# STRUCTURE STUDIES OF DISORDERED PHARMACEUTICAL MATERIALS BY HIGH-ENERGY X-RAY DIFFRACTION AND ATOMIC PAIR DISTRIBUTION FUNCTION ANALYSIS

Valeri Petkov, Physics, CMU, Mt. Pleasant, MI 48858
(Petkov@phy.cmich.edu)

Knowledge of the atomic-scale structure is an important prerequisite to understanding, predicting and improving properties of pharmaceutical materials. When those materials are perfect crystals it is easily obtained by analyzing the positions and intensities of the Bragg peaks in their x-ray diffraction patterns. However, many pharmaceutical materials are not perfectly crystalline and so pose a problem to traditional Bragg x-ray diffraction. The reason is that the diffraction patterns of disordered materials show a very limited number of Bragg peaks, if any, and a very pronounced diffuse component. The problem may be solved by employing a non-traditional approach involving high-energy x-ray diffraction and atomic pair distribution function data analysis. In the talk, the essentials of this approach will be introduced and its great potential demonstrated with results from recent studies on purely organic pharmaceutical materials such as poly and microcrystalline cellulose, lactose and others. The application of this approach to metallo-organic materials used as MRI contrast agents and anti-cancer drugs will be discussed as well.