Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Nanostructure determination from the atomic pair distribution function LUKE GRANLUND, Michigan State University, PAVOL JUHAS, Columbia University, SAURABH GUJARATHI, PHIL DUXBURY, Michigan State University, SIMON BILLINGE, Columbia University — Many materials at the nanoscale cannot benefit from crystallographic analysis and are unsuitable for refinement techniques that require an initial guess at the structure. One approach to overcoming these difficulties is the Liga algorithm, which generates structures relying solely on distances extracted from the atomic pair distribution function[1,2]. This method is shown to successfully reconstruct the buckyball from experimental data. Recent extensions to multi-component and periodic systems have also allowed reconstruction of common crystals from experimental data. The ability to handle both periodic and nonperiodic cases may make the algorithm a useful tool in the study of local structure deviations in nanocrystals in addition to noncrystalline nanomaterials. [1] P. Juhas, D. M. Cherba, P. M. Duxbury, W. F. Punch, S. J. L. Billinge. Ab initio determination of solid-state nanostructure. Nature, 440, 655-658 (2006). [2] P. Juhas, L. Granlund, P. M. Duxbury, W. F. Punch, S. J. L. Billinge. The Liga algorithm for ab initio determination of nanostructure. Acta Cryst., A64, 631-640 (2008).

Luke Granlund
Michigan State University

Date submitted: 21 Nov 2008 Electronic form version 1.4