# Advancing energy technologies by understanding material function using neutron scattering and computational methods

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Functional materials form the central part of many important energy technologies. A material's atomic structure and dynamics underpin performance characteristics, and the characterization of these is central to technology advancement.

The functional materials at the heart of energy devices often reversibly host charge or energy carriers, and characterization focuses on understanding how these guests are accommodated by the host material. Neutron scattering has made important contributions to this understanding, and is naturally complemented by first-principles calculations, with the combination particularly powerful for studying energy materials. Ideally, such studies will probe the material's functional mechanism and be performed during function within a device or during the material's response to external stimuli (*operando* and *in situ* studies), as analyses of a functional material at equilibrium can yield misleading or incomplete results. Functional materials analysis is therefore greatly benefited by modern high-speed instrumentation, which allows the rapid collection of data and real-time information concerning the functioning/responding material to be gained.

This presentation will give examples of neutron scattering and first-principles computational analysis of functional materials for energy systems under equilibrium and non-equilibrium conditions. Examples will include rechargeable battery electrodes and sorbent materials used for the separation and storage of energy-relevant gases.