Abstract Submitted
for the DAMOP12 Meeting of
The American Physical Society

**Algorithm for Reconstruction of 3D Molecular Structure from Diffraction Patterns of Laser-Aligned Molecules** JIE YANG, CHRISTOPHER HENSLEY, MARTIN CENTURION, University of Nebraska - Lincoln — Ultrafast electron diffraction from laser-aligned gas molecules is a promising method for the determination of 3D molecular structures. Reconstruction algorithms for diffraction patterns of perfectly aligned molecules have been widely studied theoretically. However, under experimental conditions only partial alignment can be achieved and the existing algorithms do not perform well when the alignment is not perfect. We develop a method to reconstruct the 3D structure of molecules with cylindrical symmetry from electron diffraction patterns of partially-aligned molecules. The evolutionary algorithm assumes a known angular distribution, which can be calculated numerically using existing theory for laser-alignment and verified by comparison with the data. Selecting $CF_3I$ as the cylindrically symmetric molecule, diffraction patterns from multiple alignment angles are used to reconstruct a single diffraction pattern corresponding to perfect alignment. The molecular structure can then be recovered from this pattern with no prior structural information required. Our results are in good agreement with previous models of $CF_3I$ structure.

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Date submitted: 26 Jan 2012 Electronic form version 1.4