

**W0032**

**Structure Refinement From Pair Distribution Functions Using a Genetic Algorithm.** Pavol Juhas, David M. Cherba, Phillip M. Duxbury, Simon J.L. Billinge, Physics & Astronomy, Michigan State Univ., 4251 Biomedical Physical Sciences, East Lansing, MI 48824-2320.

Recent developments of the synchrotron x-ray and neutron instruments and acquisition techniques allow fast and precise measurements of experimental Pair Distribution Functions (PDFs) from molecules, crystals and disordered materials. However, to extract the structure information from a PDF data is usually not simple, and the data analysis then consists of tedious trial-and-error checking of a series of structure models. Therefore it is very desirable to search for better ways of analyzing 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 examine application of genetic algorithms on a reconstruction of several single-atom molecules from their given tables of distances.