Structure Solution of Single-Element Molecules from Pair Distribution Function

Pavol Juhas[a], David M. Cherba[b], Phillip M. Duxbury[a], William Punch[b], Simon J.L. Billinge[a], [a]*Department of Physics and Astronomy,* [b]*Department of Computer Science and Engineering, Michigan State University, East Lansing, MI, USA*. E-mail: juhas@pa.msu.edu

Recent developments of synchrotron x-ray and neutron instruments and acquisition techniques allowed fast and precise measurements of experimental Pair Distribution Functions (PDFs) from molecules, crystals and disordered materials. However, it is usually complicated to extract the structure information from PDF data, and the data processing typically involves a tedious testing of a series of structure models. Therefore it is desirable to find a better way how to analyze PDF data. For single-atom molecules the PDF curves can be converted to a table of inter-atomic distances, which transforms the PDF curve-fitting to a molecular conformation problem. We have developed several algorithms on reconstruction of single atom molecules and tested them with artificial and experimental distance data.

Keywords: ab-initio structure determination, pair distribution function, molecular structure