Investigating Preservation of Local Structure in 2-D $Re_6Se_8Cl_2$ After Surface Functionalization

J. Y. Easter[1], S. H. Skjaervoe[2], S. J. L. Billinge[2], Wendy He[3], Colin Nuckolls[3], Xavier Roy[3]

[1]Department of Engineering, University of Maryland Eastern Shore, Princess Anne, MD
[2]Department of Applied Physics and Applied Mathematics, Columbia University, New York, NY
[3]Department of Chemistry, Columbia University, New York, NY

2-dimensional materials are promising candidates for next-generation technologies, and tuning their surfaces by molecular functionalization has been extensively explored for the purpose of achieving application-specific properties. Such surface functionalization often comes at the expense of other important material characteristics, such as changes in alignment and spacing of the layers. In this project, we investigate the preservation of structural integrity in 2-dimensional $Re_6Se_8Cl_2$,first, after surface functionalization that involves replacing the Cl with H and, second, when heating the material to high temperatures. We investigated the structural integrity with X-ray total scattering data collected at NSLS-II and Fourier-transformed to the atomic pair distribution function (PDF), a technique that is unmatched in its ability to solve the structure of such short-range ordered materials. The modeling of the PDF data was done using the software PDFgui, using the data of the most local structure (r<9.4Å) as well as data at higher range (r=9.4-30Å). The PDF modeling of the local structure data showed that the short-range (r=2-9.4Å) order in the structural integrity was preserved after surface functionalization, although alignment and distancing of the layers were compromised. As such, we show that this method of surface functionalization maintains the local structure of the pristine material. We also measured PDFs over a temperature range of 89K-500K, and the peaks in the most local PDF indicated that the local structure was qualitatively unchanged in the entire temperature range. However, modeling of the local structure revealed abrupt changes in lattice parameters and atomic positions at approximately 400K. These changes in the local structure occur at the same temperature where a phase transition is observed in the average structure data. Further modeling is required to explore the details of the transition.

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