

# HETSYS MATTERS

NEWS FROM THE EPSRC CDT IN MODELLING OF HETEROGENEOUS SYSTEMS

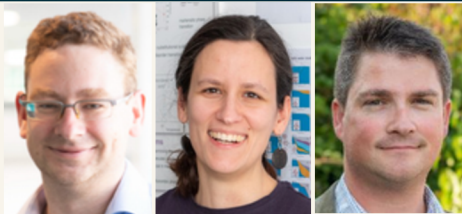
## CDT Directors' Update

Welcome to the fifth edition of HetSys Matters.

Following a productive summer that included our Annual Conference and the graduation of Cohort 2; Term 1 and the start of Term 2 have been busier still.

In October, we welcomed Cohort 7, who have settled in brilliantly and made a fantastic start to Term 1. They've been fully engaged with the training programme, meeting their supervisors, and getting to know the wider HetSys community through a variety of activities from inductions, Coffee Clubs to WCPM seminars and student socials. This summer saw excellent engagement with the Undergraduate Research Support Scheme (URSS) including projects on "Facet dependence of electron-phonon coupling of CO on metal clusters" and "Coarse-Graining of the Langevin Equation with a Quadratic Potential", exemplifying the pipeline of talent feeding into computational research in the Centre. Across the CDT, Cohort 3 have now almost all completed their studies, with two members securing Fellowship roles following a competitive process. Cohort 4 are busy defining their thesis plans, and many students from across our cohorts have been representing HetSys by presenting their work at national and international conferences, which you can read more about on page 2. We continue to deliver a broad programme of training and development: Presenting with Confidence, Applying for Fellowships, Storyology, Interview Skills, and industry seminars open to all students. For this year's recruitment, we've greatly valued input from current cohorts whose feedback on projects ensures student voices shape the process. We're also pleased that Anton Oleinik and Archie Brew from Cohort 7 have joined the SSLC, helping shape the programme and support an excellent student experience. The momentum across all cohorts is remarkable. Together, we continue to build a thriving and ambitious HetSys community.

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



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“ My time with the CDT allowed me to develop a range of skills that I can use in my current role. The support I received during the four-year period was incredible.

Katarina Blow,  
Research Fellow,  
University of Warwick  
HetSys alumna



## A warm welcome to Cohort 7:

LR: Anton Oleinik, Peter Noordman, Sindi Semanaj, Archie Brew, Stephan Gambart, Tristan McCarthy, Lucas Belz-Koeling, Jasper Allen



Cohort 7 have hit the ground running, diving into an impressive range of interdisciplinary research projects across atomistic modelling, quantum methods, and continuum mechanics. Projects cover a wide range from Lucas Belz-Koeling's machine learning of energy barriers for reaction network discovery of drug-like molecules, to Archie Brew's development of DFT methods to study atomic structure and pressure effects in f-electron materials, and Stephan Gambart's programmable fluids looking at continuum models for designing multi-stable meta-fluids. Tristan McCarthy is considering atomic-Level Defect Characterisation via Data Fusion whilst Integrating Ptchography, EELS and First Principles Calculations, while Peter Noordman is modelling ultrafast THz pumps

X-ray probe spectroscopies for ion dynamics in batteries. Anton Oleinik is modelling interfacial flows in porous media with a hybrid asymptotic-computational approach, and Sindi Semanaj is enhancing membrane-protein learning for improved factorial yield through the AMPLIFY project. A recent addition to Cohort 7 is Kunlin Cai (not pictured) who will be working on physics-informed machine learning-based swelling models for future battery cells. Anton Oleinik commented "I've thoroughly enjoyed the start to my time in HetSys. It's been fun to study together within a small cohort while also having our own projects to think about, and all of the social events with people from across the CDT have provided an amazing experience".



## HetSys at Conferences: Engagement, Collaboration, and Community

We began the summer with the HetSys Annual Conference, held in July 2025 on the University of Warwick campus. The conference brought together students from all cohorts, along with nine alumni from Cohorts 1 and 2. It provided a platform for students to share interim results from their PhD projects, celebrate milestones, and build connections across disciplines. This year's programme also included generous time dedicated to networking, giving students and alumni plenty of opportunities to build relationships, exchange ideas, and explore potential collaborations in a relaxed and supportive environment.

Highlights included insightful keynote presentations from Professor Nathan Kutz (Washington), Automated Learning of Physics from Data, and Dr Natalia Martinsovich (Sheffield), Computational modelling of materials: from fundamental properties to evaluation of photocatalytic efficiencies. A dedicated session with our alumni allowed current students to hear first-hand experiences of life during and beyond their PhDs. Coupled with a range of fascinating posters, 3D-printed models, and vibrant conversation throughout the event, the conference once again demonstrated the collaborative spirit at the heart of HetSys.



Beyond Warwick, engagement across the wider scientific community has been exceptional. Over the past six months, HetSys students have attended 40 conferences, delivered 29 presentations, and represented the CDT across 37 locations. This broad involvement reflects both the range of our research and the enthusiasm of our students to share their work. particular highlight was the strong HetSys presence at Psi-k Conference 2025 in Lausanne. Students from all cohorts, alongside several alumni, contributed to a vibrant atmosphere of scientific exchange. Contributed talks from Chris Woodgate (alumnus), Vincent Fletcher (Cohort 4), and Anas Siddiqui (alumnus), supported by a wide array of poster presentations, showcased the depth and diversity of HetSys research. HetSys Director James Kermode and Deputy Directors Nicholas Hine and Livia Bartók-Pártay further strengthened the CDT's presence by co-organising Psi-k symposia on Machine Learning, 2D Materials, and Advanced Sampling Techniques, reflecting HetSys' continued leadership within the computational materials community. Our students and academics also contributed to numerous other international meetings, including CECAM (Centre Européen de Calcul Atomique et Moléculaire), Computing Insight UK, Eurandom (Stochastics workshop centre), CoMPASS (computational materials science and mathematics at particle and atomistic scales), CCPBioSim

(Collaborative Computational Project for Biomolecular Simulation), Faraday Institution events, the CASTEP Workshop, and the Fusion of Talent Conference. These contributions spanned topics from uncertainty quantification to biomolecular simulations. At the CECAM Uncertainty Quantification workshop, work presented by George Simmons (Cohort 6) and Swathi Mahashetti (Cohort 6) highlighted the growing importance of uncertainty-aware modelling and reinforced the value of international collaboration. HetSys was also strongly represented at the CoMPASS Workshop in Edinburgh in November, with contributions from Thomas Hudson (organiser), Reinhard Maurer, Fraser Birks (Cohort 4), Geraldine Anis (alumna), George Simmons (Cohort 6), Joseph Duque-Lopez (Cohort 4), and Lakshmi Shenoy (alumna). Their presentations and posters highlighted innovative work in computational materials science, spanning coarse-graining, dislocation dynamics, atomistic fracture, and uncertainty quantification. Hubert Naguszewski (Cohort 4) also recently attended the 2025 Computing Insight UK conference, presenting research at both the CoSeC (Computational Science Centre for Research Communities) UKRI conference and the main CIUK programme on topics including machine learning and parallel Monte Carlo methods.

**The latter half of 2025 into early 2026, saw a number of research publications from Cohort 4, highlighting the breadth and impact of work being carried out the cohort.**

Jacob Eller co-authored “*Excited state deactivation in phytochemical flavonoids: astragalin and kaempferol*” (Physical Chemistry Chemical Physics). This work was selected by the RSC Physical Chemistry Chemical Physics editors for inclusion in the prestigious 2025 HOT PCCP Collection. Fraser Birks along with Matt Nutter (alumni), TD Swinburne and Prof. James Kermode published “*Efficient and Accurate Spatial Mixing of Machine-Learned Interatomic Potentials for Materials Science*” (npj Computational Materials). Vincent Fletcher, with supervisors Dr Albert Bartók and Dr Livia Pártay, released “*Autonomous thermodynamically informed database generation for machine-learned interatomic potentials and application to magnesium*” (npj Computational Materials) and Maria Radova along with WG Stark, Connor Allen (alumnus) and supervisors Prof. Reinhard Maurer and Dr Albert Bartók published “*Fine-tuning foundation models of materials interatomic potentials with frozen transfer learning*” (npj Computational Materials). In our Research Spotlight, Dr Christopher Woodgate (alumnus), Hubert Naguszewski, Dr Livia Pártay, and Prof. David Quigley published “*BraWl: Simulating the thermodynamics and phase stability of multicomponent alloys using conventional and enhanced sampling techniques*” (The Journal of Open Source Software).



Scan the QR code to view the full list of HetSys publications.

**Seminars, Industry Engagement and Teaching Innovation**

Throughout the autumn term, the WCPM Seminar Series delivered a wide-ranging programme, featuring advances in microscopy, stochastic geometry, electrochemistry, statistical modelling, infectious-disease simulations, bacterial adhesion, NMR for energy materials, and state-space inference. Term 2 is now underway with a strong industry-focused theme. Highlights include seminars from our Jaguar Land Rover partners on computational workflows in Computer-Aided Engineering and Data-Driven Battery Management Systems. Academic speakers include Balazs Ujfalussy (HUN-REN Wigner Research Centre for Physics) who will present on Majorana fermions and Josephson junctions. The evolving programme continues to reinforce the links between fundamental research and industrial application. We were also pleased to host Professor Mark van Schilfgaarde in September 2025 for a seminar exploring excitons in 2D systems and the response functions of correlated systems via Green’s

function theory. The talk attracted students across cohorts and sparked lively discussion. In addition, HetSys welcomed visiting PhD student Petter Uvdal Gothenburg, whose work at the intersection of machine learning and materials science aligns closely with our interdisciplinary ethos. His seminar, “Comparing transformers and recurrent neural networks for 3D micro-mechanical modelling,” offered valuable insights for the HetSys community. Finally, George Simmons, Luca Gasparro, and Rumesh Sudhaharan (Cohort 6) recently took part in a week-long CDT workshop at the Isaac Newton Institute in Cambridge. The event covered science communication, industry engagement, knowledge exchange, EDI and ethics, peer support, and networking with international academics. The workshop provided an excellent opportunity for students to develop key professional skills and build connections with CDT peers from across the UK.



**Life After HetSys: Alumni Updates**

Cohort 3 has had an outstanding few months, with eight members successfully passing their vivas by January 2026. Congratulations to Geraldine Anis, Tom Roche, Oscar Holroyd, Anas Siddiqui, Jeremy Thorn, Ziad Fakhoury, Matt Nutter and Matyas Parrag on reaching this major milestone in their research journeys. Several graduates have already stepped into exciting new roles. Oscar Holroyd has begun a part-time position as a Computational Mathematician at Vanellus, where he is contributing to the development of their core solver using his mathematical and programming expertise. Anas Siddiqui has joined the Physics Department at the University of York as a Postdoctoral Research Associate, continuing his work in computational and quantum materials science. We are also delighted to share that both Geraldine Anis and Matt Nutter were awarded EPSRC Postdoctoral Pathway Fellowships in late 2025. Elsewhere in the HetSys community, alumni from Cohorts 2 and 3 have also enjoyed notable successes. Alistair Soppitt is now a Postdoctoral Research Associate at the University of Liverpool, while Tadashi Matsumoto has taken up a Data Scientist role at MHRA. Tom Roche

has secured a six-month PDSI-funded post, and Adam Fisher has joined UKAEA at the Culham Centre for Fusion Energy. Ziad Fakhoury has moved into a Postdoctoral Research Associate position in Chemistry, and Joe Gilkes has also progressed into a new role. Our alumni network continues to stay connected and make impressive contributions, most recently, Lakshmi Shenoy presented Warwick-based research at the Royce Hydrogen Conference 2025. Her talk showcased results from a collaborative, machine-learning-driven project on Pt-based alloy design for hydrogen fuel cells, carried out with Connor Allen and Joe Gilkes under the supervision of James Kermode, Nicholas Hine and Scott Habershon and in partnership with colleagues at Johnson Matthey. This research grew directly from the 2024 HetSys Industry Study Group event, highlighting the continuing impact of CDT-industry collaborations. In January 2026, we were delighted to celebrate the graduation of Cohort 2 alumni Alistair Soppitt, James M. Targett, Tadashi Matsumoto, and Adam Fisher (pictured L:R above).

## Socials, Skills Development and Events

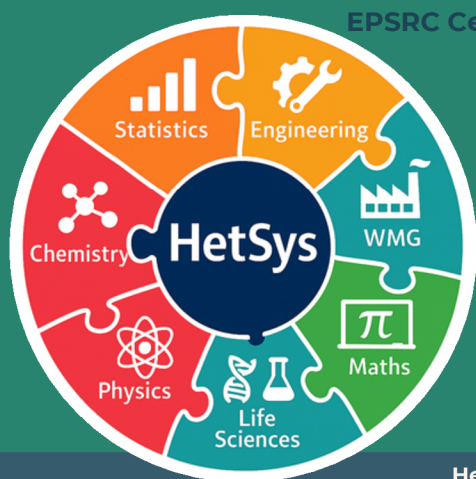
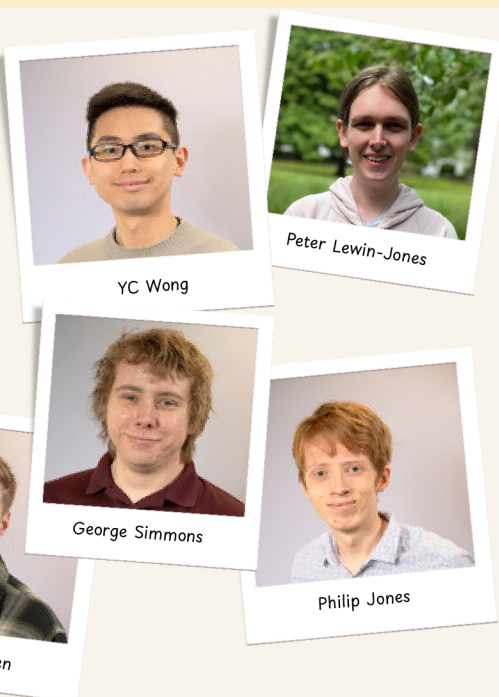
It has been a lively and productive period for the HetSys community, with a full calendar of socials, training opportunities, and cross-cohort engagement. Professional development has been a particular focus, with students taking part in a presentation and interview skills workshop led by external facilitator Simon Cain. These sessions provided invaluable preparation and contributed to the polished, confident presentations delivered by HetSys students at a range of external conferences, while also introducing techniques for giving a poised and effective interview. HetSys students also represented the CDT at a Widening Participation event on 10 September, where they highlighted the programme to prospective applicants and shared their own experiences of postgraduate research. In Term 1, we welcomed the new Cohort with an induction programme that included networking lunches, supervisor meetings, sessions on core skills, and a dedicated lunch with their student buddies to help them settle quickly into the HetSys community. Students continued to connect through the weekly Coffee Club, offering a relaxed space for socialising and networking, as well as through regular attendance at the WCPM seminars. The autumn term also included a dedicated Fellowships Workshop, during which alumni who have secured EPSRC fellowships returned to share personal advice, tips, and career insights with current students. The term concluded on a high with the Annual Quiz — enthusiastically attended by students from Cohorts 3–7 and hosted by Livia Bartók-Pártay. Looking ahead, our termly SSLC meetings will continue. In February, we are holding a workshop delivered by Storyology — an external company founded by an in-house science writer from a large research organisation — to help bring storytelling and science together. This training will be extremely valuable for writing research grants and papers, developing public engagement activities, and

using narrative techniques to communicate complex research effectively. We are also pleased to be representing HetSys at a local outreach event in February, showcasing our programme to a younger audience and encouraging the next generation of scientists to embrace a future in STEM. In March 2026, we will host our annual Research Afternoon, giving students an opportunity to present their research findings to the wider community. April 2026 will see the return of the HetSys Industry Study Group, following the success of previous years. This event enables organisations to present real-world challenges for multidisciplinary teams of researchers to explore collaboratively, developing fresh, data-driven, and model-based insights alongside our students. In 2024, Syngenta’s challenge centred on reducing adhesion of solids in manufacturing processes, prompting teams to combine theoretical modelling with scientific computing. AWE presented a multifaceted workflow-optimisation challenge for polymeric systems, inspiring innovative re-designs of simulation pathways. Johnson Matthey invited participants to explore machine-learning approaches for complex catalytic reaction networks, with students demonstrating impressive depth and agility in their solutions. This research was recently presented in December 2025 at the Royce Hydrogen Conference. The final presentations from the Industry Study Group showcased the breadth and creativity of ideas generated across the week, many of which are now being developed further with partner organisations. As we look forward to the 2026 Industry Study Group, we anticipate another energising and collaborative event—one that will continue to strengthen partnerships, spark new research directions, and give students valuable experience tackling real-world industrial challenges.

## Awards, Achievements and Wider Contributions

We are proud to share that Peter Lewin Jones (alumnus) was recently awarded the prestigious Lighthill–Thwaites Prize, recognising exceptional achievement in applied mathematics and fluid mechanics. This honour highlights the calibre of research emerging from our CDT community. We are also delighted to celebrate the success of two Best Poster Award winners. YC Wong (Cohort 5) received recognition at a research showcase held as part of the MMM conference, and Adam Fisher (alumnus) similarly impressed judges with his poster’s quality and impact. YC’s poster, titled “Machine Learning Multiscale Simulation of Defects in Correlated Oxides”, showcased his work on developing accurate machine-learning models to study Schottky defects in strontium titanate, a material system noted for its long-range electrostatic interactions. His research focuses on assessing how well these models capture such effects when applied to a particularly challenging dataset. We also extend warm congratulations to Cohort 5, all of whom achieved distinctions in their Postgraduate Diploma in Heterogeneous Modelling — a fantastic milestone that reflects their dedication and hard work.

Matt Christensen (Cohort 5) recently delivered an engaging guest session on quantum computing for the Emerging Technologies for Business module, offering an accessible and insightful introduction to current developments and real-world applications. He also presented an informative talk on quantum computing as part of the Predictive Modelling Discussion Group seminar series in Engineering, a series inspired by George Simmons (Cohort 6). Finally, we are pleased to congratulate Philip Jones (Cohort 5) on winning the ISMS Young Scientist Prize in September 2025, an impressive accomplishment that reflects both the strength of his research and his contributions to the scientific community.



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