Grand Challenges

The Materials Chemistry Consortium (MCC)

Over the next five to ten years, the MCC community will prepare materials modelling software for future computing platforms, vital for the development of Net Zero technologies in line with the UK government's plans for a cleaner world by 2050

The Community

mcc.hec.ac.uk

The High-End Computing Materials Chemistry Consortium exploits national and regional high end computing facilities in a broad programme of work modelling and predicting the structures, properties and reactivities of materials. The consortium includes over 100 research groups with over 700 users registered on the UK national supercomputing service ARCHER2, with an emphasis on modelling at the atomic and molecular level but with growing links to models at larger length and time scales.

The Challenges

A number of grand challenges aligned with government priorities that MCC will address via their current research themes as follows:

Computational Catalysis supports the wide-ranging experimental programmes of UK's catalysis, especially the Catalysis Hub and its partners in both universities and industry. The grand challenge in this area is to generate detailed structural and mechanistic information needed for catalysis optimization and design, which is vital for the development of Net Zero technologies including catalytic CO_2 conversion, ammonia synthesis and plasmonic enhanced photocatalysis.

Environmental and Nuclear Materials involve grand challenges around the development of materials to contain toxic and/or radioactive waste, capture greenhouse gases for long-term storage, remove toxins and pollutants from the biosphere. Projects include new materials for circular economy technologies and environmental protection; detection and catalytic remediation procedures for pollutants in air and water systems; CO_2 utilisation; N_2 activation; disposal and/or recycling of hazardous waste materials; and development of sustainable, non-toxic replacements for structural and functional materials.

Soft Matter and Biomaterials underpins the design of soft materials for biological applications. Understanding the superior properties of biological materials will inform the design of soft matter mimics, with applications to the pharmaceutical, drug delivery platforms, bioimaging, food and cosmetic industries.

Grand Challenges

Materials Discovery develops and applies computational approaches to find new materials with desired functional properties. Such materials include inorganic, organic (e.g. polymers and pharmaceuticals) and hybrid organic-inorganic (e.g. metal organic frameworks). The development of advanced materials is essential to growth industries including clean energy solutions and quantum technologies.

Energy Materials Modelling involves the grand challenge of battery design, including materials for high energy density cathodes, solid-state batteries and next-generation sodium-ion batteries, interacting with experimental work at the Faraday Institution (FI) and its partners in industry. Nuclear waste storage is also a grand challenge, with work on radiation damage in nuclear materials and materials degradation in partnership with the Nuclear Decommissioning Authority.

Fundamentals of Bulk Materials addresses the morphologies, atomic structure and stability of (poly)crystalline and amorphous phases of bulk materials that underpins almost all themes and assists in a diverse range of applications of materials in technology. It facilitates design and discovery of new materials with tailored properties for energy generation, transport and storage, microelectronics and carbon capture.

Fundamentals of Surfaces and Interfaces bridges method developments and applications in other themes where important processes often occur at poorly characterised interfaces between materials. Grand challenge applications include understanding the role of defects at complex grain boundaries in thin film photovoltaics to expedite optimisation for the fabrication of greener, more efficient materials.

Fundamentals in Low Dimensional Materials seeks to advance our understanding of phenomena that occur when matter is organised at the nanoscale. The predictive challenge is the need to improve our capability to design bias-free methods for evaluating such relationships, with applications including improving solar cell performance by tuning the HOMO-LUMO gap to match frequencies of visible light.

The Solution

To prepare materials modelling software for future computing platforms

To fully realise solutions to the MCC's challenges, we will need to prepare materials modelling software for future computing platforms, which will be increasingly heterogeneous, principally through use of GPUs. This requires a large and sustained effort both within MCC and through participating in related initiatives, e.g. the PAX-HPC project for particle-based simulation methods as part of the UK's ExCALIBUR exascale computing program. **Novel Algorithms for Materials Modelling** are also required and form a theme within the consortium, cutting across application-specific domains, and supporting the development and application of new algorithms for the next generation of materials simulation. This includes emerging techniques to improve on the scope, accuracy and reliability of current materials modelling, together with leveraging developments in quantum computing, machine learning and synergies with other fields e.g., quantum

chemistry. Methods beyond the limitations in cost and/or accuracy of DFT, and the materials science specific potential of algorithms designed to exploit emerging quantum computers (via their classical emulation and combination with classical resources) will require much exploration and benchmarking to assess rigorously and objectively their advantages. Large-scale simulation is needed to identify bottlenecks in current techniques and quantify the potential accuracy and range of applicability in these emerging alternatives to the field. Allied to this is the need for access to new platforms in the UK as and when they become available, which will be essential for tackling both challenges. The fact that the MCC workload managed to fill ARCHER2 when it eventually arrived demonstrates the demand from the MCC members a few years ago and this should increase.

The Outcome

Access to exascale HPC to keep internationally competitive with their science output

In three to five years from now, MCC will need access to exascale HPC to keep internationally competitive with their science output. We have been involved in the ExCALIBUR project, preparing for exascale HPC, considered quantum computers, and now looking more carefully at how best to employ AI techniques in new workflows suitable for computers like AIRR. Essentially, we aim to achieve as much impact as possible in the field of materials research with the use of national HPC resources we distribute by sharing ideas and good practices, optimising the performance (scientific throughput per CU) of our software, as well as developing and assessing new workflows and software to achieve our aims.

More Information

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