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Puzzles and promises in finding nanostructure from pair distribution function data COREY MUSOLFF, CHRISTOPHER FARROW, PHILLIP DUXBURY, Michigan State University, SIMON BILLINGE, PAVOL JUHAS, Columbia University — The pair distribution function (PDF) method provides detailed information about nanostructure and efficient software is available for refining PDF data to starting structures provided by the user. Starting structures may be developed using intuition, homologous structures from the literature, or by using ab-initio theoretical structures. However, in studies of nanoparticles good starting structures are hard to identify, particularly in systems where complex surface distortions occur. Moreover, refinement from random structures typically fails, or converges to unphysical structures. We quantify this problem through a systematic study of PDF refinement using starting structures that are randomly perturbed variants of the correct structures and identify the threshold perturbations beyond which refinement fails. To alleviate the difficulties in guessing or searching over starting structures it would be ideal if good starting structures could be found directly from PDF data. We outline our progress in this direction.

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