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Have Questions?

Type them into questions box!

"Why am I muted?"
Don't worry. Everyone is muted except the presenter and host. Thank you and enjoy the show.

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Check out the ACS Webinar Library!

An ACS member exclusive benefit

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Hundreds of presentations from the best and brightest minds that chemistry has to offer are available to you on-demand. The Library is divided into 6 different sections to help you more easily find what you are searching.

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Technology & Innovation

▶ View the Collection

From renewable fuels to creating the materials for the technology of tomorrow, chemistry plays a pivotal role in advancing our world. Meet the chemists that are building a better world and see how their science is making it happen.

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The Drug Design Delivery Series has built a collection of the top minds in the field to explain the mechanics of drug discovery. Discover the latest research, receive an overview on different fields of study, and gain insight on how to possibily overcome your own med chem roadblocks.

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Why does food taste better when it is grilled or what molecular compounds make a great wine? Discover the delectable science of your favorite food and drink and don't forget to come back for a second helping.

Popular Chemistry

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Feeling burdened by all that molecular weight? Listen to experts expound on the amazing side of current hot science topics. Discover the chemistry of rockets, how viruses have affected human history, or the molecular breakdown of a hangover.

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How do ideas make it from the lab to the real world? Discover the ins and outs of the chemical industry whether you are looking to start a business or desire a priceless industry-wide perspective.

https://www.acs.org/content/acs/en/acs-webinars/videos.html

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Learn from the best and brightest minds in chemistry! Hundreds of webinars on diverse topics presented by experts in the chemical sciences and enterprise.

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Live Broadcasts of ACS Webinars® continue to be available to the general public several times a week generally from 2-3pm ET!

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www.acs.org/acswebinars

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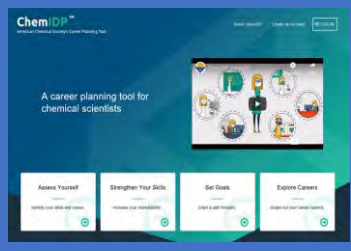

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ACS Career Navigator: Your Home for Career Services

Whether you are just starting your journey, transitioning jobs, or looking to brush up or learn new skills, the **ACS Career Navigator** has the resources to point you in the right direction.

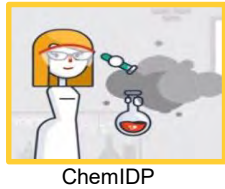
We have a collection of career resources to support you during this global pandemic:

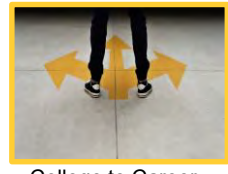

Professional Education


Virtual Career Consultants

ACS Leadership Development System


Career Navigator LIVE!


ChemIDP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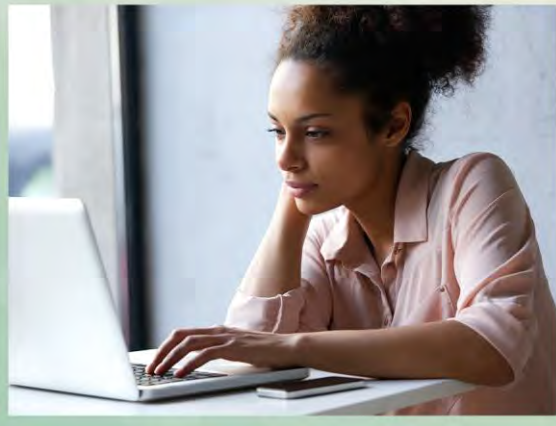
Join us in our efforts to increase the diversity of chemistry.



Valued donors like you have sustained ACS educational programs that are welcoming students from diverse backgrounds into our profession.

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ACS Office of Philanthropy
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A Career Planning Tool For Chemical Scientists

ChemIDP is an Individual Development Plan designed specifically for graduate students and postdoctoral scholars in the chemical sciences. Through immersive, self-paced activities, users explore potential careers, determine specific skills needed for success, and develop plans to achieve professional goals. **ChemIDP** tracks user progress and input, providing tips and strategies to complete goals and guide career exploration.

https://chemidp.acs.org

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If you are from an underrepresented racial or ethnic group, we want to empower you to get your graduate degree!

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ACS Department of Diversity Programs

Advancing ACS's Core Value of Diversity, Inclusion & Respect

We believe in the strength of diversity in all its forms, because inclusion of and respect for diverse people, experiences, and ideas lead to superior solutions to world challenges and advances chemistry as a global, multidisciplinary science.

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www.acs.org/diversity

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https://www.gcande.org

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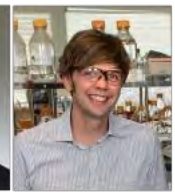
Register Today!

ACS Green Chemistry Institute
Chemistry for Life®


B. Frank Gupton

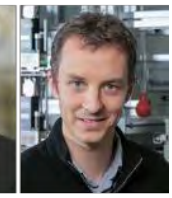

Eunice Heath


Gregg Beckham


Amy Prieto


Meagan Mauter


Jun Huang


Jeremy Luterbacher

- Daily Keynotes
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- Networking opportunities, live discussions and more!

https://www.gcande.org

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ACS Webinars
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Date: Friday, June 11, 2021 @ 1-2pm ET
Speakers: Amy Prieto, Colorado State University and Prieto Battery, Inc. and H.N. Cheng, ACS President
Moderator: Young-Shin Jun, Washington University in St. Louis

Register for Free!

What You Will Learn:

- Why battery chemistry is complex and interdisciplinary
- How the iteration of synthesis, characterization, and modeling is key for accelerating discovery
- Why there is no one perfect battery for every application

Co-produced with: ACS Committee on Science

The "Frontier Fridays" Webinar Series are organized by ACS President H.N. Cheng, Michael Morello (Division Representative, ACS Committee on Science) Retired formerly PepsiCo R&D, Young-Shin Jun of Washington University in St. Louis, and Martin G. Kociolek (Chair of the ACS Committee on Science) of Penn State Behrend.

Date: Wednesday, June 16, 2021 @ 2-3:30pm ET
Speakers: Michael Schulz, Virginia Tech and Emilie Rexeisen, 3M
Moderator: Tomonori Saito of Oak Ridge National Laboratory (ORNL) and the University of Tennessee, Knoxville

Register for Free!

What You Will Learn:

- How antiviral polymers were discovered, how the field has developed and what the future may hold for the field of antiviral materials
- What structural features give a polymer antiviral properties
- How four key aspects contribute to successful decontamination (decontamination efficacy, safety for the wearer, filtration efficiency, and respirator fit)
- How different respirator makes and models use different materials making it essential that each model is tested separately for each method

Co-produced with: ACS Division of Polymer Chemistry

Date: Thursday, June 17, 2021 @ 2-3pm ET
Speaker: Lee Polite, Axion Analytical Labs, Inc.
Moderator: Bryan Tweedy, American Chemical Society

Register for Free!

What You Will Learn:

- How to develop an HPLC method from scratch
- How to cut your analysis time in half, while preserving the quality of the results
- What are all those buttons for on your HPLC

Co-produced with: ACS Professional Education

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ACS Chemistry for Life®

co-produced with the ACS Green Chemistry Institute

Bioinspired Nanomaterials

From Discovery to Market Pipeline

FREE Webinar | TODAY at 2pm ET

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THIS ACS WEBINAR WILL BEGIN SHORTLY . . .

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ACS Chemistry for Life®

Bioinspired Nanomaterials: From Discovery to Market Pipeline

SIDDHARTH PATWARDHAN
Professor of Sustainable Chemical and Materials Engineering, and Head of the Green Nanomaterials Research Group, Department of Chemical and Biological Engineering, The University of Sheffield, United Kingdom

DAVID CONSTABLE
Science Director, Green Chemistry Institute, American Chemical Society

Presentation slides are available now! The edited recording will be made available as soon as possible.

www.acs.org/acswebinars

This ACS Webinar is co-produced with the ACS Green Chemistry Institute.

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Discovery to market pipeline for bioinspired nanomaterials

Siddharth V. Patwardhan
Professor of Sustainable Chemical and Materials Engineering,
Green Nanomaterials Research Group,
Chemical and Biological Engineering, University of Sheffield, U.K.
S.Patwardhan@sheffield.ac.uk
www.svplab.com @GreenNanoRes
Director of Sipat Consulting and Training

www.sipatconsulting.co

Sheffield

City
- "*Natural amphitheatre*" created by 7 hills & 5 rivers
- 61% area is green space (~2 million trees)
- 1/3rd within the Peak District national park
- >250 parks, woodlands & gardens in the city
- Highest ratio of *trees : people* of any city in Europe

University
- Founded in 1879
- Academic departments: 54
- Students: 29,000

Department of Chemical and Biological Engineering

One
of the largest departments for chemical engineering in the UK

1st
in the UK for research environment, top 5 in the UK for Chem Eng output
* REF 2014

2nd
in the Russell Group for student satisfaction
*NSS 2019

£3.5 million
invested in new research facilities

750
delegates at our conference in 2019

87
funders

29
live grants

Research themes tackling 21st century challenges:

Processes and systems

Biological engineering

Sustainability

Materials and products

What You Will Learn

- The need for bioinspired functional nanomaterials
- Design of bioinspired nano-products
- The importance of integrating scale-up at discovery stage in reaching the markets

Green Nanomaterials Research Group

The University Of Sheffield.

Nanomaterials Production

- Green chemistry has started to see impact on **organic chemistry**
- But, nanomaterials have not received much attention, despite their multi-billion £ market
- Traditional methods for nanomaterials production are environmentally damaging

J. Ind. Ecol., ***12***, *316, 2008.*

The University Of Sheffield.

Why green manufacturing?

Industry sector	Production *tonnes*	E-factor*
Oil refining	10^6 - 10^8	~0.1
Bulk chemicals	10^4 - 10^6	<1-5
Fine chemicals	10^2 - 10^4	5-50
Pharmaceuticals	10 - 10^3	25 to >100
Nanomaterials	10^2 - 10^3	100-100,000

** Mass of waste produced per mass of product*

J. Chem. Technol. Biotechnol. **68**, 381-388, (1997).
J. Ind. Ecol., **12**, 316, 2008.

The University Of Sheffield.

Audience Survey Question

ANSWER THE QUESTION ON BLUE SCREEN IN ONE MOMENT

Nanomaterials production is so wasteful because of the high precision needed and the difficulty in controlling at the nanoscale.

- True
- False

Industry sector	Production *tonnes*	E-factor[1]
Oil refining	10^6 - 10^8	~0.1
Bulk chemicals	10^4 – 10^6	<1-5
Fine chemicals	10^2 – 10^4	5-50
Pharmaceuticals	10 – 10^3	25 to >100
Nanomaterials	10^2-10^3	100-100,000

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Reasons for wastefulness

Case study of silica for illustration

Specialty silicas are worth $2-4 billion per annum

Synthetic amorphous silica

Porous & Functional

Low value ← → **High value**

High value → **Current markets** ← → **Emerging markets**

Approved by the EMA and the FDA as ***Generally Recognised As Safe*** for cosmetics and food additives.

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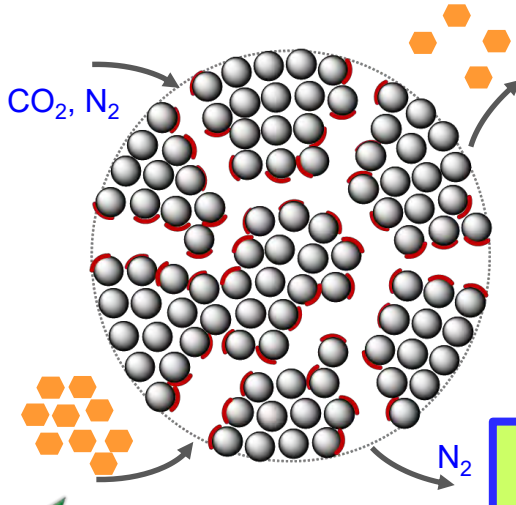
The needs for emerging applications



- These depend on complex pore **structure** and **functionality.**
- This leads to more **uneconomical** and/or **unsustainable** synthesis.
- Hence high-value nanomaterials are **difficult to manufacture.**

➔ There is a tension between *functionality, sustainability* and *scalability*

The University Of Sheffield.

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Audience Survey Question

ANSWER THE QUESTION ON BLUE SCREEN IN ONE MOMENT

How can wastefulness of nanomaterials production be fully addressed?

- Reducing reaction temperature
- Using renewable feedstock
- Using plant extracts as catalysts
- Consider downstream processing e.g. separation or purification
- Taking a systems approach

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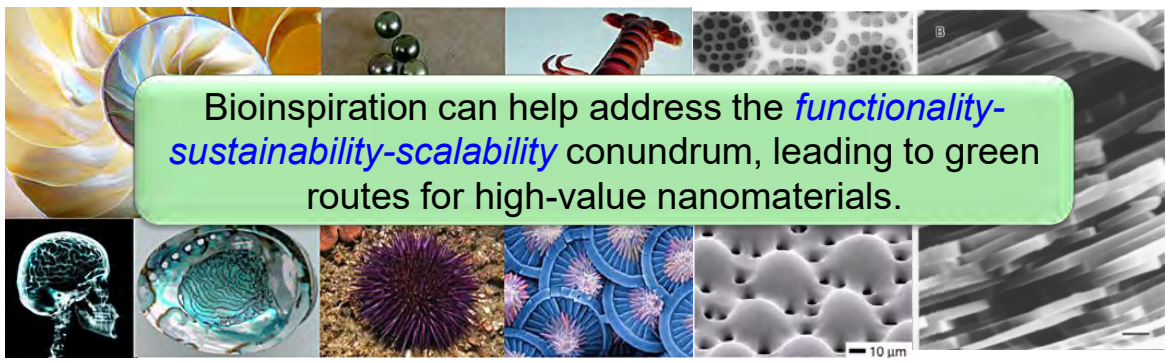
Bioinspiration at rescue

Biology produces functional nanomaterials under eco-friendly conditions and at large scale!



Cur. Opin. Green Sus. Chem., **2018**, *12*, *110*.

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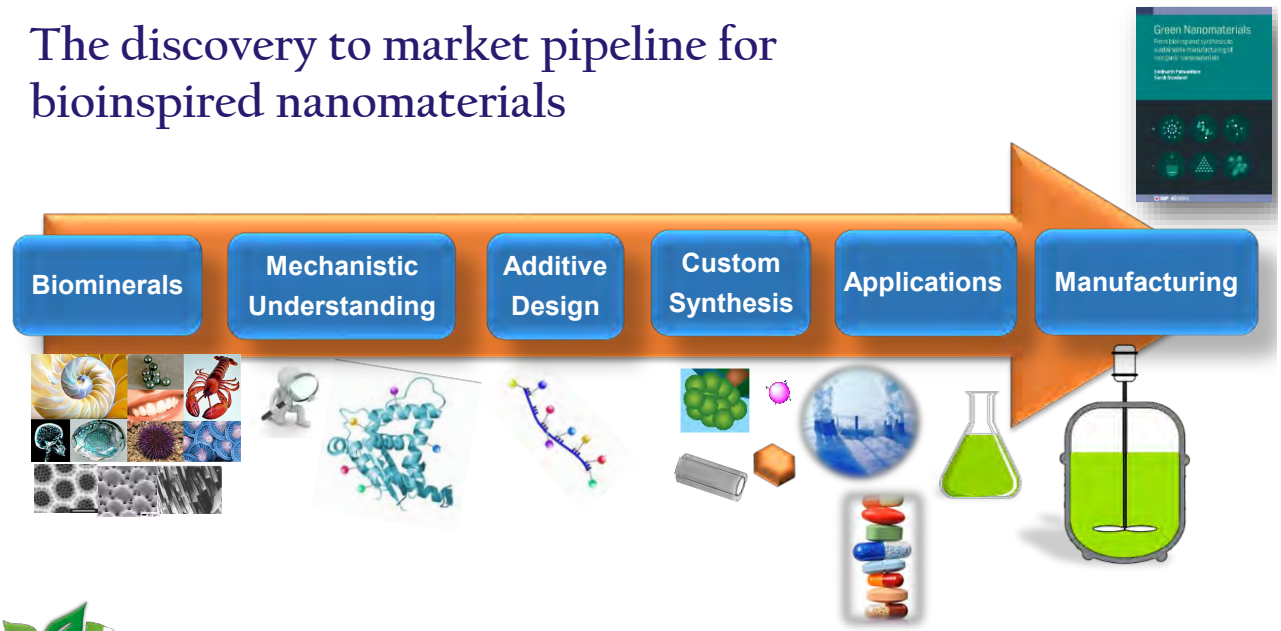
Biosilica

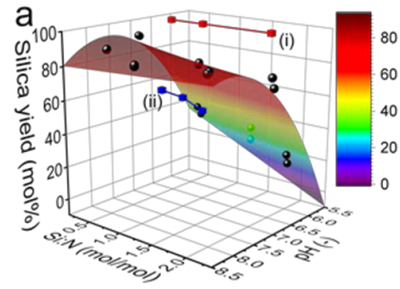
The discovery to market pipeline for bioinspired nanomaterials



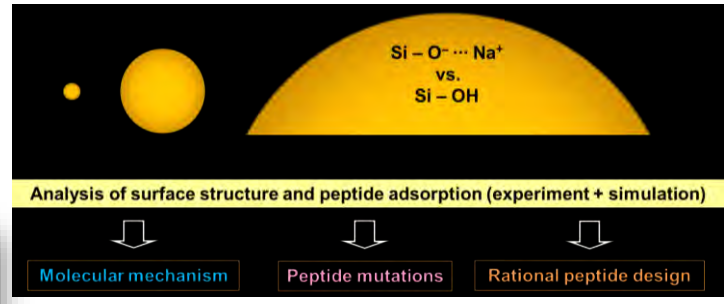
Patwardhan & Staniland, *Green Nanomaterials*, IoP Publishing, 2019.
Cur. Opin. Green Sus. Chem., **2018**, *12*, *110*.

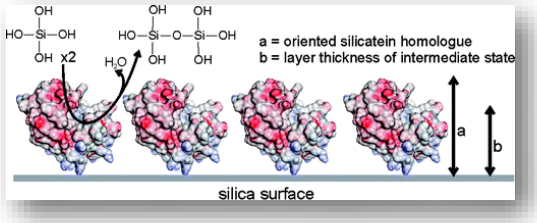
What You Will Learn

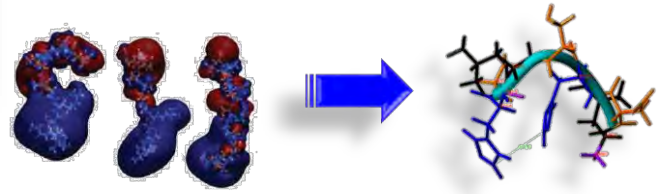
- The need for bioinspired functional nanomaterials
- Design of bioinspired nano-products
- The importance of integrating scale-up at discovery stage in reaching the markets



Gaining molecular understanding



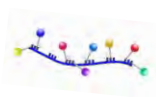


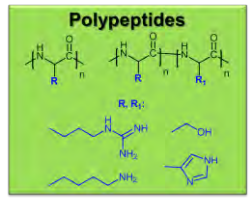


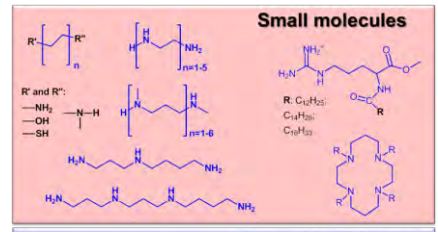
J. Mater. Chem, 2005, **15**, 4629.
Biomacromol., 2010, **11**, 3126.
JACS, 2012, **134**, 6244.

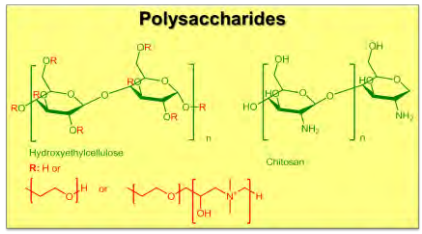
Chem. Mater., 2014, **26**, 2647.
Chem. Mater., 2014, **26**, 5725.

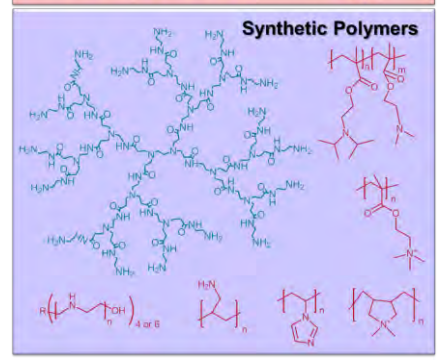
Designing synthetic *additives*

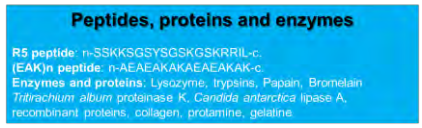












Chem. Commun. 2011, **47**, 7567

The University Of Sheffield.

Bioinspired synthesis

The use of additives enabled the invention of a green method that is:

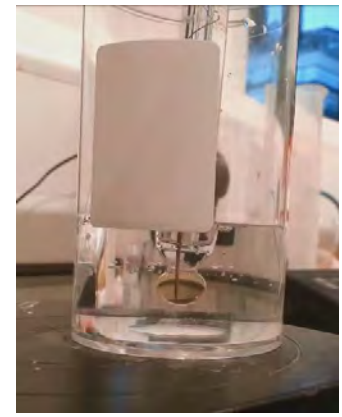
- *Simple,*
- *rapid,*
- *all-aqueous*
- *at room temp.*
- *pH7 and*
- *offers control.*

Silica precursor
+
'Additive'

pH = 7
Water

t < 5min
T = 20°C

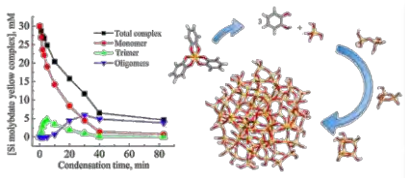
Green Nanosilica (GN)

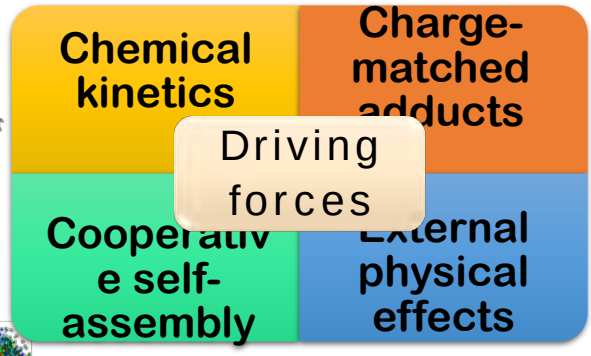


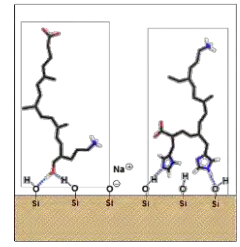
J. Vis. Exp., **138**, e57730, 2018.
Cur. Opin. Green Sus. Chem., **12**, 110, 2018

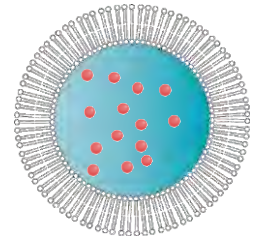
The University Of Sheffield.

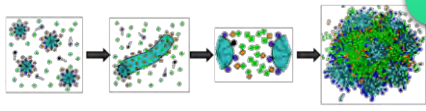
Understanding the driving forces











The fundamental knowledge gained on bioinspired synthesis can enable materials design and manufacturing.

J. Phys. Chem. B, 2010, **114**, 9947. *JACS*, 2012, **134**, 6244.
Mater. Horiz., 2019, **6**, 1027. *Mol. Syst. Des. Eng.*, 2021, **6**, 170.

The University Of Sheffield.

Application-driven product design

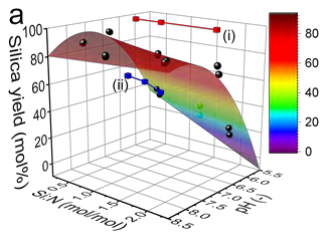
Applications → **Quality attributes/ performance** → **Properties** → **Materials design & Synthesis**

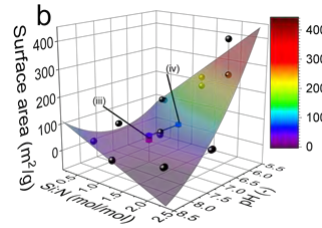
Pharma Excipient	Pure Nontoxic Hydrophilic, …..	Purity Safety Surface area and chemistry, ….
Rubber filler	Blends well Good friction and heat stable, Competitive price	Surface chemistry Wear & thermal testing, Yield & cost

The University Of Sheffield.

Statistical approach to design

- A unique sequential Design of Experiments strategy was developed
- It enabled reliable models connecting synthesis with properties
- Used for optimisation of synthesis for desired products



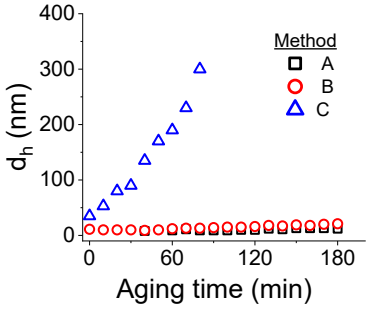


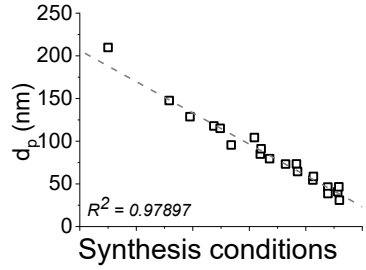
$$\textbf{Yield}\ (mol\%) = A + B \times \textbf{Si:N} + C \times \textbf{pH} + D \times \textbf{Si:N} \times \textbf{pH} + E \times \textbf{pH}^2$$

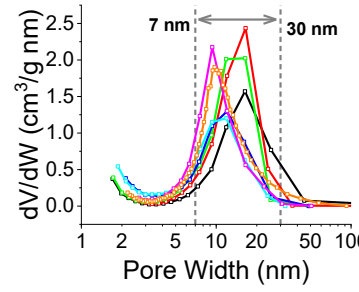
$$\textbf{Surface area}\ \left(m^2/g\right) = P + Q \times \textbf{Si:N} + R \times \textbf{pH} + S \times \textbf{Si:N} \times \textbf{pH} + T \times \textbf{pH}^2$$

Mol. Syst. Des. Eng., 2021, **6**, 293.

Discovery of "green" colloidal & mesoporous silica





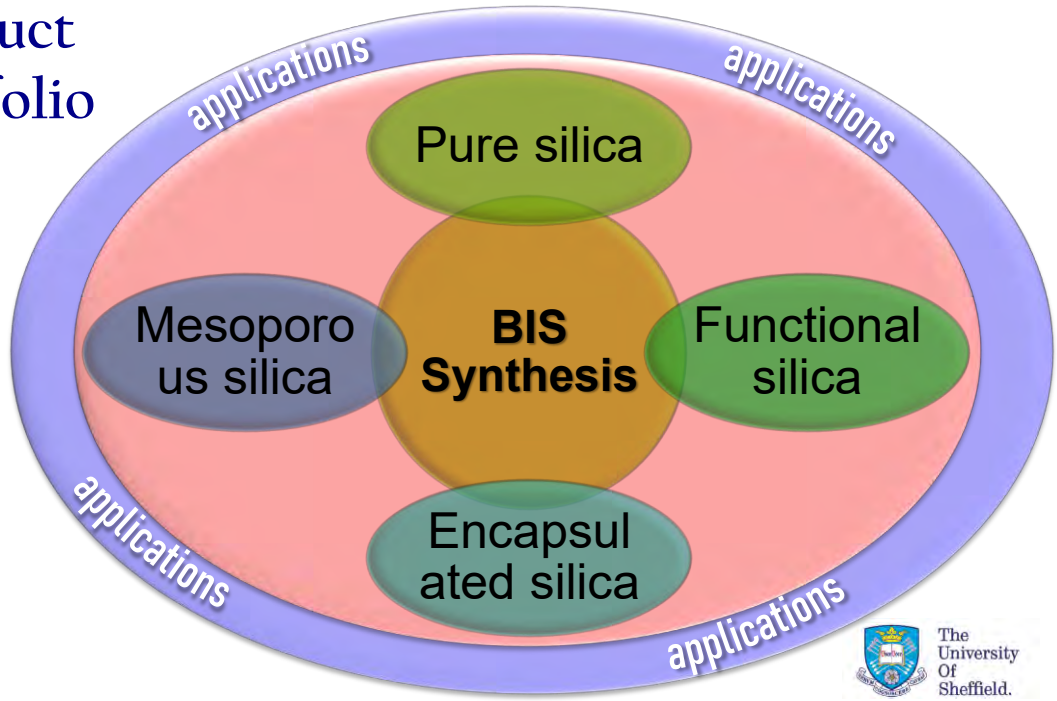


The **first report** of colloidal or mesoporous silica synthesis at room temp., in water, pH7 & within 15 min.

J. R. H. Manning, PhD thesis, 2019. *Dalton Trans.*, 2020, **49**, 1334.

Basis for a spin-out company

Product portfolio



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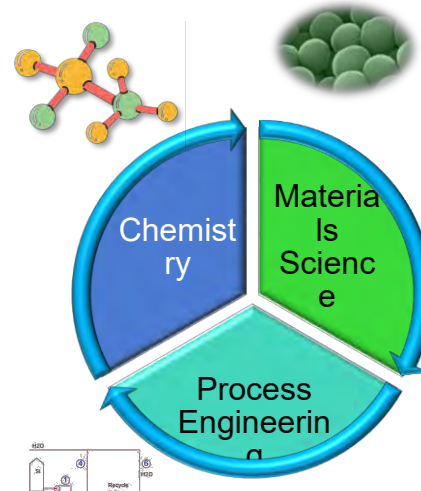
What You Will Learn

- The need for bioinspired functional nanomaterials
- Design of bioinspired nano-products
- The importance of integrating scale-up at discovery stage in reaching the markets



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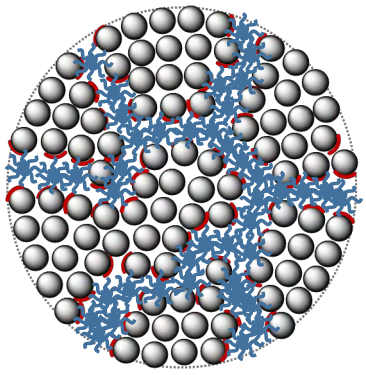
Energy intensive purification



- Low porosity
- Additive impurities

- High porosity
- 100% purity
- Energy intensive
- **>10^3-10^6×** wasteful and **1000×** costly
  - Not always effective
  - Energy intensive (reflux)
  - Hard to transfer between systems

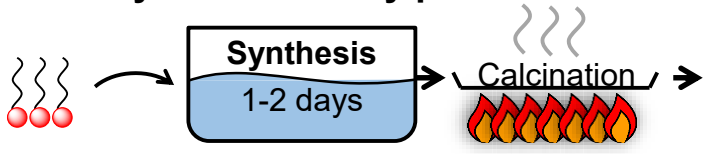
E.g. Mesoporous silica: invented in 1992, they cannot be manufactured at large scales!

Patarin, *Angew. Chemie Int. Ed.*, 2004 (**43**), 3878

The University Of Sheffield.

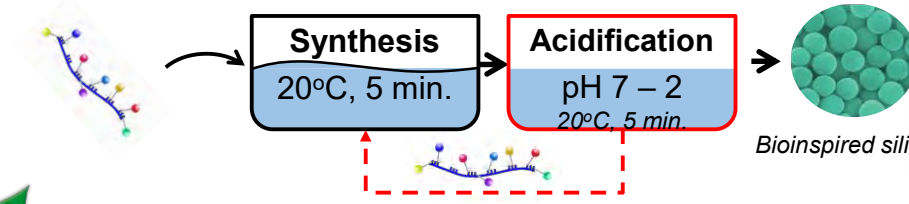
Avoiding calcination

Current synthesis of any porous silica

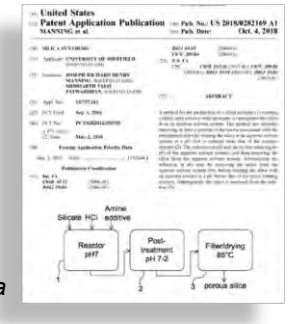


Templated silica

New process chemistry



Bioinspired silica



Up to 95% solvent & additive **recycling**

WO/2017/037460. *ChemSusChem*, 2017, **10**, 1683

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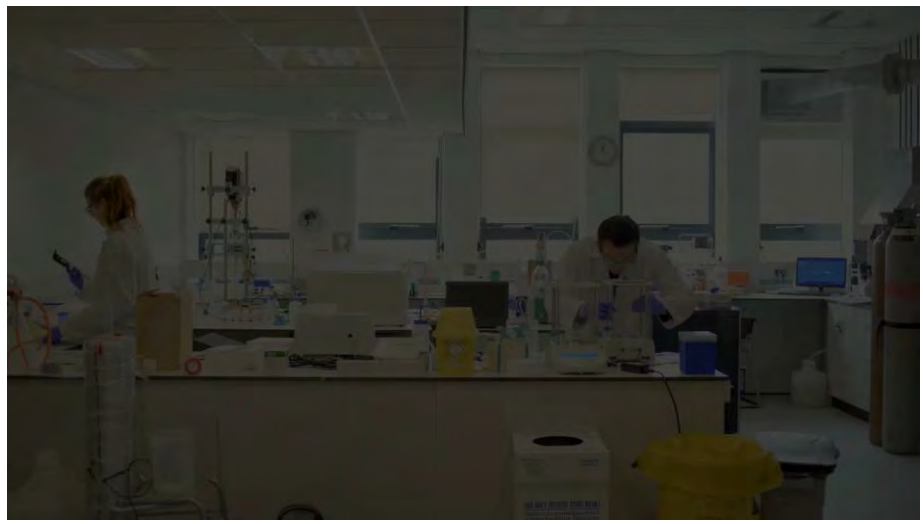
Scale-up

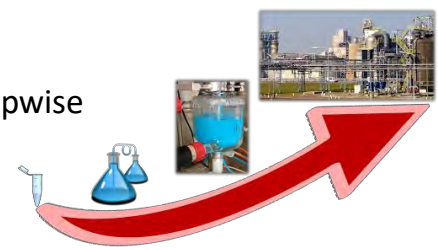


Audience Survey Question

ANSWER THE QUESTION ON BLUE SCREEN IN ONE MOMENT

What is ONE key way to ensure effectively scale-up a reaction?

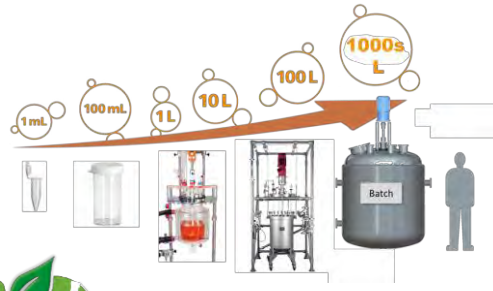
- Using flow chemistry
- Maintaining equipment geometry
- Maximize the stirring speeds
- Trial and error when going up in scale stepwise
- No meddling by chemists

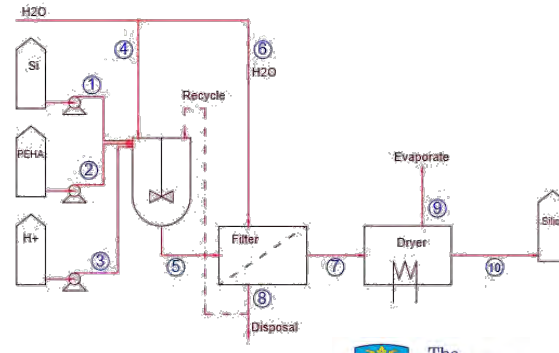


Process Design

As product discovery follows scale-up, we need to:

- design a process flow diagram,
- perform techno-economic analysis,
- [refine the synthesis]…

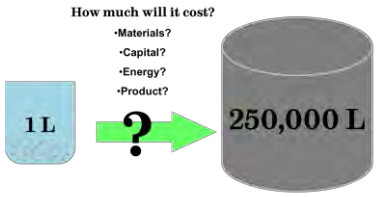


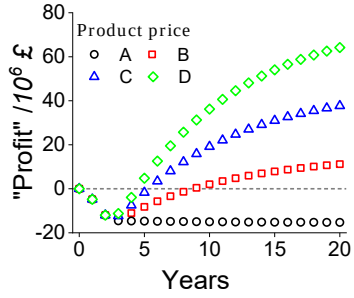


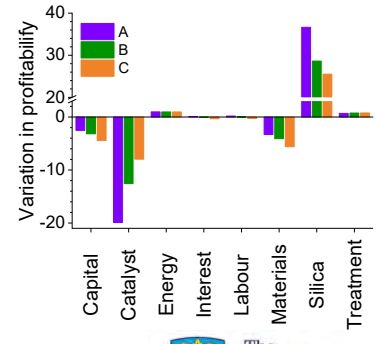
Economic feasibility

Technoeconomic analysis is performed to answer these Qs:

- Is the process economically favorable, and for which products/markets?
- Is it more sustainable (energy, waste, feedstock, …)?
- Are there any improvements needed?







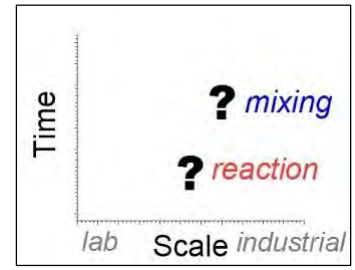
Chem. Eng. J., 2014, **244**, 483.
Asher Smith MEng Project

Audience Survey Question

ANSWER THE QUESTION ON BLUE SCREEN IN ONE MOMENT

With scale-up, the time needed to achieve the same mixing is?

- does not change
- changes linearly with the scale
- changes non-linearly with the scale
- changes but independent of the scale



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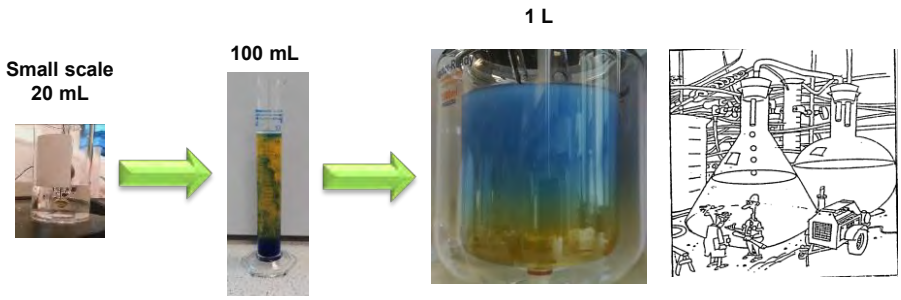
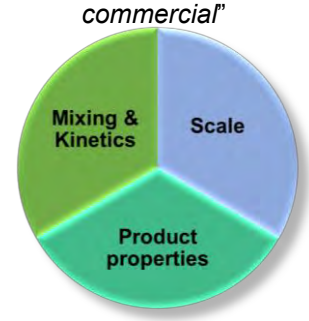
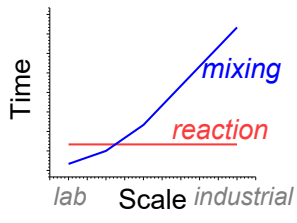
Scale-up challenges

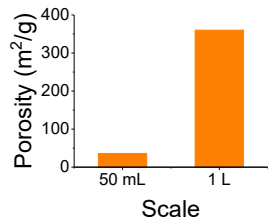


"We've got a few problems going from lab scale to full scale commercial"



- Simply going from $<10^{-1}$ L (mg) to 10^4 L (tonnes) **does not work**!
- Science that controls materials properties, changes with scales.





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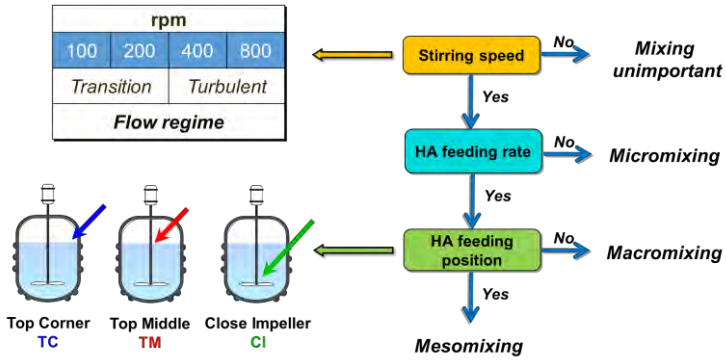
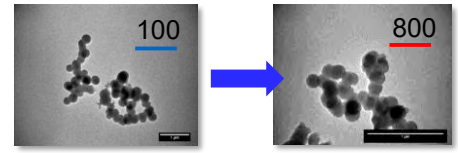
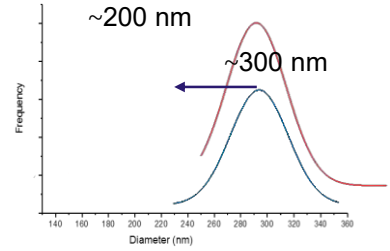
A simple way to study effects of mixing

An established protocol can be used to identify mixing mechanisms.







J. R. Bourne, *Org Process Res Dev*, 2003, **7**, 471

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Scale-up by design

The mixing mechanisms can help design scale-up, yet attaining desired product attributes.

Batch: **1-40L** (~1 kg)
Continuous : ≈200 kg/day.m^3

PCT/GB2016/05270 5

www.synbim.co.uk

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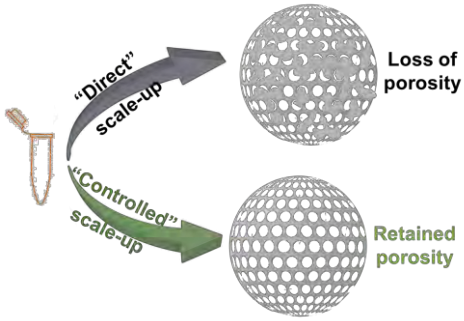
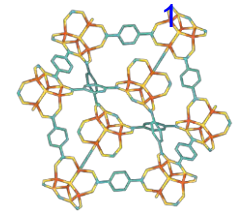
Other scale-up examples from the group

Battery anodes (porous silicon)

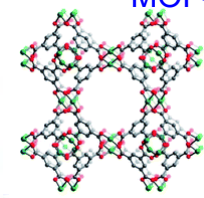


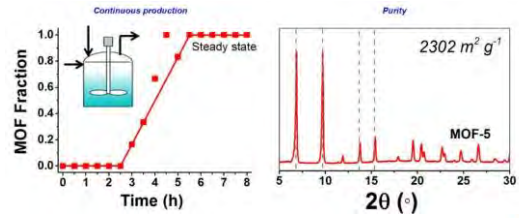
Metal organic framework materials

HKUST-1



MOF-5





Chem. Eng. J., **326**, 570, 2017. *Chem. Eng. J.*, **285**, 718, 2016. *RSC Adv.*, **11**, 3801, , 2021

Summary

Application areas

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Silicon 2021, doi: 10.1007/s12633-020-00924-1
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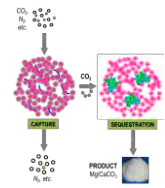

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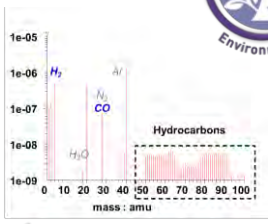

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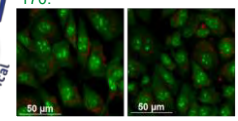

Silicon, **2010**, 2, 33
Chem. Eng. J. **2014**, 244, 483
ChemSusChem **2017**, 10, 1683
Mol. Syst. Des. Eng., **2021**, 6, 293

J. Mater. Chem. B, **2013**, *1*, 1164.
Macromol. Biosci., **2014**, *14*, 1619.

J. Mater. Chem. B, **2014**, 2, 5028.
ACS Biomater. Sci. Eng., **2016**, 2, 1493

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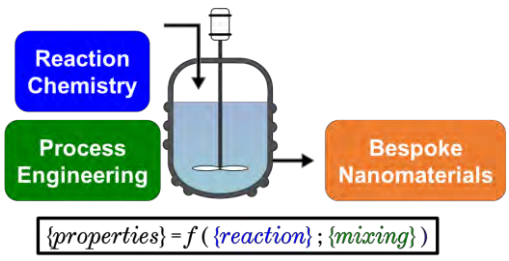
Future challenges – *digital twins*

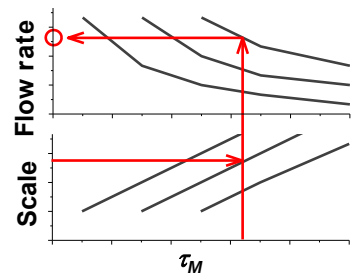
Quantification and integration of

- process chemistry,
- materials discovery and
- scale-up design.

$$Critical\ Quality\ Attributes = f(\tau_M, \tau_R)$$

$$kinetics, \tau_{R_i} = f(C, k_i, pH, T, \ldots)$$





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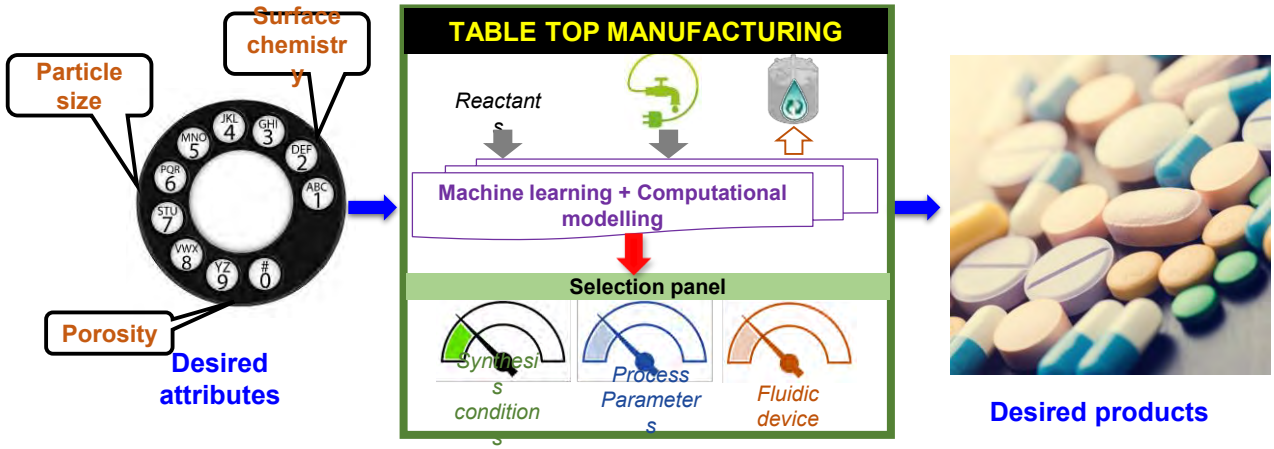
Future challenges – *on-demand manufacturing*



Acknowledgements

- Present and past group members
- Numerous collaborators across the world
- Colleagues who discussed and helped develop ideas
- Funders

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Chemical and Biological Engineering, University of Sheffield, U.K.
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Moderator: Young-Shin Jun, Washington University in St. Louis

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What You Will Learn:

- Why battery chemistry is complex and interdisciplinary
- How the iteration of synthesis, characterization, and modeling is key for accelerating discovery
- Why there is no one perfect battery for every application

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Speakers: Michael Schulz, Virginia Tech and Emilie Rexeisen, 3M
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What You Will Learn:

- How antiviral polymers were discovered, how the field has developed and what the future may hold for the field of antiviral materials
- What structural features give a polymer antiviral properties
- How four key aspects contribute to successful decontamination (decontamination efficacy, safety for the wearer, filtration efficiency, and respirator fit)
- How different respirator makes and models use different materials making it essential that each model is tested separately for each method

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Date: Thursday, June 17, 2021 @ 2-3pm ET
Speaker: Lee Polite, Axion Analytical Labs, Inc.
Moderator: Bryan Tweedy, American Chemical Society

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What You Will Learn:

- How to develop an HPLC method from scratch
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