Town Hall meeting – discussion notes

Discussions surrounding the future trajectory of the UK Catalysis Hub highlighted several key themes essential for its continued success and impact. Participants emphasized the need for the hub to evolve its priorities over time, ensuring alignment with emerging challenges and opportunities in catalysis. This evolution should be accompanied by adequate resource allocation to support ambitious goals, including enhancing collaboration between academia and industry. Suggestions included organizing joint conferences, offering industry placements, and facilitating technology transfer through mentorship programs. Additionally, there was a call to establish the hub as an integrated institute with clear strategic focus areas, akin to the Rosalind Franklin Institute, while expanding its global reach and maintaining existing networks.

Skill development emerged as a crucial aspect of supporting the community, especially Early Career Researchers (ECRs). Discussions emphasized the importance of cross-disciplinary training, including AI and computational skills, and the provision of structured training programs aligned with industry demands. Strategies for engaging with SMEs and smaller businesses were also discussed, highlighting the hub's potential role as a focal point for technology transfer and collaboration. Looking ahead, participants envisioned the hub as a catalyst for fundamental research and innovation, driving progress towards net-zero emissions and addressing global challenges. By embracing these principles and initiatives, the UK Catalysis Hub can continue to play a leading role in advancing catalysis research, supporting the next generation of researchers, and driving innovation towards a sustainable future.

What are the key challenges and deliverables for Net Zero and Sustainability

In discussions surrounding the challenges and deliverables for catalysis research in achieving Net Zero and sustainability goals, several key points emerged. One prominent challenge identified is the need for addressing issues related to plastics and circular economy initiatives through catalytic research. This involves exploring new technologies and techniques for characterizing materials, particularly focusing on plastics, while also considering the decarbonization of processes such as steel and ammonia production. Additionally, there is a recognized barrier to adopting new catalysts in industry, stemming from historical practices and economic considerations, which underscores the importance of enhancing existing catalysts and overcoming barriers to their implementation. In addition to these challenges, reducing the total emissions of the Chemicals industry, particularly Scope 3 emissions, to zero by 2050 emerged as a critical objective. This endeavour faces complexities such as water use, reducing emissions to air/water, and emerging issues with forever chemicals and microplastics. Among these challenges, achieving Scope 3 Net Zero is particularly daunting due to its intricacies and the need for comprehensive strategies to mitigate indirect emissions associated with the supply chain and product lifecycle.

Furthermore, the discussions highlighted the complexity of feedstock selection and the necessity for catalysts capable of accommodating various feedstocks, including biomass, which presents logistical challenges. Accelerating catalyst production and testing, as well as improving high-throughput screening methods under relevant conditions, emerged as critical deliverables for catalysis research.

Moreover, ensuring access to and standardization of information, both in literature and patent databases, is essential for advancing research effectively. Establishing informed policies to guide research direction and enhancing the quality and consistency of reporting are also imperative. Overall, the Catalysis Hub aims to balance breadth and specificity in addressing these challenges, fostering collaboration across disciplines, and promoting fundamental research to drive the transition towards Net Zero and sustainability.

Efforts are underway to integrate fundamental concepts with macroscopic effects in modelling, necessitating multidisciplinary collaboration and the development of realistic modelling systems by computational scientists and software engineers. The urgency of achieving Net Zero requires accelerating learning and leveraging the Catalysis Hub as an opportunity to facilitate this transition. It is crucial to cultivate multifaceted scientists capable of bridging communication gaps between disciplines and understanding the entire life cycle of catalytic processes. While specialization is important, there is a growing recognition of the need for diverse expertise and a strong commitment from younger generations to drive change in catalysis research for sustainability.

What are the key challenges and deliverables and opportunities in Digital chemistry including AI, Automation, and computational methods?

In the realm of catalysis research, the advent of digital chemistry, bolstered by AI, automation, and computational methods, presents both challenges and opportunities that necessitate concerted future efforts. Key challenges identified include the need to streamline computational time for diverse catalytic systems and complex materials, particularly in the context of biocatalysis where acceleration of discovery is fundamental. Harnessing AI for predicting new enzymes or catalysts and implementing high-throughput screening and automation processes are imperative but underutilized opportunities. A pivotal deliverable for the future involves establishing a framework for sharing computational results effectively, while also addressing validation concerns and enhancing accessibility and availability of data. Standardizing data formats and developing algorithms to optimize data usage for the benefit of the community are essential steps forward, with the UK Catalysis Hub poised to take a leadership role in proposing and implementing such initiatives.

Moreover, the future of digital chemistry in catalysis research hinges on bridging the gap between experts and non-experts, ensuring effective communication and collaboration. This entails developing shared languages for communication, facilitating networking events, and providing platforms for knowledge exchange. Additionally, there is a pressing need to integrate AI training into the scientific community, particularly for mid-career researchers, and to design interactive software tools that streamline research processes. The role of human intuition in AI applications cannot be overlooked, necessitating innovative approaches such as voice recognition and virtual collaboration. The UK Catalysis Hub can play a pivotal role in fostering multidisciplinary interactions, providing funding and opportunities for early career researchers, and advancing policy perspectives to steer digital chemistry towards catalysing sustainable solutions. Ultimately, by embracing digital technologies and collaborative frameworks, catalysis research can achieve greater efficiency, transparency, and impact in addressing global challenges.

What are the key challenges and deliverables in Advanced Techniques for Catalysis including the Use of facilities?

In advancing techniques for catalysis research, a key challenge lies in streamlining the validation process for in situ and operando equipment within research facilities. Currently, this validation process can be time-consuming, often taking between 8 months to 1 year, thereby impeding timely experimentation. Future efforts should prioritize educating facility managers to strike a balance between safety requirements and facilitating research activities efficiently. Moreover, addressing the increasing bureaucratic hurdles is essential to expedite experimental setups and minimize delays. Collaborative initiatives between the UK Catalysis Hub and facility engineers, possibly through joint positions with certified chemical engineers, can enhance trust and streamline validation processes, ensuring quicker access to advanced research techniques.

Furthermore, future endeavours should focus on democratizing access to advanced techniques and facilities for a broader community of researchers. Implementing a hub and spoke model, linking expertise across the country, can facilitate knowledge sharing and accessibility to specialized equipment. This approach, coupled with digital twinning initiatives, can effectively onboard new users and expand the utility of existing facilities. Strategic investments in automation and digital twinning for remote access and analysis present promising avenues for enhancing efficiency and scalability in catalysis research. Additionally, targeted funding schemes, such as seed funding for equipment acquisition, can empower early career researchers to explore new research fields, including sustainable alternatives like biosolvents and green hydrogen, addressing global demands and contributing to carbon footprint reduction initiatives. By demystifying access to central techniques, fostering collaborations, and strategically deploying resources, the UK Catalysis Hub can spearhead transformative advancements in catalysis research, driving innovation and sustainability.

What are the Emerging areas, Interdisciplinary areas, and new opportunities in Catalysis?

In navigating the emerging areas and interdisciplinary opportunities in catalysis, a paradigm shift towards holistic catalyst design and integration of diverse catalytic methods is imperative. This entails exploring innovative approaches such as blending different types of catalysis, including bio and heterogeneous catalysis, for efficient biomass conversion. To ensure the reliability and reproducibility of research findings, there is a pressing need to enhance reporting standards, particularly in electrochemistry and beyond. Implementing rigorous measurement protocols, including the inclusion of error bars and triplicate measurements, can bolster the credibility and trustworthiness of research outcomes. Moreover, fostering interdisciplinary collaborations is paramount to harnessing synergies between catalysis and other domains such as big data and AI. By reaching out to diverse communities and integrating insights from engineering, life cycle assessments (LCAs), and emerging interdisciplinary areas, the catalysis community can unlock new avenues for innovation and address complex challenges effectively.

Furthermore, catalysis research must adapt to evolving technological landscapes and societal demands, particularly in the context of renewable energy integration and waste utilization. Proactively engaging with initiatives like biomass networks and collaborative platforms such as BBSRC NIBBs and PoCs facilitates industry partnerships and short-term engagements, fostering rapid translation of research into real-world applications. Embracing advancements in AI and exploring

novel coupling reactions, as well as simplifying procedures, can streamline catalytic processes and enhance their applicability in intermittently powered plants fuelled by renewable sources like wind or solar energy. Collaborating with other hubs and prioritizing safety considerations are also paramount, ensuring responsible and sustainable catalysis practices in line with broader societal and environmental objectives. By embracing interdisciplinary collaboration, adopting innovative methodologies, and aligning research efforts with emerging societal needs, the catalysis community can navigate towards a more impactful and sustainable future.

What strategic Equipment should the Hub invest in to support the community (Academia and Industry)

To strategically invest in equipment that best supports both academia and industry within the catalysis community, it's crucial to prioritize accessibility, functionality, and community engagement. A consensus among discussions suggests that any new equipment acquisitions should align with existing capabilities while enhancing experimental efficiency and data quality. High-throughput reactors have been proposed as a unique and valuable addition to the Hub's equipment inventory, offering versatile usage and real-time product analysis capabilities. However, the effectiveness of such investments hinges not only on the acquisition of equipment but also on ensuring proper setup, operation, and utilization. Therefore, investing in equipment must be accompanied by adequate training and support to enable widespread access and utilization, akin to the operational model of national facilities. Additionally, the selection process for new equipment should be collaborative, with input solicited from the catalysis community to define principles and priorities that align with the evolving needs and objectives of Phase 3 initiatives.

In navigating equipment acquisition and utilization, the Hub can leverage its position to foster collaborations, facilitate funding applications, and enhance research capabilities. Community engagement is paramount, with stakeholders advocating for active involvement in decision-making processes regarding equipment selection and administration. Moreover, initiatives such as shared PhD student pools and PDRA sharing programs can bolster resource utilization and enable broader access to expertise and facilities. By streamlining access to equipment and providing support for proof-of-concept work and preliminary experiments, the Hub can play a pivotal role in catalysing innovation and advancing research efforts across academia and industry. Ultimately, strategic investments in equipment should not only enhance experimental capabilities but also foster a collaborative and inclusive research environment that drives meaningful progress in catalysis research and development. Suggestion such as long duration equipment a, electrolysers, sample environments and equipment to support access to facilities need to be considered

What mechanisms should there be to utilise the flexible funding to support the community?

To effectively utilize flexible funding to support the community, mechanisms must be established to address various career stages, promote networking, and facilitate skill development. Initiatives such as mentorship programs for early-career researchers (ECRs) can provide invaluable guidance and support, with efforts made to ensure diverse representation and access to mentors outside of the mentees' home institutions. Implementing best practices in mentorship, including training for both mentors and mentees, can enhance the effectiveness of these programs. Networking events tailored

to new starters, along with workshops on fellowship applications and proposal writing, can empower researchers with the knowledge and resources needed to advance their careers and secure funding. Additionally, leveraging the expertise of successful facility users to share insights on proposal writing and collaborative opportunities can further enrich the community's skillset and promote collaboration across disciplines.

Furthermore, the flexible funding should be allocated to address various needs within the research community, including covering journal charges, investment studies, and impact assessments. Efforts should be made to bridge interdisciplinary gaps by inviting participation from other departments, such as biology, and aligning grant eligibility criteria to avoid conflicts. Initiatives like interruption of studies for PhD students to engage in research assistantships and targeted training programs in management, project management, and mentoring skills can further enhance the professional development of researchers. Additionally, to maximize the impact of grants, mechanisms such as small pots of funding with a decent success rate and sandpit-style workshops can be implemented to foster innovation, facilitate collaboration with industry partners, and address emerging challenges in catalysis research. By embracing these mechanisms, the hub can effectively leverage flexible funding to foster a dynamic and collaborative research environment that drives impactful advancements in catalysis science.

How can the Hub engage more with industry?

The UK Catalysis Hub can enhance its engagement with industry through various strategies aimed at fostering collaboration, addressing industry needs, and promoting knowledge exchange. One approach is to facilitate joint academic-industry conferences and meetings, maintaining a balanced representation to encourage networking and collaboration opportunities. Emphasizing poster sessions at these events can further encourage interaction and potential collaborations between academia and industry. Additionally, the hub can play a pivotal role in highlighting industrial strategic priorities, providing clarity on industry objectives and requirements to align research efforts effectively. Training programs tailored to industry needs can equip researchers with the necessary skills, fostering a workforce adept at addressing industrial challenges. Initiatives such as joint industry postdoctoral research associates (PDRAs) and PhDs, as well as short-term industry internships facilitated by the hub, can provide valuable hands-on experience and facilitate mutually beneficial collaborations between academia and industry. By showcasing the breadth of career opportunities in catalysis, including SME involvement, through dedicated events like "Careers in Catalysis," the hub can attract industry interest and talent, further strengthening collaboration efforts.

To optimize engagement with industry, the UK Catalysis Hub can adopt several strategic measures and mechanisms. Showcasing hub activities at industrial shows can increase visibility and attract industry partners, while providing a comprehensive list of competencies on the website can guide industrial partners to the appropriate contacts within the hub. Clear signposts on how industry can engage better, emphasizing factors like speed of turnaround and mechanisms for wider partnership, can streamline collaboration processes and enhance industry buy-in. Collaboration opportunities with industry consortia, manufacturing hubs, and technology translators can broaden the scope of engagement and facilitate problem-solving across various sectors. Moreover, initiatives like sandpit workshops, co-creation projects, and prosperity partnerships can provide avenues for collaborative

research projects that address specific industry challenges while fostering long-term partnerships between academia and industry. Demystifying research facilities and leveraging advancements like high throughput techniques and AI can further enhance industry collaboration by providing innovative solutions and insights into complex industrial problems.

What might the Hub look like after 7 years

In envisioning the future trajectory of the UK Catalysis Hub over the next seven years, several key considerations and aspirations emerge from the discussions. It is imperative that the hub's priorities and drivers evolve over time, adapting to emerging challenges and opportunities. One crucial aspect is ensuring that resources align with the hub's ambitions, addressing any challenges related to linkages with facilities and resourcing issues. Enhancing engagement with other UK universities is essential for fostering broader collaboration and maximizing the hub's impact across academia. Affiliation with the hub should serve as a catalyst for attracting additional funding, leveraging its capabilities as a seed for obtaining further financial support. Moreover, forging evidence-backed partnerships is paramount in achieving the hub's ambitious goals, transforming it into an integrated institute with clear collaborations akin to established entities like the Rosalind Franklin Institute.

To solidify its position as a catalyst for impactful research, the hub should aim to operate as an incubator, facilitating connections with entities for transitioning research outputs to commercial applications. The integration of a Business Development Manager within the hub could bolster efforts in this direction. Additionally, increased representation at conferences and proactive engagement with industry stakeholders are pivotal for broadening the hub's reach and impact. Strategically, establishing clear mission areas and deliverables, particularly in the context of addressing challenges related to net-zero emissions, can enhance the hub's visibility and influence, positioning it as a go-to institute for catalysis-related initiatives. Continued emphasis on public engagement, networking internationally, and leveraging achievements to secure funding and international recognition are essential components in shaping the future trajectory of the UK Catalysis Hub towards greater prominence and impact on a global scale.

What Skills and training should the Hub be providing to support the community especially ECRs

The UK Catalysis Hub aims should aim to provide comprehensive skills and training support to the community, especially Early Career Researchers (ECRs), to enhance their interdisciplinary capabilities and prepare them for industry engagement. This includes fostering expertise in cross-disciplinary communication, such as facilitating dialogue between process engineers and fundamental scientists, and equipping researchers with essential AI and computational skills for data sciences. Industry placements and structured training frameworks tailored to industry demands are essential for preparing ECRs for diverse career pathways, whether in academia or industry. Additionally, formalized training programs, aligned with existing Centres for Doctoral Training (CDTs), can enrich the skill sets of Postdoctoral Research Associates (PDRAs) within the hub, ensuring a depth of expertise coupled with a breadth of understanding across disciplines. Collaborative initiatives, such as roadshows bringing facilities to industry and mentorship schemes linking researchers with experts, can streamline access to resources and facilitate knowledge exchange, contributing to the professional development of ECRs and fostering a vibrant and interconnected research community.

Furthermore, the hub should prioritize fundamental research while offering avenues for career progression and industry engagement, ensuring a balance between beamtime-focused activities and the development of transferable skills. Efforts to engage with SMEs and interconnect smaller businesses with the hub can broaden industrial involvement and facilitate technology transfer, enhancing the hub's impact on the broader economic landscape. By maintaining a career carousel and continually elevating new talent, the hub can sustain its momentum in catalysing groundbreaking research and driving innovation across academic and industrial domains. Through strategic initiatives and collaborative partnerships, the UK Catalysis Hub can position itself as a dynamic hub of excellence, empowering ECRs and fostering a culture of interdisciplinary collaboration and impactful research in catalysis.

Other points raised

International engagement

e.g., Horizon consortiums : Mission integrated biorefineries? The hub should provide a focus for these international funding opportunities. E.g., Royal Society international exchanges, NSF-UKRI funding schemes.

International entities may also benefit from engagement form the hub e.g.

- The Capex Pioneer centre in Denmark, a £30 million research initiative on catalysis for power to x with a heavy focus on automation and AI. I have strong links to the PI, Tejs Vegge, so happy to make connections there.
- The DOE's Sunlight Alliance https://www.liquidsunlightalliance.org/welcome
- Mission Innovatoin https://mission-innovation.net
- Sunergy, an EU initative on sustainable fuel and chemical production https://sunergy-initiative.eu

UK wider excellence

The UK has are incredible centres of excellence in the capability behind catalysis. Outside of Harwell (of course) we have not tapped into flow/process methods (Leeds in particular), NMR (York, Cambridge), Mechanochemistry (Birmingham), AI/ML (Manchester), Industrial Catalyst Characterisation (Drochaid), Chemical Biology. There are many more: Perhaps a model where the concept of CORE PDRA is extended to these other capabilities is one where real progress can be made? If the largest single component of the EPSRC portfolio is catalysis, then there are plenty of projects that can use such capability. People bid for a PDRA time for 2,3,4 months to solve or explore a particular problem in catalysis (even better if related to Net Zero, UK security). This would also be a way to engage with industry - it de-risks exploratory studies and also provides a source of income/industrial engagement.

Engagement with other communities

There are many people in the Hub that could be utilised to strengthen and build links with other communities so the Hub can link to other UK entities with overlapping remits to avoid replicating efforts Some of these may include for example

- The RSC Electrochemistry and Materials Chemistry groups
- The Henry Royce Institute, which holds a lot of events in relation to catalysis and has a lot of relevant equipment for catalysis researchers.
- The Solar Chemicals Network, which also represents a large group of catalysis researchers.

This could be done through joint events, workshops and invitations to speak to encourage dissemination and collaboration an s could lead to grant proposals.