

# > **Alchemy** News: Autumn Edition

## Launch, Funding, & More

### Welcome to the Alchemy Autumn Edition Newsletter!

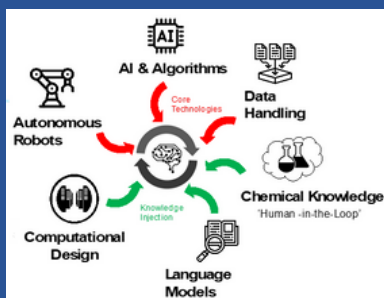
Our first newsletter marking the digital launch of Alchemy, a UK, EPSRC funded Hub pioneering AI-driven chemistry. In this issue, we will cover our latest funding call, recap on our inaugural webinar, and meet Professor Kim Jelfs in our "Meet the Team" spotlight.

### > **AICHEMY'S DIGITAL LAUNCH (5 SEPT)**

At our digital launch, the Alchemy Hub unveiled our vision for integrating AI into chemistry, attracting nearly 150 attendees. Co-Director Professor Kim Jelfs introduced Alchemy's mission: conducting cutting-edge research and normalising the use of AI in chemistry.

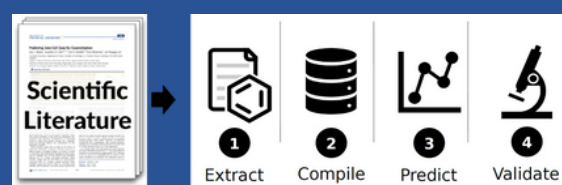
The hub has kicked off with five forerunner projects:

1. Human-in-the-Loop Platform – A real-time platform where researchers inject insights as robotic searches evolve, scaling to global crowdsourced experiments.

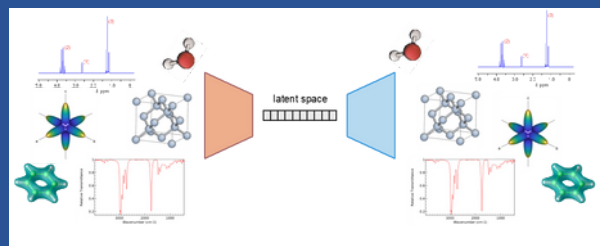


2. Large-scale crystal structure prediction (CSP) – creating large-scale data, to describe relationships between crystal structure, molecular structure, and functional properties.

3. Data-Driven Materials Discovery – Developing a 'design-to-device' pipeline that uses AI, machine learning, and high-throughput testing for materials discovery for chemical applications.



4. Generative AI for Materials – Scalable generative models that harvest chemical knowledge from large-scale multi-modal chemistry data.



5. Multi-Fidelity Reaction Optimisation – An automated platform using AI to identify and optimise reaction mechanisms.

These projects set the stage for collaborative, data-driven chemistry innovation

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We outlined activities aimed at fostering a collaborative community, such as annual conferences, hackathons, workshops and training organised by the Early Career Researchers (ECR) committee. The hub also announced a Flexible Fund for research grants, with the first funding call opened in October (see further below for more details).

Co-Director Professor Andy Cooper discussed the importance of industry engagement within the hub. Alchemy encourages collaboration across sectors, offering engagement opportunities for co-funded projects and secondments. These partnerships will play a key role in advancing innovation within the AI and chemistry research, bridging the gap between industry and academia. The response from attendees during our interactive session highlighted a real need for community-building around AI in chemistry, guiding our future events and initiatives.

### > **FUNDING OPPORTUNITY: AICHEMY PUMP PRIMING FUND**

The Alchemy Pump Priming Fund is now open for applications, offering up to £25,000 per project (award made at 80% FEC) to support short-term research at the AI-Chemistry interface.

This funding aims to help researchers develop and test innovative ideas in areas such as AI applications in chemistry, software development, and data improvements.

The deadline for applications is Friday, **6th December 2024 at 5:00 pm.**

Full details, including eligibility and the review process, can be found in the Funding Call Document Pack on our website. The webpage also includes some frequently asked questions which you may find useful.

### > **AICHEMY'S INAUGURAL WEBINAR - (23 OCT)**

We recently hosted the inaugural webinar in our monthly webinar series, organised by the AIChemistry ECR Committee.

The webinar featured two amazing talks, Annabel Basford, a PhD student at Imperial College London shared her work on automating the synthesis of porous organic cages, showcasing how robots and high-throughput systems can speed up material discovery and improve efficiency.

Then, Professor Anna Slater from the University of Liverpool talked about the wonders of flow chemistry, which allows for precise control over complex reactions, leading to better yields and quicker processes.

[\*\*APPLY AND FOR MORE INFO\*\*](#)



[\*\*WATCH THE TALKS HERE\*\*](#)



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### >\_UPCOMING WEBINAR

Don't miss out on the chance to hear from leading experts in the AI-Chemistry field!

**Sign up Now to our November webinar.**

📅 20th November 2024, 13:00-14:00

📍 MS Teams Webinar

**REGISTER NOW**



#### Speakers:

- Dr. Adam Clayton - Self-Optimising Approaches for Flow Synthesis
- Abdoulatif Cisse - HypBO: Accelerating Black-Box Scientific Experiments Using Experts' Hypotheses

### >\_CHEMICAL AND MATERIALS MACHINE LEARNING SCHOOL 2025

📅 31st March - 4th April 2025

📍 Daresbury Laboratory

💷 Fee: £350 (includes 4 nights' accommodation and catering)

Applications are now open, this in-person training covers ML basics, graph networks, generative models, ML potentials—specifically tailored for chemistry and materials science.

**APPLY AND FOR MORE INFO** [↗](#)

### >\_SAVE THE DATE - UPCOMING AICHEMY CONFERENCE

📅 17th March 2025

📍 Imperial, White City Campus

Join us for a day of great talks, innovative research, and networking opportunities. Speakers to be announced!

### >\_MEET THE TEAM - SPOTLIGHT

#### PROF. KIM JELFS



Professor Kim Jelfs,  
Co-Director of  
Alchemy Hub and Co-  
Director of the  
Institute for Digital  
Molecular Design and  
Fabrication ([DigiFAB](#)).

She is a leader in Computational Materials Chemistry, fusing calculations with robotics, connecting AI to synthesis, generative models and explainable ML. Recognised with prestigious awards like the Royal Society of Chemistry Harrison-Meldola Memorial Prize (2018) and the Philip Leverhulme Prize (2019). As an Associate Editor for Chemical Communications and a key member of several influential research networks, she is dedicated to advancing materials science and chemistry.

**Thank you for reading and we look forward to engaging with the wider community as we advance the Alchemy mission!**

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