-folding strategy can be significantly enhanced to enable accurate and robust prediction of heterogeneous folding paths by (i) introducing a novel topologically informed metric for comparing two protein contact maps, (ii) reformulating their graph-represented folding path generation, and (iii) introducing a new and more reliable structural back-mapping algorithm. These changes improve the reliability of generating structurally sound folding intermediates and dramatically decrease the number of physically irrelevant folding intermediates generated by the previous simulation strategy. Most importantly, the paper demonstrates how the authors' enhanced folding algorithm can successfully identify the alternative folding mechanisms of a multifolding-pathway protein, in line with direct molecular dynamics simulations.

## HetSys Community



Our students thrive not just in research but in life beyond academia, proving that whether it's sports, music, martial arts, or student societies, they pursue a wide range of passions that enrich their experiences and strengthen our sense of community.

In May, #TeamWarwickUni took on the Cotswold Hilly 100—a challenging 100-mile relay race. HetSys was proud to be represented by alumnus Chris Woodgate (cohort 1), Peter Brommer (Management Team), and Matt Christensen (cohort 5), who helped the team finish in 14:22:34—an impressive 50-minute improvement over last year. Matt and Peter pictured left. Elsewhere, Luca Seaford (cohort 6) practices Aikido and Sebastian Dooley (cohort 4) balances his academic work with martial arts and a keen interest in Formula 1. Oscar Holroyd (cohort 3) takes on ultra marathons, pushing physical limits with the same discipline he brings to research. In the arts, Tom Rocke (cohort 3) plays French horn in the orchestra, David Bewicke (cohort 6) brings depth on the tuba, and Dylan Morgan (cohort 3) lends his voice to the choir.

## Life After HetSys: Journeys Beyond the PhD

We are delighted to confirm that the first cohort of the CDT have already made their mark—venturing into impactful careers across academia, industry, research, and beyond. These alumni are living proof of HetSys’ mission: producing versatile, computationally skilled researchers equipped to tackle real-world challenges with cutting-edge modelling and interdisciplinary thinking.

Achieving a PhD is a significant milestone, reflecting years of hard work, dedication, and substantial contributions to the field.

Our first HetSys cohort have gone on to shape the future of computational science across sectors. Dr Andrew Angus has worked on data-driven modelling to hydrogen pipelines and battery storage systems. Dr Aravinthen Rajkumar now works as an algorithm developer in the aerospace industry, building predictive multiscale models. Dr Carlo Maino is enjoying a new role focused on sustainable energy transitions, continuing his commitment to impactful science at the intersection of data, the environment, and society.

At ETH Zürich, Dr Idil Ismail is advancing high-throughput cheminformatics for chemical reaction prediction. Dr Jingbang Liu is modelling membrane dynamics in cellular processes at the University of Oslo, blending mathematics with molecular simulations. Dr Katarina Blow applies her computational expertise to life sciences research at Warwick, focusing on molecular crystallisation. Dr Christopher Woodgate leads a research project at the University of Bristol, exploring magnetic materials and high-entropy alloys. Dr Matthew Harrison now works as a hydrogeologist at Piteau Associates, modelling subsurface transport and groundwater systems.

We’re incredibly proud of all they’ve achieved. Though their paths now span academia, industry, and beyond, they remain an integral part of the HetSys community—and we look forward to staying connected as their careers continue to grow.

*Pictured L:R Christopher Woodgate, Idil Ismail, Matthew Harrison.*



“ I really value my time at HetSys. It gave me a solid interdisciplinary foundation in computational sciences and prepared me to work in an interdisciplinary research environment. The skills and experience I gained there continue to be useful in my career. ”

Idil Ismail, Alumnus

## Presentation Prizes and Awards

We’re delighted to share recent achievements from several of our outstanding students. Joe Gilkes (cohort 2) has received two prestigious awards for his doctoral work: The Faculty of Science, Engineering and Medicine Thesis Prize from the University of Warwick, presented at the Chemistry Postgraduate Symposium, and the AWE/Armourers and Brasiers Prize for Best Doctoral Thesis. Joe attended the Armourers and Brasiers Cambridge Forum on the 23rd of June to receive his award in person. Peter Lewin-Jones (cohort 2, current IAS Early Career Fellow), won the Young Scientist Award for his conference presentation at the 1st International Symposium on Non-Equilibrium Transport Phenomena (netp.scimeeting.cn), which was held in Beijing in April 2025 along with the G-Research 2025 award for his quantitative research in fluids dynamics.

Fraser Birks (cohort 4) was recognised at the COSIRES radiation damage conference in Kingston, Ontario, winning the prize for best student presentation for his innovative work on accelerating simulations using QM/MM-style machine-learned potentials. Fraser also won best student talk at the COSIRES Conference (June 2024), as well as the best performance prize at the HetSys Research Day event, (March 2025).

Meanwhile, Jacob Eller (cohort 3) presented at both the Computational Molecular Science 2024 conference in Warwick and the AI in Computational Chemistry meeting in Sheffield. His talk on the ESTEEM Python package sparked engaging discussions around AI applications in chemistry. Jacob also explored a potential future in Intellectual Property law through Venner Shipley’s Summer of IP taster day in Cambridge, which further piqued his interest in the field.

Valdas Vitartas (cohort 5) for won the Best Poster Award at the 2024 GAP/(M)ACE Developers & Users Meeting in Berlin. His poster, based on his HetSys summer project “Hamiltonian Surrogate Model of Gold Based on the Atomic Cluster Expansion,” was well-received by the international research community – a testament to the quality and impact of HetSys research.

James Kermode, HetSys Director has been appointed as a trustee of the Psi-k charity, as chair of the CoSeC advisory board, and sits on the EPSRC Centre for Doctoral Training in Developing National Capability in Materials 4.0 with the Henry Royce Institute External Advisory Board. Livia Bartók-Pártay, HetSys Deputy Director has joined the External Advisory Board of the CDT in Digital and Automated Materials Chemistry based in Liverpool giving us a great opportunity for collaborative working and best practice with other EPSRC funded CDTs.

And finally, congratulations to Professor Julie Staunton, founding director of HetSys, who has received the 2025 Wohlfarth Memorial Lecturer Award from the IoP Magnetism Group delivering a plenary lecture at the Magnetism 2025 conference which took place in Sheffield earlier this year. Julie has been named as this year’s lecturer in recognition of her many contributions to the theory and simulation of magnetism and magnetic materials within the framework of first-principles electronic structure calculations. Some of her recent work included the description of the subtle temperature dependence of the magnetic properties of rare earth-transition metal permanent magnets, such as  $\text{SmCo}_5$  and  $\text{Nd}_2\text{Fe}_{14}\text{B}$ .

Julie commented “It was a great pleasure and honour to give the lecture. Very early in my career I spent a year as a post-doc in Peter Wohlfarth’s group – not only was he a brilliant physicist but he was also a kind and supportive mentor to his junior colleagues.”

Julie has brought these same qualities—intellectual excellence, mentorship, and a deep commitment to fostering a collaborative and inclusive research environment into our community. Her involvement continues to shape HetSys in ways that reflect the very values she so eloquently attributes to her former mentor.

### EPSRC Centre for Doctoral Training in the Modelling of Heterogeneous Systems (HetSys)

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