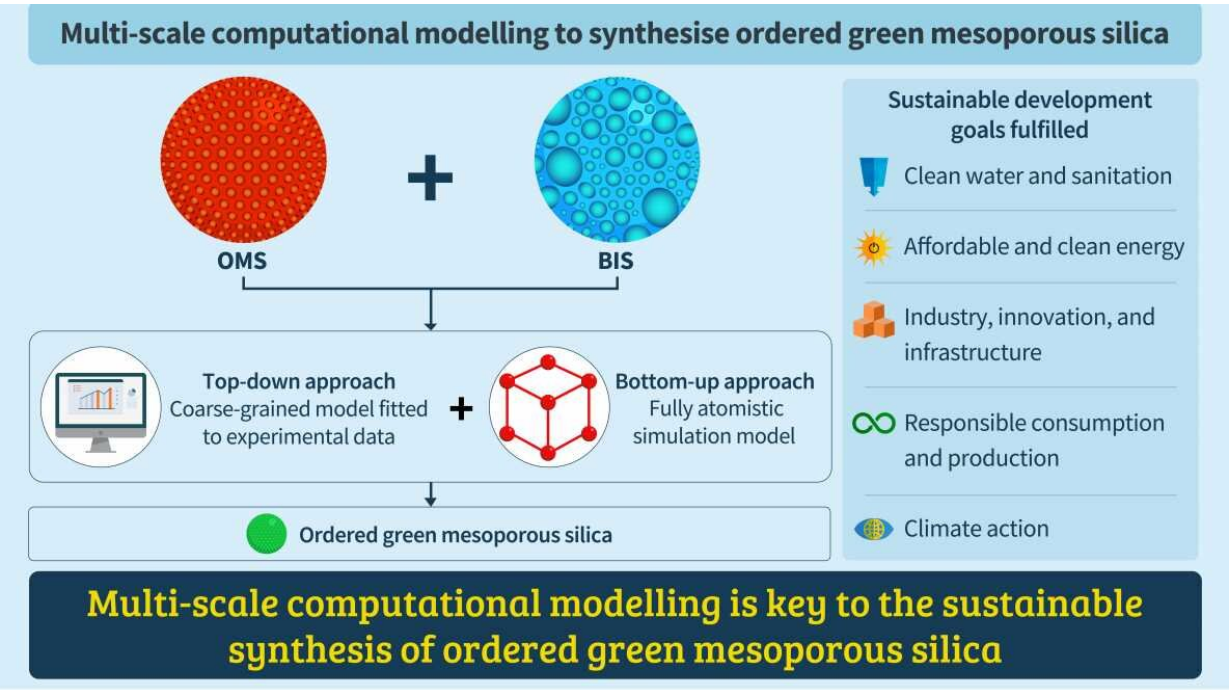
Paper highlights critical need for collaborative approach to green chemistry research

April 5 2023



Credit: University of Sheffield

Tom Stavert, a joint Ph.D. researcher between Sheffield and Strathclyde, has published an article in the journal *RSC Sustainability* exploring how combining computational modeling with green chemical principles can enable sustainable manufacture.

Novel research methods critical to the decarbonization of industry have been highlighted in a new paper published by a Sheffield-Strathclyde research team.

Tom Stavert is a postgraduate researcher whose Ph.D. is a joint collaboration between the University of Sheffield and the University of Strathclyde, supervised by Prof. Siddharth Patwardhan and Dr. Miguel Jorge, respectively, who also contributed to the new paper alongside Dr. Robert Pilling.

The focus of Tom's research is combining novel experimental and computational approaches to produce sustainable nanomaterials.

His recent research has culminated in the publication of the article titled "Unlocking the holy grail of sustainable and scalable mesoporous silica using computational modeling," in *RSC Sustainability*.

Ordered mesoporous silica (OMS) has applications in the likes of gas separation, catalysis, drug delivery in patients, and biosensors—the latter can be used for disease monitoring among other things.

However, despite the discovery of OMS 30 years ago, it's not yet possible to produce such materials sustainably because they require high temperature and pressure, extreme pH, and harsh, toxic chemicals, as well as forming polluted water, making it a highly energy and resource intensive process.

Bio-inspired methods offer a great alternative for the design of high-value mesoporous silica under more environmentally considerate conditions, allowing for both sustainable and economic scale up. However, at present, synthesis of bio-inspired silica (BIS) is not fully understood, which creates barriers to achieving products comparable in quality to traditional mesoporous silica.

As such, this article summarizes key findings in the development of OMS and BIS synthesis, with focus on the challenges in the development of scalable routes for the production of these materials. It also highlights recent triumphs in improving the mechanistic understanding of syntheses using computational modeling, as well as how modeling can be used for the predictive design of BIS.

Through combining computational modeling with the principles of green and sustainable chemistry, there is the potential to transform material discovery and sustainable manufacture. This approach can reduce production costs by two orders of magnitude in some cases.

With OMS having a wide range of applications, future outcomes from this work align with multiple of the UN's sustainable development goals (SDGs): SDG 6—clean water and sanitation, SDG 7—affordable and clean energy, SDG 9—industry, innovation and infrastructure, SDG12—responsible consumption and production, and SDG 13—climate action.

On his recent publication, Tom said, "Being part of a collaborative Ph.D. project has given me a fantastic perspective of the importance of taking a multi-disciplinary approach to solving research challenges as it combines both experimental and computational methods.

"In this article we highlight how seemingly unrelated strands of research can be joined together to create novel and effective research methods, drawing on expertise from researchers with diverse skillsets. This combined approach will be critical to decarbonising industry and effectively tackling climate change."

More information: Tom Stavert et al, Unlocking the holy grail of sustainable and scalable mesoporous silica using computational modelling, *RSC Sustainability* (2023). DOI: 10.1039/D3SU00019B

Provided by University of Sheffield