

#### *In situ/operando neutron and X-ray studies of functional materials*

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Functional materials are central to many technologically-important devices and systems. Such materials are often multifunctional and highly responsive. Developing experimental approaches that specifically target functional materials is essential in obtaining a mechanistic understanding of how properties and behavior occur, and leads directly to materials advancement. This is particularly relevant given the increasing power and speed of characterization instrumentation that enables real-time and non-equilibrium measurement of the material during operation.

This presentation will give examples of the application of X-ray and neutron techniques of analysis, in combination with computational density-functional-theory-based methods, to understand materials function. Example in situ and operando studies of functional materials will be presented, focusing mostly on rechargeable battery electrodes and multifunctional porous framework materials.

Results of rechargeable electrode studies presented will focus on structure across a range of length-scales, from local to powder particle morphology. Examples presented will include real-time measurement of the location of charge-carrying ions within the structure during charge-discharge cycling of whole batteries, and how the host electrode structure responds to this. A case where operando powder diffraction and microscopy are combined to reveal a complete picture of how function arises and to understand capacity decay will be presented [1].

Results of porous framework material studies presented will include experimental measurements of local and average structure, as well as dynamics, with these measurements being coupled with density functional theory-based computations to gain functional insight. These studies are aimed at understanding behaviors supporting application as solid porous sorbents (such as gas-adsorption and temperature effects [2]), and to understand how interesting fundamental mechanical properties arise (such as compression [3]).

[1] Chen, C. -J.; Pang, W. K.; Mori, T.; Peterson, V. K.; Sharma, N.; Lee, P. -H.; Wu, S.-h.; Wang, C. -C.; Song, Y. -F.; & Liu, R. -S. (2016) *Journal of the American Chemical Society*, 138, 8824-8833.

[2] McCormick, L. J.; Duyker, S. G.; Thornton, A. W.; Hawes, C. S.; Hill, M. R.; Peterson, V. K.; Batten, S. R.; & Turner, D. R. (2014) *Chemistry of Materials*, 26, 4640-4646.

[3] Duyker, S. G.; Peterson, V. K.; Kearley, G. J.; Studer, A. & Kepert, C. J. (2016) *Nature Chemistry* 8, 270 - 275

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