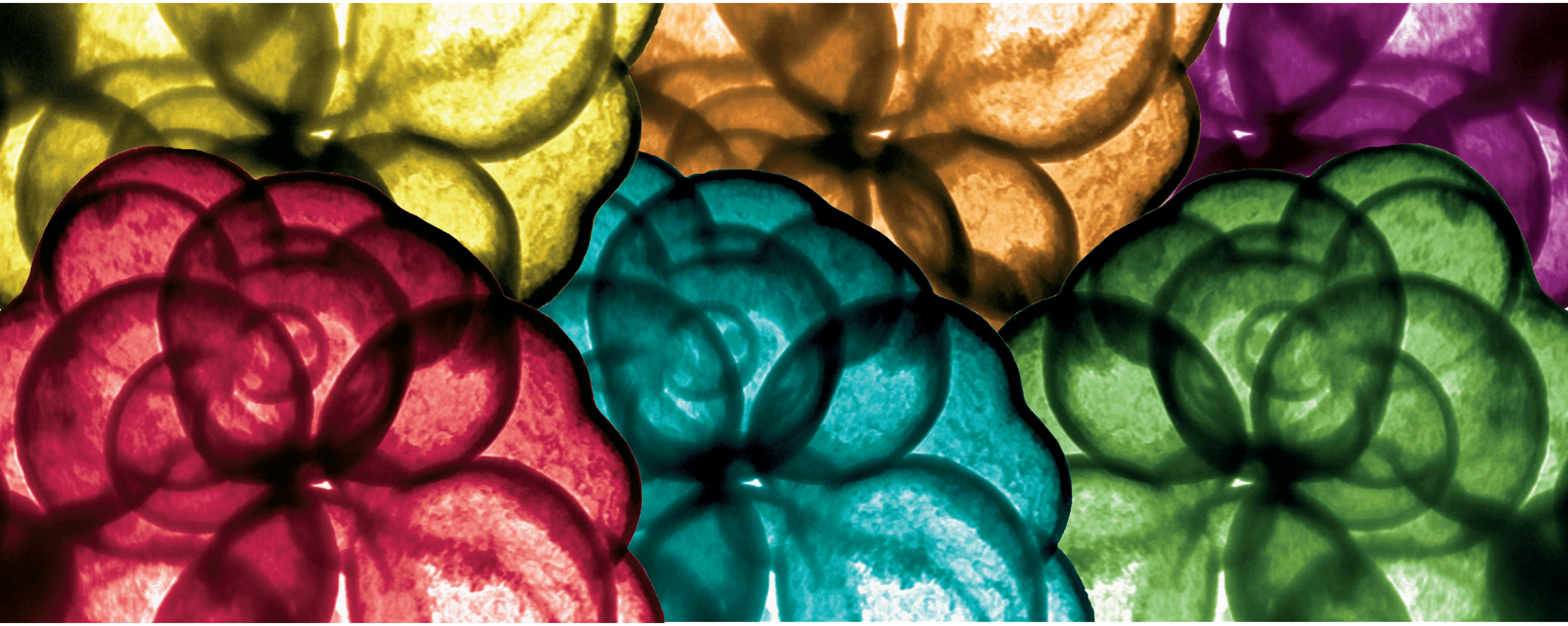
SynBIM



Report from the Symposium on

Bridging the gap:

bioinspired nanomaterials and sustainable manufacture

Bridging the gap: bioinspired nanomaterials and sustainable manufacture.

This is a report from the symposium organised in Manchester on 22-23 Jan 2020.
This report is written for public dissemination.

March 2020.
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All photos from the entire symposium are available at https://tinyurl.com/qng38ke.

Contents

Executive summary

The SynBIM project combines experiments and modelling, creating transformative knowledge and toolsets, to enable larger-scale tunable manufacturing of nanomaterials using a bioinspired "green" approach.

Research focusses on establishing laws both for governing de novo design of nanomaterials, and also for how processing conditions and production scale affect material attributes. The work responds to the challenge that, despite the benefits of bioinspired chemistry, cost-effective, reproducible commercial-scale manufacturing remains elusive due to challenges associated with scale-up.

The symposium reported progress made by the SynBIM project and brought together stakeholders interested in driving discovery-to-scale-up of nanomaterials. The event combined talks and posters from academia and industry from both within and beyond the project. It also included a half-day development workshop, which explored future challenges and responded with project ideas and proposals.

Delegates **identified a number of research challenges** associated with driving discovery of nanomaterials to sustainable manufacturing. Four broad themes emerged in the areas of **analytics** (e.g. measuring time-scales for various processes over relevant length-scales), **dial-a-product/process** (e.g. predictive design of materials and processes), **data science** (e.g. data mining and machine learning) and **sustainability** (e.g. systems-level evaluation of sustainability and life cycle for driving innovation).

A number of projects were envisioned to address these challenges and three top voted projects were developed further into outline proposals. They included *Britain's Next Top Modeller*, *SubSIDe (Sustainable, Scalable Incredible Database)* and *ForMA (Ferromagnetic for Medical Applications).*

In recognising the scale of both the significant opportunities and also the corresponding challenges associated with realising the SynBIM vision, further substantial work and investment is required. For success, this will require effective collaborations over extended time frames. Consequently, a further challenge is how to achieve this.

This report is provided to inform the scientific community across academia and industry, as well as funders and policy makers, about important future challenges and opportunities. Those who attended the event are encouraged to lead in developing associated partnerships, collaborations and funding applications.

Left: photo taken on day-2 of the symposium shows all attendees on that day.

1. The SynBIM project

Commercial manufacturing of high value nanomaterials is energy and resource intensive. In contrast, biomineralisation, which occurs in nature, produces a wide range of nanomaterials under ambient conditions. The development of corresponding synthetic biology (synbio) offers the potential of more sustainable production though so far has only delivered at lab-scale.

The aim of this collaborative and interdisciplinary project is to create transformative knowledge and toolsets needed to enable larger-scale manufacturing of tuneable nanomaterials using an eco-friendly "green" synbio approach. Specifically, the project aims to increase the knowledge and understanding of how we can translate natural processes into materials produced in the laboratory and how we can translate the developed science into industrially relevant products. Work is organised by three research themes:

Particle formation pathways

Experiments and modelling to probe nanomaterial formation pathways, clustering and self-assembly under static and dynamic flow conditions. Also, the characterisation of resulting nanomaterial properties, building synthesis-property relationships and scaling laws.

Product design

Scalable synthesis of nanomaterials by specifying the chemistry and synthetic conditions to produce products with desired properties that are ready for industry.

Scale up and manufacturing

Validation, at larger scale, of the relationships between nanomaterial formation pathways, clustering, optimised synthetic conditions, effects of fluid dynamics and scaling laws.

IMPACT SUMMARY

Selected publications

- *Mol. Phys.*, 2018, **116**, 3231
- *Curr. Opin. Green Sustain. Chem.*, 2018, **12**, 110
- *Nanomaterials*, 2019, **9**, 1729
- *Colloid Surface A*, 2019, **579**, 123633
- *Mater. Horiz.*, 2019, **6**, 1027

The project is creating significant academic and non-academic impact via a book, and other publications, by disseminating research at conferences, by engaging public and schools in science through a wide range of outreach activities and creating strong academic and industry collaborations to facilitate fundamental research and its translation to industry

SynBIM

• 4 years • £1.9 million • 3 themes
• 3 universities • 15 researchers.

2. The SynBIM symposium

The symposium reported progress made by the SynBIM project and brought together stakeholders interested in driving discovery-to-scale-up of nanomaterials.

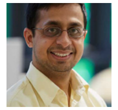
The event combined talks and posters from academia and industry from both within and beyond the project, giving emphasis to the full scope of experimental and modelling interests, and to both translational and fundamental research. There was also a half-day development workshop, through which participants explored future challenges and responded to them with project ideas and proposals.

Session	Title	Description
Session 1	Inspired by Nature	Tracked the synbio concept from its biological origins through chemical discovery towards targeted market applications. It also reviewed progress on associated mechanistic investigations and understanding.
Session 2	Harnessed for Market	Reversed the thinking of session one, starting with a view of the selected markets and exploring how synbio inspired processes are enabling engineers to respond with novel technology and commercially relevant solutions. It also considered the role of fundamental work alongside.
Session 3	Enabled by Research	Reflected upon the major research challenges emerging from the first two sessions and considered them in the context of the UK research, development and funding landscape.
Session 4	Workshop	The workshop provided an opportunity to build on project learnings and discussions from day 1, to consider emerging research challenges and explore possible future work and collaborations.

The feedback on the symposium was overwhelmingly positive on all aspects including the scientific relevance and quality, planning and communication, and the project outcomes and future directions. Delegates expressed a clear desire to make this a recurring event. See appendices for delegate list and feedback summary, the full programme and a list of abstracts for oral and poster presentations. **Further information can be found at: http://www.synbim.co.uk/symposium.html.**

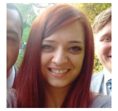
3. Session 1: Inspired by Nature

Session 1 explored the inspiration researchers draw from nature, analysing natural processes in order to build understanding and extract design rules for materials and applications. It provided examples of how to translate *bio* knowledge into innovative *synthetic* methods by combining experimental and theoretical approaches.



Siddharth Patwardhan (University of Sheffield), provided an **overview of the SynBIM project,** explaining its origins, scope and main collaborators. He reported good progress, highlighting academic outputs, industrial collaboration and a range of outreach activities (see section 6).

Marc Knecht (University of Miami) presented work on the **understanding and utilisation of bio-nano interactions in designing materials.** Inspired by the concept of bio-recognition, he showed the ability to fabricate multifunctional materials with desired properties on demand, including the examples of the design and performance of bespoke nano-catalysts.

Sarah Staniland and **Laura Norfolk** (University of Sheffield) presented work on **magnetic nanoparticles** (Magnetite), which, as they explained, form in nature inside bacteria. Taking inspiration from these magnetotactic bacteria, the pair's work has led successfully to **bioinspired synthesis of magnetite** in the laboratory using an array of organic additives selected by identifying key chemical functions and motifs from biomineralisation proteins: simpler than the proteins, these additive have the potential environmental benefits over traditional approaches. Their screening work, supported by Design of Experiments, demonstrates successful control of particle growth and material properties. Early results also show successful translation to a continuous scaled-up production of magnetic nanoparticles.

Paul Southern (Reasonant Circuits Ltd) talked about **medical applications of magnetic nanoparticles,** associated product characteristics and market perspectives. His own company is developing the use of cell-bound magnetic nanoparticles for hyperthermia-based treatment of cancer. His talk surveyed a wider range of possible applications and recognised a signficant market demand with large scale production of these materials becoming increasingly important into the future.

Georgina Zimbitas (University of Strathclyde) shared latest findings from within the SynBIM project relating to understanding the **fundamentals of particle formation pathways** using bioinspired additives. She elaborated on experimental and modelling results on clustering and self-assembling of the additives and how we can build, develop and calibrate predictive models for designing the synthesis of bespoke nanomaterials.

Miguel Jorge (University of Strathclyde) reported on the use of molecular dynamic simulations for synbio approaches. He talked specifically about multi-scale modelling for mechanistic understanding of bioinspired silica, taking into account the importance of different time and length scales. Research from his group shows that the neutral templating mechanism for porous silica fomation is incorrect. Validation from experiments is leading to the development of novel computational design for this class of materials.

4. Session 2: Harnessed for Market

This session focussed on what the market needs and explored the potential for bio-inspired materials and processes to meet these needs, whilst also improving sustainability. Overcoming scale-up challenges was acknowledged as a key development challenge for nanomaterials. Case studies of and principles for scaling-up for industrial manufacturing were presented.

Siddharth Patwardhan explained the **discovery to market pipeline** for bioinspired silica, including colloidal and mesoporous silicas. He explained how integrating scalability, market perspective and the techno-economics at discovery stage is beneficial. The **results from scale-up** were presented using a range of reactors in both batch and continuous mode, reaching the kg scales, thereby demonstrating how using the knowledge developed from the SynBIM project is enabling green manufacturing.

Rohan Vernekar (University of Edinburgh) presented work on **mesoscale modelling** applied to understand the influence of **fluid dynamics** on **nanoparticle growth,** and consequently how different flow regimes may affect scale-up. He presented the use of lattice Boltzmann algorithm to model the growth of nanoparticles, taking into account hydrodynamics, solute transport and particle dynamics. The model in its current form has been validated using benchmarks cases, thus indicating its potential to advance scale-up of nanoparticle synthesis.

Ian Houson (CMAC Future Manufacturing Research Hub) reviewed **scale-up principles for industrial manufacturing,** drawing upon a variety of examples and considering a range of perspectives including science, safety, product quality and business. He emphasised that scaling-up is not trivial and needs a multi-disciplinary approach. His key message was to think, plan, and consider rate processes very carefully because, while chemical processes are scale-independent, physical processes (e.g. mixing) change with scale and equipment.

Stuart Coles (International Manufacturing Centre, University of Warwick) presented a new, green chemistry-based classification model for the **assessment of sustainability** of nanomaterials synthesis, using **Multiple Criteria Decision Making** with information derived from literature and experts. He described a second, independent model based on **Stochastic Multiple Criteria Acceptability Analysis,** using relative indices based on a survey of experts. He illustrated both methods using the example of silver nanoparticles. Validation studies support wider application as part of product based sustainability assessment.

The second session concluded with flash presentations from early career researchers.

Andrea Laybourn (University of Nottingham) introduced herself and her work on the manufacturing of **metal-organic frameworks** using microwaves.

Jonathan Foster (University of Sheffield) did likewise on **metal-organic nanosheets** that can be applied for sensing, catalysis, separation and electronics, focusing on the need for scalability and future opportunities.

5. Session 3: Enabled by Research

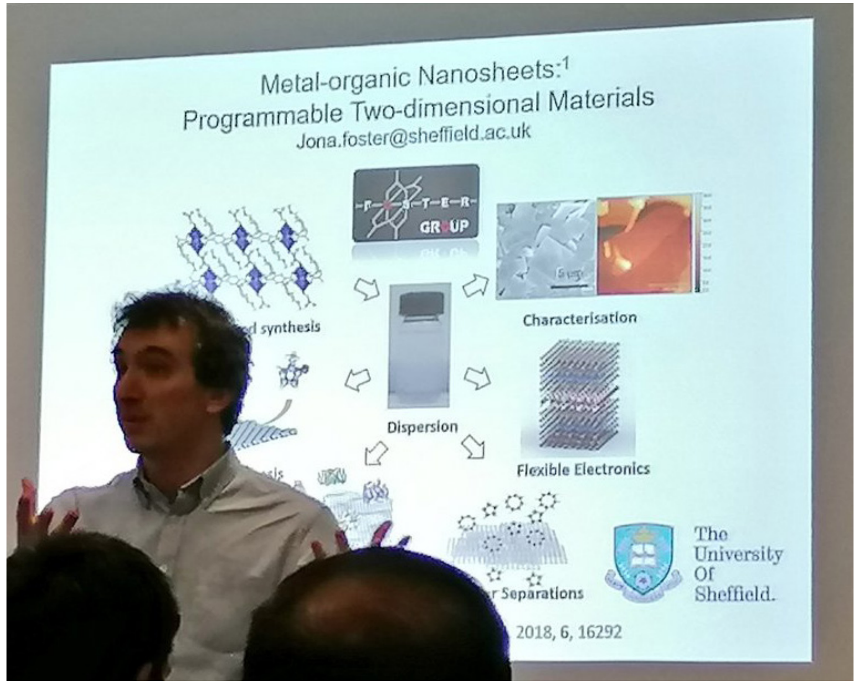
This session included presentations from the EPSRC, KTN and Directed Assembly Network about funding and networking opportunities to enable future research. There followed a discussion on the future challenges emerging from the whole day.

Becky Cheesbrough, representing the Manufacturing the Future theme at the Engineering and Physical Sciences Research Council (EPSRC), provided an overview of the council's priority framework, focussing on **funding schemes** relevant to the topic of the symposium such as the Standard Research Proposals, New Horizons Call and UK-USA collaboration scheme.

Mark Littlewood from the Knowledge Transfer Network (KTN) introduced the Network and its place within the UK research and innovation landscape. He also introduced KTN's new Nature Inspired Solutions Special Interest Group and emphasised how **learning from nature** offers important opportunities to solve industrial and societal challenges. KTN is leading the way in the UK to build an associated community across academia and businesses in this area.

Martin Elliott, Network Manager of the Directed Assembly Network (DAN) explained how it is bringing together researchers to tackle grand challenges from materials discovery through to scale-up and commercial translation. DAN is organised into five themes and three challenges. Their **Roadmap of Innovation** was constructed by the DAN community and presents areas of common interest, identifying challenges and aims to foresee scientific advancements over the next 50 years.

This session finished with discussion of the **challenges** faced in taking sustainable nanomaterials to manufacturing and market. These discussions and challenges formed the basis for developing future projects in the workshop on day 2 (see section 7 for detail of the challenges and other workshop findings).



6. Poster session and outreach activities

During the day, a range of posters were displayed. The judges awarded prizes to Laura Norfolk (1st), David Ashworth (2nd) and Manasi Mulay (3rd) on the basis of the quality and attractiveness (see photo below).

[LEFT} The three winners of the poster competition, Laura Norfolk, David Ashworth and Manasi Mulay, with the judges, Mark Littlewood of KTN (far left) and Marc Knecht from Miami (far right).

A range of outreach and public engagement activities developed during the SynBIM project were also showcased. Members of the SynBIM team and co-workers have been active in disseminating research to the wider public and communicating the science behind the project on numerous occasions. The topics included bioinspiration, the effects of mixing, scale-up and uses of silica and magnetic nanoparticles, which were presented in the form of hands-on activities, videos/ animations, public talks, school visits and dance in big events such as:

- **British Science Week,**
- **Discovery Night,**
- **Pint of Science,**
- **Festival of the Mind**
- **Manchester Science Festival.**

In total, the SynBIM project engaged with nearly 1000 people through these activities and events.

SynBIM

PRODUCT CHALLENGES

- **Larger-scale manufacturing of tunable nanomaterials**
- **Sustainable synthetic biology (synbio) approach**
- **Focus on silica nanoparticles and magnetite nanoparticles**

RESEARCH CHALLENGES

- **Understanding, prediction, optimization and control of complex chemical and physical processes operating over multple time- and length-scales, from lab-scale upwards towards pilot and manufacture.**

PIPELINE

- **Development process conceptualized as an interdisciplinary pipeline running from natural nanoparticles through to sustainably manufactured nano-materials.**

PROJECT

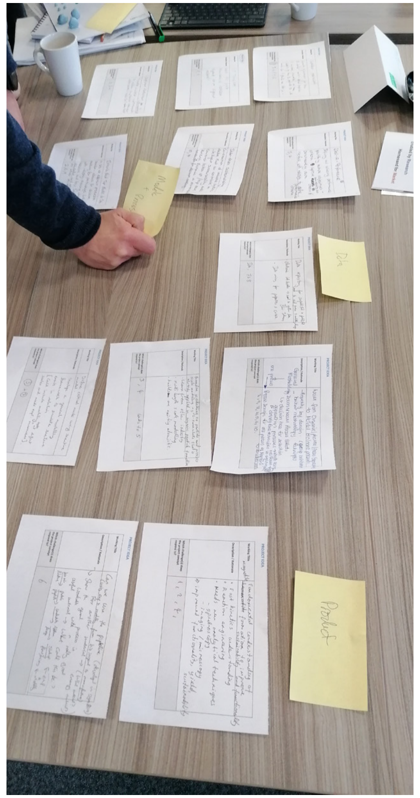
- **The SynBIM project enagages academia and industry across multiple groups, institutions and organisations on work spanning translational and fundamental, theoretical and practical chemistry and engineering.**

Fig 1: SynBIM project framework and product pipeline

7. Development Workshop

The second day included sandpit and road-mapping activities, aiming to engage funders and R&D specialists from industry and academia to identify research challenges, and explore future opportunities, new directions and collaboration. Building on the list of research challenges established on day one, participants brainstormed **project ideas** to respond to the challenges and drive forward the SynBIM vision. Ideas were collected and clustered into **related areas.** Participants were invited to choose the area(s) of most interest to themselves and form corresponding **working groups.** These groups elaborated the clustered ideas into **outline proposals,** which were finally presented and discussed in **plenary.** The workshop reinforced the important contributions made by the SynBIM project and also a clear need for follow-up research.

Outputs from the session are reported in three parts: general recommendations relating to the **SynBIM project framework and development pipeline** (section 7.1), list and elaboration of the identified **research challenges** (section 7.2) and the responding **research project proposals** (section 7.3). Finally section 7.4, looks **beyond the project level,** exploring a strategic view for the way ahead.



7.1. Project Framework and Development Pipeline

SynBIM elaborates both an ambitious vision and a practical framework for realising the larger-scale manufacturing of tunable nanomaterials via sustainable synbio methods. Good progress has been made across its work streams, both contributing directly to the development goals and also to a deeper understanding of the opportunities, uncertainties and barriers to success.

Workshop discussions confirmed that the framework and pipeline remains important and valid. Associated opportunities and suggestions emerged:

- It is important to continue to develop **silica and magnetite nanoparticles.** There is also potential for expansion to explore further systems, chemistries and functionalisation.

- **The bio-inspired approach** has demonstrated its value. There are useful opportunities to build stronger links with **the wider bio-inspired community**. Equally, for silica specifically and to some extent magnetite, the research focus has now moved down the pipeline with reduced emphasis on biological investigations.

- The central research challenge remains as **bridging the gap between chemistry and commercial products and manufacturing.** Achieving this *translation* takes longer and is more difficult than might be recognised, with many physical and chemical rate processes to be considered (e.g. different stages in the nanomaterial formation pathways). Success requires complete control of these processes and a deep understanding of the implicated chemistry and physics. Even where this has been achieved for lab-scale preparations, increasing the scale towards manufacture is rarely straightforward.

- Scale-up efforts so far have tended to concentrate on **main reactions and reactors.** Downstream processes, such as separations, are equally important from a process engineering perspective. **Incorporating the effects of downstream processes** on product properties and economics is therefore very important. One approach is to consider full process flow diagrams from an early stage of discovery.

- More broadly, recognising that the ultimate goal is to take discoveries pertaining the chemistry and synthesis of nanomaterials all the way to manufacturing highlights the importance of **Systems Engineering** (i.e. taking a systems-level approach, which encompasses the breadth of production processes and economics).

- There is a need to strengthen **modelling capabilities** to span wider time and length scales and also to combine empirical and fundamental approaches. Developing fully **empirical models,** although useful, may not provide the desired scientific insights and may provide limited predictability for wider systems. **Fundamental modelling** addresses these limitations but is time intensive and requires full understanding of the underpinning chemistry and physics. A **combined approach** offers the benefits of both (i.e. accuracy, predictability and practicality), however, care is needed in aligning workflow and timescales, especially within relatively short individual projects.

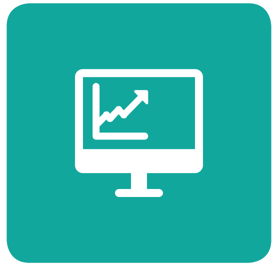
- Continued **collaboration and engagement** is vital. End user engagement in the formulation of research as well as in knowledge exchange was highlighted to be an important need. The **end users** include those developing applications of nanomaterials, who require the ability to control properties "on-demand". They also include those focussing on **manufacturing**, who need to engage with the scale-up science. There are important opportunities for learning from organic/pharma industries, especially with regard to the adoption quality-by-design.

- The synbio-nanomaterial community is small yet leading the way. It is important to build wider **networks both nationally and internationally.** More broadly, rising demand for knowledge on manufacturing of nanomaterials requires continued efforts both to engage the **public** and develop **educational resources.**

7.2. Research Challenges

Responding to the future needs, a number of specific **research challenges** emerged as crucial for progressing towards the goal of sustainable nanomaterials manufacturing. These were grouped in four Challenge Themes: **Analytics, Dial-a-product/process, Data Science** and **Sustainability.** The challenges are listed against each theme in Box 1. Themes are elaborated in the following text and summarised in fig 2.

BOX-1: Research Challenges



ANALYTICS

1. Measuring time scales for various chemical and physical processes over the relevant length scales.
2. In-situ monitoring of particle formation pathways to understand the process and develop process control strategies.
3. Coupling simulations using reactive ensemble with length and time scales of the reaction/synthesis.

DIAL-A-PRODUCT (or PROCESS)

4. Inclusion of detailed chemistry in simulations and matching real world parameters in simulations to enable predictive design of materials.
5. Designing high performance materials. Developing the underpinning science, defining the performance and linking it to properties (features vs benefits/property-performance relationship).
6. How to generalise the chemical understanding to make it transferable to other systems (predictively)?

DATA SCIENCE

7. Need for relevant experimental data for advanced modelling, sustainability evaluation and scale-up.
8. How to identify which data is needed and how to quantify uncertainties?
9. How to combine the use of data-driven models and modelling from the 1st principles?
10. Data mining and criteria defining

SUSTAINABILITY

11. Systems-level evaluation of sustainability as a means to drive innovation – Sustainability by Design (SbD).

Fig 2: Challenge Themes

SynBIM Challenge Themes

Challenge Theme 1: Analytics

Chemical processes, such as reaction kinetics, are scale independent however physical processes, such as mixing and heat transfer, are dependent on both the production scales and the equipment used. For a given scale (or at different manufacturing scales during scale-up trials), it is of vital importance to identify the rate-determining process/phenomenon.

This knowledge will help design suitable process and equipment for a given production scale in order to maintain the product quality. An example of this is that, at lab scale, the mixing of reagents is usually much faster than the time taken for the reaction, hence mixing has very little effect on the outcome of the reaction. At larger scales, given the larger volumes, mixing becomes slower than the reactions and hence specialised designs are required to maintain the reaction outcomes. The identification of rates of various processes requires significantly improvement analytical accuracies and capabilities. The needs are in three specific areas.

- The first is designing a combination of existing analytical instrumentation to measure critical processes. This also requires the adaptation of existing measurements and their analyses.
- Secondly, measuring the appropriate and multiple time scales for various chemical and physical processes is important because some processes can occur within microseconds, while others can take minutes to hours
- Finally, the techniques should be able to measure across the relevant length-scales. In particular for nanomaterials, the analytical capability should span from atomic (angstrom) agglomerate (micrometer) length scales because properties and the performance of nanomaterials is determined by properties across these length-scales.

These capabilities will be greatly beneficial in building in situ monitoring of particle formation pathways, in understanding the process and in developing process control strategies for large-scale manufacturing.

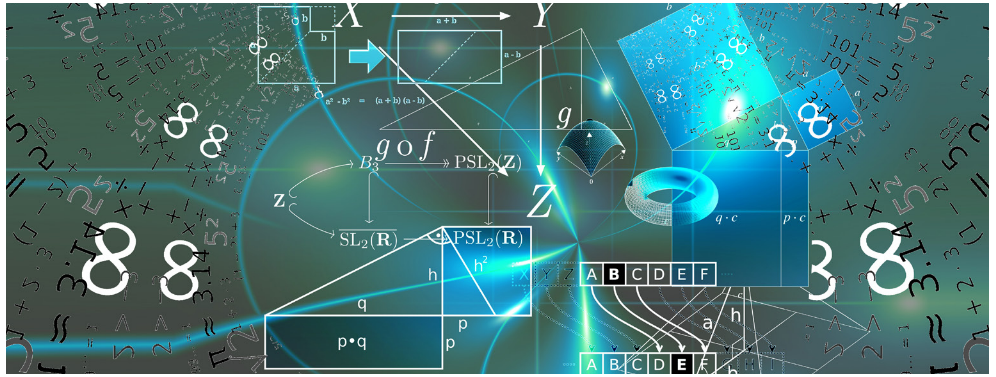
Challenge Theme 2: Dial-a-product/process

In recent years, the importance and the benefits of quality by design (QbD) has been realised in many sectors. Implementation of QbD requires a deep knowledge of a given system, including the process and the products. Developing predictive designs of nanomaterials and processes to produce them at a range of desired scales is hence a key research challenge. In the case of nanomaterials, their physicochemical properties are important as they control the performance of nanomaterials. As a result, developing the science to enable "dial-a-property" or property by design is required, which has also been identified as a key priority by the Directed Assembly Network. Three future directions were identified in this theme:

- A centrally important aspect is to build predictive capabilities using modelling and simulations across the length- and time-scales relevant to the reactions and syntheses. This requires the inclusion of detailed chemistry and matching real world parameters in simulations. There is a need to actively integrate the outcomes of analytics with simulations – to this end a two-way collaboration and communication is essential.
- Efforts in developing fundamental chemistry in order to design high performance nanomaterials needs to continue. A key challenge in this is defining critical quality attributes (CQAs) that are desired in given applications. Further, it is also important to link CQAs to measurable properties and build property-performance relationships. Addressing these challenges will help engage with industry/end-users by articulating the features and the benefits of the nanomaterials.
- Ultimately, these efforts should aim to develop generalised chemical understanding and methodologies that are transferable to other systems. This will enable wider and faster adoption of the outcomes as well as it will fast-track nanomaterials discovery to the marketplace.

Challenge Theme 3: Data science

With the progress made in field of big data and Industry 4.0, there are key challenges to address for nanomaterials manufacturing pertaining to identifying which data to collect and how to better use existing data. These efforts should help build advanced models.



- With increased analytical capabilities, it becomes important to identify which data are critically important. Creating chemical/syntheses repositories and developing standards for nanomaterials characterisation and testing are equally important. This need for relevant experimental data arises from building advanced models for predictive design of nanomaterials and scale-up methodologies. They also are important for systems level evaluation (see Theme 4). With model data being generated, it becomes important to develop tools and methods that are suitable to quantify uncertainties in the context of nanomaterials.
- The effective use of mining existing and new data is crucial. The outcomes can help better understand the synthesis, define the CQAs and address the challenges from Theme 2. For example, for a given nanomaterial, there are typically numerous published synthesis protocols. Data mining can help unify these into scientific principles and build structure-property-performance relationships. Such knowledge can also feed into Theme 4.
- Developing fully empirical models, although useful, may not provide the scientific insights and may have limited predictability for wider systems. On the other hand, modelling from the 1st principles, although desirable, can be time consuming and requires all underpinning physics to be known. Hence the challenge is to combine the use of data-driven models with fundamentals to impart the desired predictability with necessary accuracy.

Challenge Theme 4: Sustainability

The challenge is to use systems-level evaluation of sustainability and life cycle to drive innovation. As detailed by the ACS Green Chemistry Institute with various case studies, adopting the principles of sustainability can also offer significant economic benefits. In order to achieve systems level approaches, designing new tools and methodologies to compare the sustainability of various nanomaterials is required. Given that the CQAs for nanomaterials are typically complex and include more than just purity (e.g. shape, size, surface chemistry, crystallinity, porosity, etc.), such tools should be able to incorporate details about nanomaterials synthesis, properties, performance and environmental impact.

7.3. Project Proposals

A number of project ideas were developed to address the research challenges. The three most popular ideas were then developed into outline proposals. These are listed and briefly described below:

Britain's Next Top Modeller	SubSIDe (Sustainable, Scalable Incredible Database)	ForMA (Ferromagnetic for Medical Applications)
Building a modelling pipeline throughout scales (from fundamental mechanisms to manufacturing) by engaging with experiments to feed into and validate models.	Creating an online resource by data-mining literature in order to interface with industry, academic researchers and other stakeholders to enable sustainability and scalability decision making.	Applying quality by design principles linking particle properties / attributes to manufacturing process for magnetic nanoparticles for hypothermia therapies.

Details on each project were captured and have been shared with those attending. These individuals are encouraged to lead in developing associated partnerships, collaborations and funding applications.

For information, SynBIM project members who participated in these respective discussions were: SubSIDe (Siddharth Patwardhan, s.patwardhan@sheffield.ac.uk), ForMA (Sarah Staniland, s.s.staniland@sheffield.ac.uk) and Top Modeller (Timm Krueger, timm.krueger@ed.ac.uk).

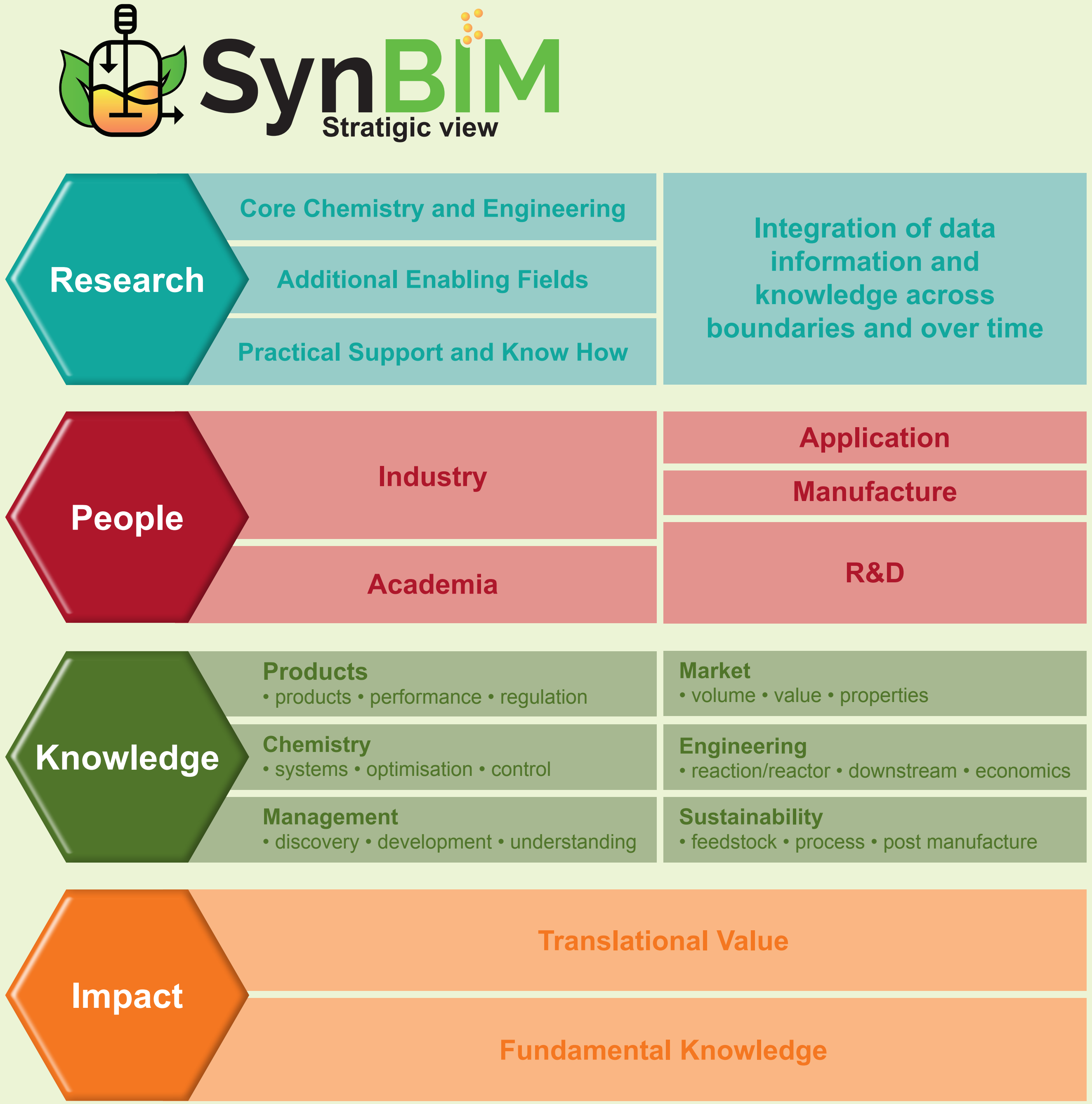


Fig 3: Supra-project processes and relationships

7.4. Beyond Project Level

Tackling the various research challenges and realising larger-scale manufacture of tunable nanomaterials via sustainable synbio methods requires the collaboration of researchers from multiple backgrounds, expertise and experiences, combining core chemistry and engineering with enabling fields such as data science and sustainability appraisal. These efforts require support from and grounding within industry, both manufacturers and product end-users (Fig 3 – **Research** relies on **People** who have **knowledge** and want **impact**).

Individual research projects, such as those envisioned in section 7.3, have potential to provide important contributions towards both fundamental and translational goals. Such combined approaches are possible, though aligning project timescales and impact pathways can be challenging (Fig 3 – **Research** moving/creating **knowledge** and achieving **impact**)

Ultimately, there are limits to what can be achieved within typical project budgets and timescales, which in turn necessitates compromise between breadth and depth of activity. Fortunately, progress also occurs beyond the project level through the linking, integration and application of outputs and learning cumulatively over time.

These cumulative processes may occur through ad hoc academic interaction or through actively managed initiatives at community level (e.g. review or discussion papers, organic network development) or policy level (e.g. targeting funds, national road mapping, network funding). It is also possible to envision development of physical tools, standards or data systems, which would automate or enable specific aspects.

Irrespective of the mechanisms at play, realisation of the SynBIM vision relies on significant and rapid progress beyond the level of individual projects. Opportunities to coordinate and accelerate progress through strategic intervention therefore deserve consideration

8. Summary

The **SynBIM project framework and product pipeline** (section 7.1) elaborate an ambitious and attractive vision for realising the larger-scale manufacturing of tunable nanomaterials via sustainable synbio methods. Good progress has been made across its work streams, both contributing directly to the development goals and also to a deeper understanding of the opportunities, uncertainties and barriers to success.

The **project symposium** (sections 2-7) enabled wider discussions and contributions, and lead both to important **general suggestions** (section 7.1) and also a list of specific **research challenges** (section 7.2). Workshop participants responded to these by creating and developing a range of **research proposals** (section 7.3).

In recognising the scale of both the opportunities and challenges associated with the SynBIM vision, it is clear that further **substantial work and investment** is required. For success, this will require effective collaborations over extended time frames and beyond the project level. Associated **strategic interventions** deserve consideration (section 7.4).

This report is provided to inform the scientific community across academia and industry, as well as funders and policy makers, about these important future challenges and opportunities. Those who attended the event are encouraged to lead in developing associated partnerships, collaborations and funding applications

9. Acknowledgements

The SynBIM project and this symposium could not have been realised without the support of our team members, partners and collaborators.

We are deeply thankful to the following institutions and companies for their support during the SynBIM project.

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University of Cincinnati
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Resonant Circuits Limited
Svenska Aerogel
Merck
Glantreo
Directed Assembly Network – Beyond the Molecule
EPSRC – Engineering and Physical Sciences Research Council

We are also deeply thankful to the sponsors who funded our symposium.

Royal Society of Chemistry
UK Fluids Network
Innovate UK – Knowledge Transfer Network
EPSRC – Engineering and Physical Sciences Research Council

Appendix 1: Delegates list

Name	University / Company
David Ashworth	The University of Sheffield
Edidiong Asuquo	The University of Manchester
Yahaya Baba	The University of Sheffield
Joan Cardiner	The University of Sheffield
Rebecca Cheesbrough	EPSRC
Mauro Chiacchia	Nexeon
Stuart Coles	University of Warwick
Marc-Olivier Coppens	University College London
Luc Dewulf	The University of Sheffield
Martin Elliott	Directed Assembly Network
Jonathan Foster	The University of Sheffield
John Hanrahan	Glantreo
Ian Houson	University of Strathclyde / CMAC
Miguel Jorge	University of Strathclyde
Amber Keegan	The University of Sheffield
Marc Knecht	University of Miami
Timm Krueger	The University of Edinburgh
Andrea Laybourn	University of Nottingham
Mark Littlewood	Knowledge Transfer Network
Vincenzo Lombardi	The University of Sheffield
Joseph Manning	University of Bath
Manasi Mulay	The University of Sheffield
Linh Nguyen	University College London
Laura Norfolk	The University of Sheffield
Siddharth Patwardhan	The University of Sheffield
Rob Pilling	The University of Sheffield
Eleni Routoula	The University of Sheffield
Jan Sefcik	University of Strathclyde
Paul Southern	Resonant Circuits
Sarah Staniland	The University of Sheffield
Rohan Vernekar	The University of Edinburgh
Anietie Williams	University of York
Max Yan	The University of Sheffield
Georgina Zimbitas	University of Strathclyde

Appendix 2: Summary of feedback

The delegates were asked to provide feedback on the symposium. Their responses to specific questions are given below in the form of average scores *(5 = very positive / 1 = poor)* with selected comments.

1. **How useful do you feel the event was? Score 4.2 / 5.0**
   - *New and interesting ideas.*
   - *Great talks of very high quality.*

2. **How would you rate the overall content and quality of each session? Score 4.7 / 5.0**
   - *It was enjoyable to work with everyone. It was scientifically satisfying.*

3. **How would you rate the event organisation and communication? Score 5.0 / 5.0**
   - *Great communication at all levels, especially before the meeting for organisation.*

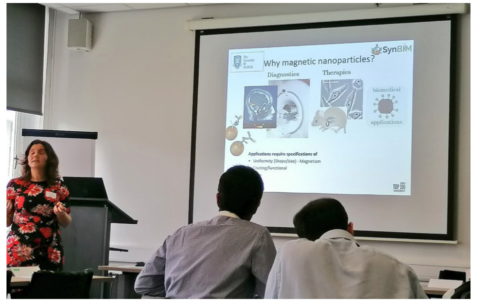
4. **How was your experience of the meeting venue? Score 4.5 / 5.0**

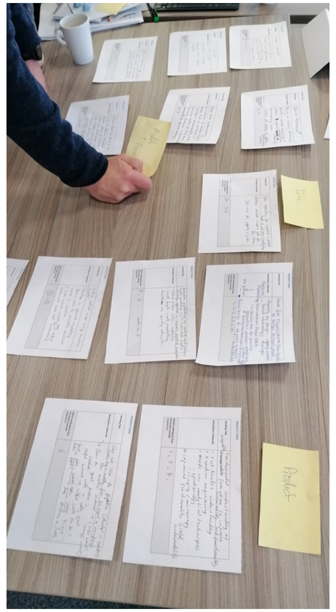
5. **From what you know of the SynBIM project, what priorities would you suggest to the project team for the final nine months?**
   - *Keep up the good work, plan succession*
   - *Extend modelling capabilities*
   - *How to ensure continuation of the project*
   - *How to connect issues in lab scale with scale up*

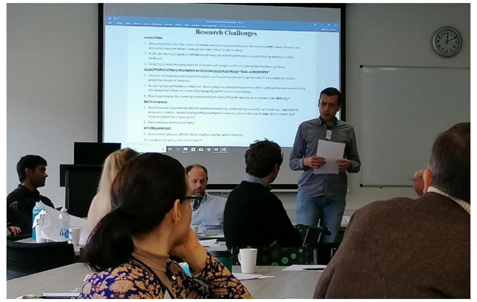
6. **SynBIM pursues the multidisciplinary challenge of translating bio-inspired chemistry through research from lab-to-market. Which do you perceive as the most significant challenges faced?**
   - *Finding the market where added value of nanomaterials justifies development costs for scale-up*
   - *Understanding fundamentals of the bioinspired chemistry*
   - *Scale-up, process transfer, thorough understanding of chemistry*
   - *Making sure end users (market, industry, people) understand*

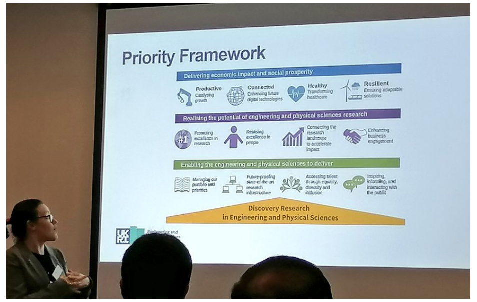
7. **Any further comments about the event, the project and/or synbio-inspired sustainable nanomaterials?**
   - *This was a great symposium. Future ones along this line to continue the discussion would be great.*
   - *Very successful, learnt a lot*
   - *Really great event. Excellent timing (1.5 days, start time, end time). Excellent balance of speakers, posters, networking. Really lovely format to receiving outcomes of sessions. Would definitely come to something like this again.*

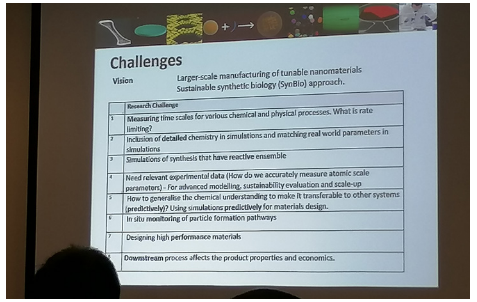
Appendix 3: Photos from the symposium

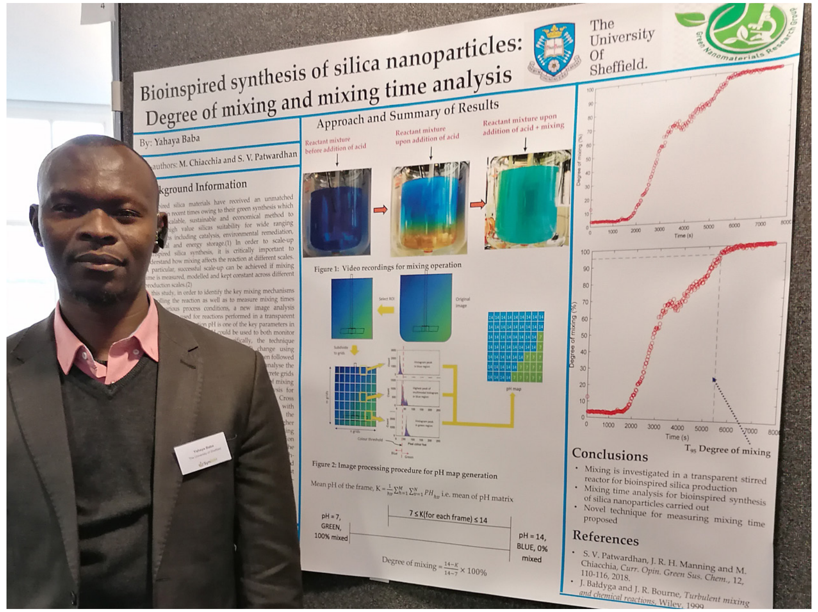


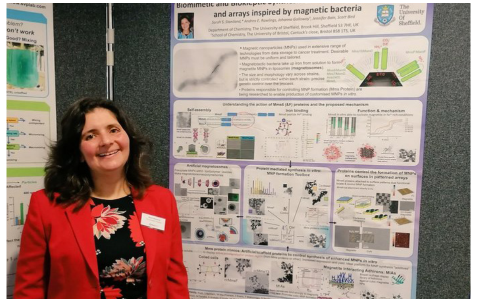


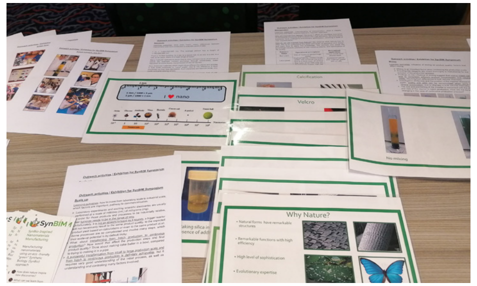


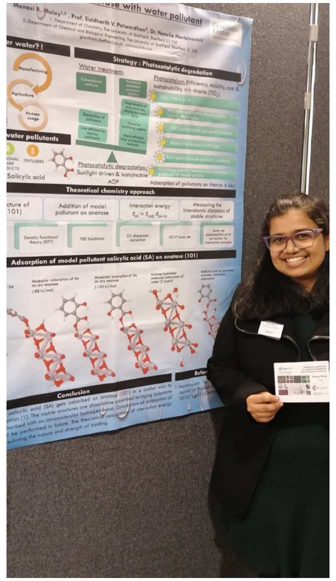


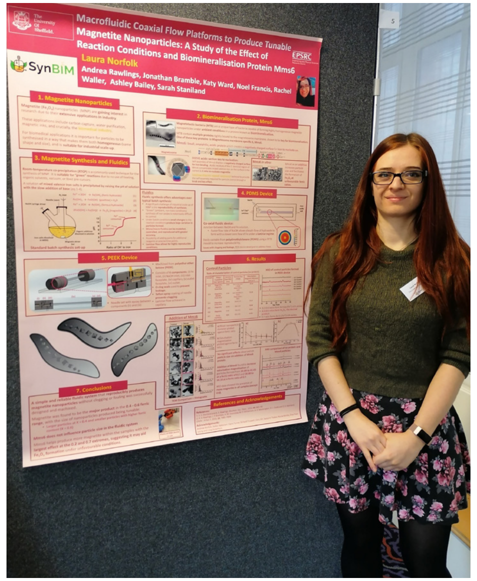












Appendix 4: Talks

Session 1 - Inspired by Nature — *Chair: Timm Krueger*

- **Welcome and Overview**
  Siddharth Patwardhan (the University of Sheffield)
- **Bio-nano interactions in designing materials**
  Marc Knecht (University of Miami)
- **Magnetic Nanoparticles – discovery and developmental chemistry**
  Sarah Staniland & Laura Norfolk (the University of Sheffield)
- **Magnetic Nanoparticles – products and market perspective**
  Paul Southern (Resonant Circuits)
- **Clustering and Self-Assembly of SynBIM additive**
  Georgina Zambatis (the University of Edinburgh)
- **Multi-scale Modelling of Bio-inspired Silica Material Synthesis**

Session 2 - Harnessed for Market — *Chair: Sarah Staniland*

- **Designing bioinspired syntheses of silica and understanding their scalability**
  Siddharth Patwardhan (the University of Sheffield)
- **Mesoscale modelling of nano-particle growth under flow**
  Rohan Vernekar (the University of Edinburgh)
- **Process design and scale-up**
  Ian Houson (University of Strathclyde)
- **Green chemistry-based classification model for silver nanoparticle synthesis**
  Stuart Coles (University of Warwick)
- **Flash Presentations from selected poster presenters**

Session 3 - Enabled by Research — *Chair: Marc-Olivier Coppens*

- **EPSRC: Manufacturing the Future**
  Rebecca Cheesebrough (EPSRC)
- **Knowledge Transfer Network: Emerging Technologies**
  Mark Littlewood (KTN)
- **The Directed Assembly Network: Research and Network Activities**
  Martin Elliott (Directed Assembly Network)
- **Emergent Research Challenges: Distillation & Discussion**
  The SynBIM Project Team
- **Day 2 Workshop: Preamble**
  Rob Pilling (the University of Sheffield)

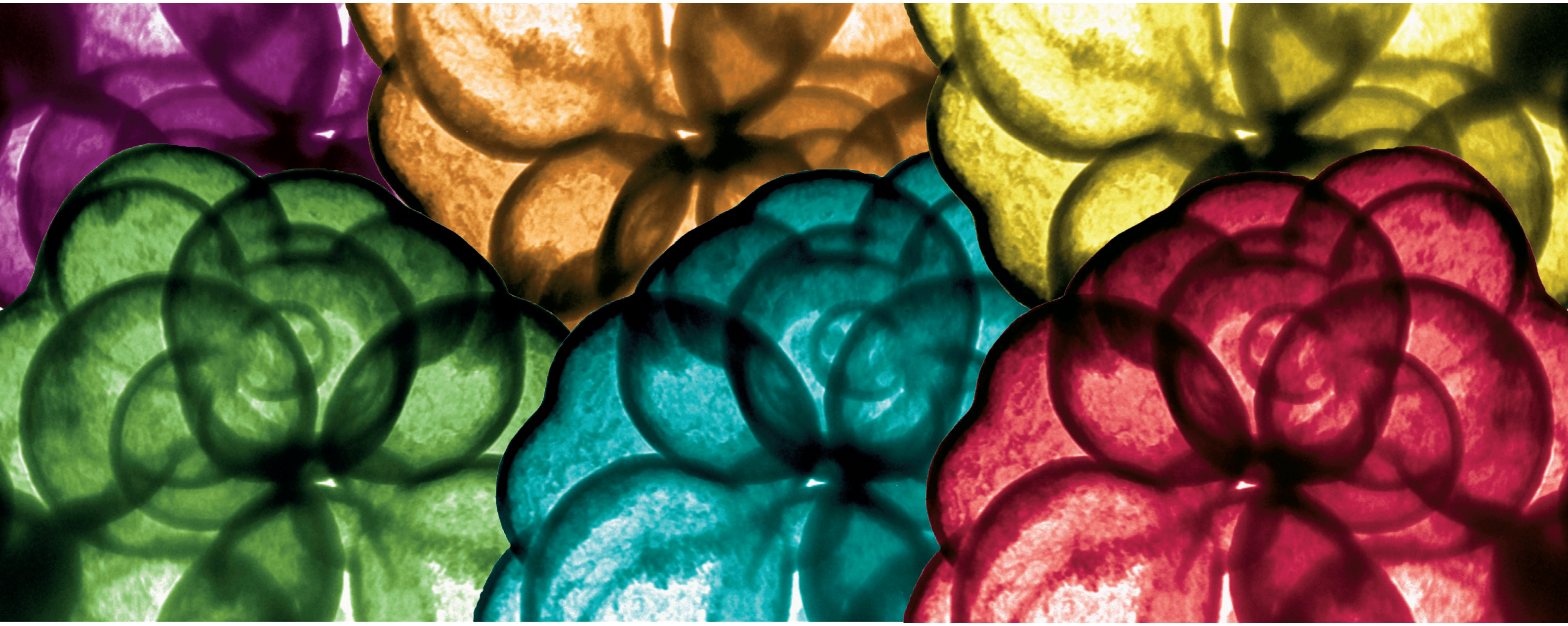
Posters

Poster No.	Poster title	Presenter	University
1	Manufacture of Metal-Organic Frameworks using Microwaves: Science to Scale up	Andrea Laybourn	Nottingham
2	Lab-scale process intensification of bioinspired silica nanomaterial synthesis	Joseph Manning	Bath
3	Morphological Control of Magnetite Nanoparticles Under Green Reaction Conditions	Laura Norfolk	Sheffield
4	Bioinspired synthesis of silica nanoparticles: degree of mixing and mixing time analysis	Yahaya Baba	Sheffield.
5	Macrofluidic Coaxial Flow Platforms to Produce Tunable Magnetite Nanoparticles: A Study of the Effect of Reaction Conditions and Biomineralisation Protein Mms6	Laura Norfolk	Sheffield
6	Programmable 2D materials for sensing, catalysis, separation and electronics applications	Jonathan Foster	Sheffield
7	Searching for the Sweet Spot: Optimising Bioinspired Silica Properties via Design of Experiments	Luc Dewulf	Sheffield
8	Biomimetic and Biokleptic Synthesis of Magnetic nano particles and array inspired by magnetic bacteria	Sarah Staniland	Sheffield
9	Versatile, scalable and green synthesis of nanomaterials: an approach to engineer functional products	Mauro Chiacchia	Sheffield
10	Interaction of anatase with water pollutants	Manasi R. Mulay	Sheffield
11	Small organic molecule aqueous solutions' colloidal scale solute clustering dependence on concentration & pH	Georgina Zimbitas	Strathclyde
12	Fundamental modelling challenges of nanoparticle growth	Rohan Vernekar	Edinburgh
13	Clustering of Pentaethylenehexamine (PEHA) in Aqueous Solutions: Molecular Dynamics Study	Nasser Afify	Edinburgh
14	synbio-Inspired Nanomaterials Manufacturing	SynBIM	Sheffield

Notes

Symposium organised by the EPSRC funded project: SynBIM - Synbio-Inspired Nanomaterials Manufacturing

Symposium funded by:



Bridging the gap:
bioinspired nanomaterials and
sustainable manufacture.