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Understanding the properties of energy materials from their local structure

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Numerous energy materials with improved properties often show nano- or heavily disordered structural features which are hardly characterized by the conventional crystallographic technique alone. By using the atomic pair distribution function (PDF) analysis [1]on X-ray and neutron total scattering data, we have investigated various energy materials to elucidate structural features closely linked to their properties. Some of the examples are heavily disordered V1-xTixH2 for hydrogen storage [2] and layered Li1.2Mn0.567Ni0.166Co0.067O2 cathode material for lithium ion batteries. These materials possess an intricate structure and could easily lead to misleading results if one relies on only one structure probing technique. In this talk, I will show how their structural information was extracted from the x-ray and neutron PDFs obtained at BL22XU at SPring-8 and NOVA at J-PARC, respectively and how it was used with information available from other techniques to understand the properties of these energy materials.

[1] *T. Egami and S. J. L. Billinge, Underneath the Bragg Peaks: Structural Analysis of Complex Materials: Pergamon Press Elsevier: Oxford, England, 2003.,* ***[2]*** *H. Kim et al., J. Phys. Chem. C 117 (2013) 26543-26550.*

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