Data-Driven Chemistry: Accelerated Design and Discovery

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The landscape of chemistry is transforming with the integration of new techniques and tools from the artificial intelligence (AI) community. These changes are being facilitated by progress in hardware, including classical supercomputers and emerging quantum computers, alongside software advancements incorporating advanced algorithms and statistical machine learning models [1]. Recent developments such as large language models and generative diffusion techniques are unlocking application areas ranging from multimodal characterisation to self-driving laboratories. This seminar will introduce the field of data-driven chemistry, highlighting its potential to enhance chemical discovery and expedite the identification of compounds essential for advancing the next generation of clean energy technologies [2]. I will include insights from recent progress in characterising materials relevant to solar energy applications, while addressing obstacles such as reliable structure-property databases to enable more powerful models that are repeatable and reproducible [3].

[1] "Machine learning for molecular and materials science" Nature **559**, 547 (2018) [link]
[2] "Has generative artificial intelligence solved inverse materials design?" Matter **7**, 2355 (2024) [link]
[3] "Open computational materials science" Nature Materials **23**, 16 (2024) [link]

Biography

Aron Walsh began his career at Trinity College Dublin (Ireland) where his PhD focused on the computer simulation of solids. Following a postdoctoral stay at the National Renewable Energy Laboratory (USA), he held a Royal Society University Research Fellowship at the University of Bath (UK), and joined Imperial College London as the Chair in Materials Design. He was awarded the EU-40 Prize for his work on the theory of solar energy materials and the RSC Corday-Morgan Prize for his contributions to computational chemistry. Aron features in the Clarivate Highly Cited Researchers list and is an Associate Editor for the Journal of the American Chemical Society covering energy materials and artificial intelligence.