Grand Challenges

The Collaborative Computational Project for NMR Crystallography (CCP-NC)

Over the next 5-10 years CCP-NC aims to leverage the power of modern computational chemistry to facilitate materials characterisation and discovery using NMR to produce a reproducible ecosystem enabling non-experts to apply NMR crystallographic methods to complex materials.

The Community

CCP-NC Collaborative Computational Project for NMR Crystallography

www.ccpnc.ac.uk

CCP-NC was established in 2010 to support researchers using nuclear magnetic resonance (NMR) to understand and characterise materials. This community increasingly relies on computational methods (particularly electronic structure codes) to connect structural models with experimental methods, an approach described as “NMR Crystallography”. CCP-NC develops the software tools and provides training to allow a largely experimental community to exploit the power of modern computational chemistry. Through its software and its website resources, CCP-NC is at the forefront of research internationally in this rapidly developing field.

The Challenge

To leverage the power of modern computational chemistry to facilitate materials characterisation and discovery using NMR

The ability to link experimental NMR data with predictions from quantum chemistry calculations has transformed our ability to characterise materials and relate experimental features to three-dimensional structure. Advances in computational chemistry, such as machine learning (and AI more generally) and quantum computing offer the prospects of applying these methods to significantly more complex materials, such as amorphous drugs and energy materials. Simultaneously, these developments make it increasingly difficult for experimental researchers to apply these sophisticated computational tools efficiently and effectively.

Grand Challenges

The Solution

Equipping experimental researchers with state-of-the-art computational tools

CCP-NC will use its position at the interface of computational chemistry and experimental NMR to provide tools and training for the next generation of materials researchers, both in academia and industry. Working with developers of quantum chemistry codes, we develop protocols and workflows to ensure that calculations are both robust (delivering trustworthy results) and efficient (using computing resources with maximum energetic efficiency). Building on our existing work on standard file formats and databases of calculation results, we develop tools and working practices to ensure that results are FAIR-ly available and reusable by AI-enabled researchers. By providing a variety of training activities and web resources, we will ensure that best practice is disseminated effectively, to both established and new researchers.

The Outcome

An accessible, reproducible ecosystem enabling non-experts to apply NMR crystallographic methods to complex materials

A coordinated suite of interoperable computational tools, workflows and training resources will be delivered by 2030, enabling experimental and computational researchers to apply NMR crystallographic methods routinely and reproducibly to complex and disordered materials. Integrated, end-to-end workflows will link experimental NMR data with predictions from quantum chemistry, incorporating machine-learning and AI-enabled methods to accelerate structure generation, ensemble exploration, spectral simulation and quantitative comparison. These workflows will deliver robust, trustworthy results while making efficient use of GPU-enabled Tier-1 and Tier-2 high-performance computing resources, preserving methodological transparency and lowering barriers to adoption by non-specialists.

These capabilities will be complemented by community-endorsed protocols for provenance tracking, spectral benchmarking and FAIR data deposition, ensuring that computational results are reusable for data-driven and AI-enabled research. Together, these developments will establish CCP-NC as the UK hub for NMR crystallography and the computational–experimental study of structurally complex materials, strengthening links with crystallography, structure prediction and materials informatics, and supporting long-term UK leadership in materials science.

More Information

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