Abstract for IAS International Conference on Energy Materials (January 19-23, 2026)

Characterizing Energy Materials: Understanding Function by Studying Material Change

Vanessa K. Peterson

Australian Centre for Neutron Scattering,

Australian Nuclear Science and Technology Organisation, Australia

Email: vanessa.peterson@ansto.gov.au

The performance of materials central to energy devices including gas separation and storage technologies, fuel cells, and batteries, is determined largely by materials structure-dynamic-function relations. Most energy materials function by undergoing change, such as the compositional change in rechargeable battery electrodes that host charge-carrying ions and in porous sorbent materials that host gas molecules. These materials are structurally complex, and the compositional change they accommodate is continuous and large.

Robust characterization methods that quantitatively and accurately capture representative changes in these materials are essential to understanding functional processes and informing the strategic design of superior materials. Ideally, the detailed characterization of these materials would be gained while the material is undergoing change within a device that is operating under application representative conditions. However, rapid characterization, particularly of materials within operating devices, limits the level of detail that can be gained. This challenge is sometimes alleviated by studying model systems in which material function is not representative of that in the device. Importantly, the characterization of materials and the functional understanding gained must include a careful choice of methods and a consideration of the limitations of methods and approaches used [1].

This talk will highlight some methods and approaches useful in studying materials undergoing change with the aim of understanding their function in energy systems. Example studies of battery [2-7] and porous solid framework materials used for gas separation [8-15] will be presented that highlight the understanding of function that can be gained, with a focus on *in situ* and application representative methods using instrumentation at the Australian Centre for Neutron Scattering.

References:

- [1] V. K. Peterson, J. E. Auckett and W. K. Pang IUCrJ 4 540-554 (2017).
- [2] G. Liang, C. Didier, Z. Guo, W. K. Pang and V. K. Peterson, Adv. Mater. 32 1904528 (2020).
- [3] N. Sharma, V. K. Peterson, M. M. Elcombe, M. Avdeev, A. J. Studer, N. Blagojevic, R. Yusoff and N. Kamarulzaman, J. Power Sources 195 8258-8266 (2010).
- [4] C. Didier, W. K. Pang, Z. Guo, S. Schmid and V. K. Peterson Chem. Mater. 32 2518-2531 (2020).
- [5] W. K. Pang, V. K. Peterson, N. Sharma, J. J. Shiu and S. Wu, Chem. Mater. 26 2318-2326 (2014).

Abstract for IAS International Conference on Energy Materials (January 19-23, 2026)

- [6] W. K. Pang and V. K. Peterson, Appl. Crystallogr. 48 280-290 (2015).
- [7] C. Didier, J. P. Mata, E. P. Gilbert and V. K. Peterson, Adv. Energy Mater. 13 2301266 (2023).
- [8] S. Lee, H. Chevreau, N. Booth, S. Duyker, S. Ogilvie, P. Imperia and V. K. Peterson, J. Appl. Cryst. 49 705-7112016 (2016).
- [9] H. Chevreau, S. G. Duyker and V.K. Peterson, Acta. Cryst. B 71 648-660 (2015).
- [10] V. K. Peterson, Y. Liu, C. M. Brown and C. J. Kepert, J. Am. Chem. Soc. 128 15578-15579 (2006).
- [11] V. K Peterson, C. M. Brown, Y. Liu and C. J. Kepert, J. Phys. Chem. C. 115 8851-8857 (2011)
- [12] C. M. Brown, Y. Liu, T. Yildirim, V. K. Peterson and C. J. Kepert, Nanotechnology 20 204025 (2009).
- [13] Y. Liu, C. M. Brown, D. A. Neumann, V. K. Peterson and C. J. Kepert, J. Alloy Compd. 446 385-388 (2007).
- [14] H. Chevreau, W. Liang, G. J. Kearley, S. G. Duyker, D. M. D'Alessandro and V. K. Peterson, J. Phys. Chem. C. 119 6980-6987 (2015).
- [15] L. Zhang, R. Röß-Ohlenroth, V. K. Peterson, S. G. Duyker, C. Li, J. Luiz Fiorio, J.-O. Joswig, R. Dinnebier, D. Volkmer and M. Hirscher, Nat. Commun. 16 5941 (2025).