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Ultrafast Imaging of Molecules with Electron Diffraction

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Ultrafast imaging of isolated molecules in three dimensions and with atomic resolution is important for elucidating intermediate states in molecular reactions. Electron diffraction has been the main tool to determine the structure of molecules in the gas phase. Diffraction patterns from randomly oriented molecules in the gas phase contain only one-dimensional information, and thus input from theoretical models is needed to recover the structure. We have shown experimentally that three-dimensional structural information of symmetric top molecules can be retrieved from multiple electron diffraction patterns of aligned molecules. The molecules are aligned impulsively with a femtosecond laser pulse and probed with a femtosecond electron pulse two picoseconds later, when the degree of alignment reaches a maximum. Furthermore, we show that our method can be extended to asymmetric molecules using diffraction from partially aligned molecules and a new structure retrieval method. Previous reconstruction algorithms had two major limitations: First, they require diffracting from a single molecule or an ensemble with very high degree of alignment that is generally incompatible with diffraction experiments, and second, each algorithm is only applicable for a specific type of molecules. We have developed a two-step reconstruction comprising a genetic algorithm that corrects for the imperfect alignment followed by an iterative phase retrieval method in cylindrical coordinates. Our simulations show that the full 3-D structure of trifluorotoluene, an asymmetric-top molecule, can be reconstructed with atomic resolution.