

Abstract Submitted
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Violation of centrosymmetry in time-resolved coherent x-ray diffraction from ro-vibrational states of diatomic molecules¹ HUA-CHIEH SHAO, ANTHONY F. STARACE, University of Nebraska - Lincoln — Owing to increasing applications of x-ray scattering for the investigation of molecular reaction dynamics, we theoretically study coherent x-ray diffraction to characterize features in time-resolved diffraction images that reflect nuclear motion in molecules.² Contrary to the conventional theory of time-independent x-ray diffraction, our model shows that the diffraction images can exhibit asymmetric angular distributions when the nuclei are in motion. In order to illustrate this violation of centrosymmetry (VOC), we simulate the diffraction images from two oriented diatomic molecules undergoing ro-vibrational motion: deuterated lithium hydride (LiD) and hydrogen (HD). We further investigate how the VOC relates to the nuclear motion and the nature of such asymmetry. Our analysis indicates that the VOC is a general phenomenon in time-resolved coherent diffraction whenever a molecular motion breaks the inversion symmetry.

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²H.-C. Shao and A.F. Starace, Phys. Rev. A **99**, 033413 (2019).

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