Trailblazing Training Adds to Chemistry's Attraction

When designing new molecules for pharmaceutical and other uses, the key is to combine the right elements in the right way. The same is true of the training vital to nurturing the skills needed to make it happen.

A perfect example has seen Southampton University join forces with Oxford and Bristol to establish an EPSRC Centre for Doctoral Training (CDT) integrating two vital aspects of chemistry in a powerful new way.

With strong links to industry ensuring its work feeds into the real economy, the Theory and Modelling in Chemical Sciences (TMCS) CDT is producing tomorrow's research leaders and equipping them to tackle today's research challenges.

Where Two Worlds Meet

In chemistry, theory is the bedrock of everything – understanding structures, predicting properties and explaining behaviour. Modelling & simulation, meanwhile, is an invaluable tool for examining and exploring ideas fast and cost-effectively – testing, validating and improving, and often revealing unknown phenomena. As well as their individual importance, the two disciplines provide crucial mutual support:

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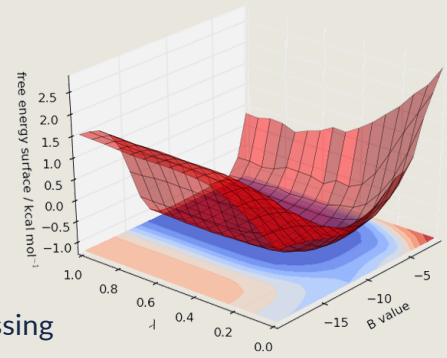
>
> *Professor Jon Essex, TMCS CDT Co-Director*

"Modelling must be underpinned by sound theoretical understanding, but it can also refine that understanding and stimulate fresh theoretical insights," says Jon Essex, Professor of Computational Chemistry at Southampton and the CDT's Co-Director, as well as Chairman of its Industry Board. "Industry and academia increasingly need researchers skilled in both fields. **That's why the training we provide dovetails the two disciplines, drawing on three universities' expertise because single institutions don't have the critical mass to do it on their own**."

Under its Director David Logan, Professor of Theoretical Chemistry at Oxford, the TMCS CDT delivers a four-year training programme including:

- **A one-year MSc course** that broadens perspectives and builds key skills, with modules such as 'Computer Programming', 'Electronic Structure Theory' and 'Computer Simulation Methods'.
- **A three-year doctoral research project**, supplemented by activities such as public engagement and training in high performance computing (HPC). The CDT has two dedicated HPC clusters: one based on CPU (central processing



unit), the other on GPU (graphics processing unit) technology.

"We have around 20 industrial partners," Jon Essex adds. "Including names like AstraZeneca, Johnson Matthey and Microsoft, they support the CDT, help shape our plans and offer potential employment opportunities for our graduates. Our work is hugely enriched by these close links with companies that recognise and value the breadth and depth of the training we provide."

Student Stories

Hannah Bruce Macdonald (Southampton)

Hannah was part of the first cohort accepted into the CDT in 2014. "When I joined, I knew virtually nothing about computational chemistry," she says. "It does come up in undergraduate courses but tends to get squeezed into 'physical chemistry'. The CDT gave me a crash course in coding, which set me up with the skills I needed." After completing her initial year, Hannah joined Jon Essex's group at Southampton. Here she harnessed the experience of colleagues specialising in the development and application of computer simulation in the field of organic and biological molecules, and molecular association in particular. Hannah's PhD set out to shed new light on the way that drug molecules interact and bind with water molecules in proteins – a process vital to many drugs' effectiveness.

"Computational chemistry enables you to take things down to the scale of atoms and electrons, which you just couldn't do experimentally," Hannah explains. "Modelling & simulation can help locate where water molecules might be within protein complexes and reveal how tightly connected they are. It was great to be able to develop codes with important practical uses, and Southampton has been the perfect place to do it."

Visits to pharma companies gave Hannah the opportunity to demonstrate the codes' capabilities and suitability for industrial application. "It was quite daunting but the sessions went very well. The methods that pharma firms currently use to generate the same results are limited in effectiveness and existing software is expensive. That makes the process of drug development more costly and increases time-to-market. **The codes I've worked on offer a better potential route to new therapies**."

> *"I now have a varied skillset that will help me pursue a career in the pharma sector when I've finished my PhD."*
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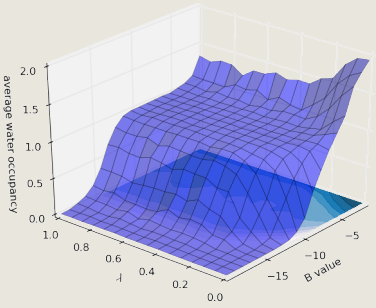
> *Hannah Bruce Macdonald, Southampton University*

And the best thing about the TMCS CDT? "Being part of a close-knit cohort from different backgrounds – maths, physics, biology, as well as chemistry – really helps to widen perspectives. I now have a varied skillset that will help me pursue a career in the pharma sector when I've finished my PhD."

Tim Naginey (Oxford)

Tim joined the CDT after completing his physics degree in the US. “The first year was critical in getting me to the point where I could start my PhD research”, he says. His PhD aims to enhance the capabilities of electron microscopes, which use electron beams to scan samples and are used in the development of advanced materials, for instance.

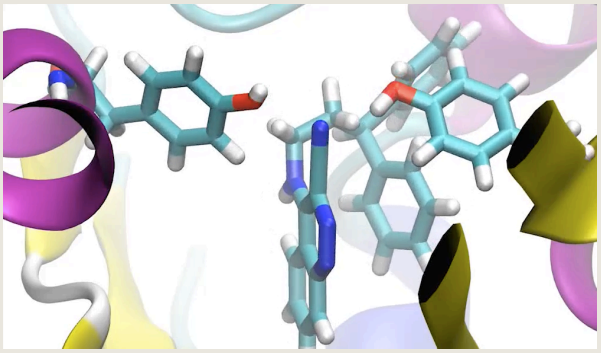
“My goal is to develop software tools that produce more detailed images by predicting how the electrons will distribute themselves in samples and revealing atomic bonding**. My supervisors work closely with companies who need tools like these, and microscope manufacturers themselves could incorporate them into the software used with their products**.”



Tim is in no doubt about the CDT’s strengths. “It’s not easy to bring theoretical and computational chemistry together and deliver an education embracing both,” he says. “The CDT’s ability to do this, which is rooted in the cross-institutional collaboration between the three universities, underpins the unique experience it delivers”.

Personal Chemistry

Innovation isn’t just about cutting-edge laboratory facilities, next-generation software and state-of-the-art computers – fundamentally, it’s about equipping people with the skills and vision to harness them and unlock their full potential. “In the world of chemistry, important discoveries will be made at the interface of theory and experiment – exactly the place where modelling & simulation sits,” Jon Essex concludes. “Integrating disciplines so that researchers’ expertise breaks down traditional boundaries has to be the way forward. The TMCS CDT is blazing a trail towards that future.”



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