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Uncovering Structural Features Related to the Material Properties by the PDF Method. Wojtek Dmowski[1], Karen E. Swider-Lyons[2], Takeshi Egami[1,3], [1]Dept. of Materials Science and Engineering, Univ. of Tennessee, Knoxville, TN 37996, [2]Code 6170, Naval Research Laboratory, Washington, DC 20375-5342 USA , [3]Oak Ridge National Laboratory, Oak Ridge, TN 37831.

Atomic pair-density function (PDF) analysis is an ideal approach for examining the local- and medium-range atomic structures of materials. PDF has been widely used in the studies of glasses and liquids and has also been applied successfully to characterize the local and complex structures of crystalline solids. Using PDF analysis, we demonstrate that important conclusions can be drawn about how the short-and long-range atomic structure of several materials, including catalysts, structural materials and ferroelctrics, relates to their physical and electrochemical properties. We demonstrate that PDF can be extended to study local atomic dynamics.