## FROM KNOWLEDGE TO ACTION APPLICATION

Title: Sustainable Ammonia for a Net Zero Society

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## Other investigators:

#### Category

From Science to Society

### Problem (max. 50 words):

Ammonia as a fertiliser has both positive and negative effects on society. It is positive as it sustains over 40% of global population but has a negative impact as current ammonia production is highly energy-intensive and carbon-emitting. Sustainable, distributed ammonia synthesis is essential for society and will be our focus.

### Unmet Need (max. 50 words):

Ammonia is an essential chemical for fertiliser production and an emerging energy vector. Sustainable, scalable production methods compatible with intermittent renewable energy are lacking. Overcoming catalytic limitations and mechanistic barriers is critical to decarbonising ammonia production and enabling its wider use in sectors such as aviation and energy storage.

## Project Description (max. 200 words):

This project will develop novel catalytic approaches for low-energy ammonia synthesis, by linking computational and experimental methods bridging fundamental research and real-world impact. We will focus on metal nitride catalysts that offer pathways beyond traditional scaling limitations, potentially enabling associative mechanisms akin to enzymatic nitrogen fixation. Well-defined catalysts will be systematically synthesised, characterised, and tested using advanced experimental techniques.

Computational modelling will guide catalyst design, with insights feeding back to experimental work. This interdisciplinary effort links chemistry, materials science, and digital methods, aligned with the Net Zero agenda. The work supports decentralised ammonia production for sustainable agriculture, green energy storage, and fuels for hard-to-decarbonise sectors like aviation. It fosters collaboration across academic disciplines, promoting knowledge transfer and career development for young researchers.

Led by the UK Catalysis Hub we will ensure that the findings will be disseminated to society through outreach events (e.g. the Royal Society Summer Science Exhibition) and science fairs.

# Hypothesis (25 words):

Metal nitride catalysts can enable novel associative mechanisms for sustainable ammonia synthesis,

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overcoming current performance barriers and facilitating decentralised, low-carbon production compatible with renewable energy.

### Implication for Practice (50 words):

The project will inform the design of catalysts and processes for distributed, low-carbon ammonia production, supporting decarbonisation of agriculture, energy, and transport. It will directly contribute to Europe's Net Zero goals, while fostering practical pathways for integrating green ammonia into energy infrastructure and emerging clean fuel markets.

### Implication for Research (50 words):

Our work will advance fundamental understanding of nitrogen activation and associative ammonia synthesis. By combining experimental, computational, and AI approaches, we aim to develop predictive models for catalyst design. The research will stimulate cross-disciplinary collaborations and contribute to broader efforts in sustainable catalysis and digital chemistry across Europe.

Training of Early Career Researchers (ECRs):

The project will support early career researchers to develop interdisciplinary skills in catalysis, computational modelling, and sustainable technologies, preparing the next generation of scientists to tackle real-world energy and environmental challenges.

Formation of New Collaborations:

By fostering interdisciplinary partnerships, the project will stimulate knowledge exchange, build networks, and accelerate the translation of research into impactful societal applications.

Increased Public Awareness of Sustainable Ammonia and Green Chemistry:

Through engagement activities such as science fairs and public exhibitions (e.g. Royal Society Summer Science Exhibition), the project will raise awareness of sustainable chemistry and its role in the Net Zero transition.

In the slightly longer term we propose

Acceleration of Technological Readiness:

Proof-of-concept catalytic systems developed under this project could inform the early design of next-generation ammonia production technologies, laying the groundwork for industrial trials and scale-up.

Contribution to Policy and Industry Dialogue:

results could inform discussions on Green ammonia, net Zero and clean fuel strategies, contributing to national and European policy development for energy and agriculture sectors.