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***Ab initio* Structure Determination from Pair Distribution Function.** Pavol Juhas, Phillip M. Duxbury, Simon J.L. Billinge, Michigan State Univ., East Lansing, MI.

A vast majority of all known structures has been obtained by reciprocal space methods that require periodic long-range order in the material. However, many important systems, such as nanomaterials or non-crystallized molecules, have no periodic order at all and their structures cannot be solved using crystallographic methods. The analysis of the atomic Pair Distribution Function (PDF) is not limited by periodic order and it has yielded important atomic scale information on nanomaterials. However, PDF analysis is not simple and it typically consists of time consuming trial-and-error tests of different structure models. Our recent work [1] presents another way of extracting structure from PDF data and it demonstrates a complete *ab-initio* structure solution of a single-component molecule from PDF data alone. We will describe the extension of *ab-initio* PDF method to general, multi-component molecules and to periodic systems with large supercells. The application of chemical information, such as bond angle restraints or known structure fragments will also be discussed.

[1] P. Juhas, D. M. Cherba, P. M. Duxbury, W. F. Punch, S. J. L. Billinge, *Ab initio* determination of solid-state nanostructure, Nature (to be published in 2006).