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Field-free molecular alignment for studies using x-ray pulses from a synchrotron radiation source PHAY HO, Argonne National Laboratory, MICHELLE MILLER, Northwestern University, ROBIN SANTRA, Argonne National Laboratory and University of Chicago — A short, intense laser pulse may be employed to create a spatially aligned molecular sample that persists after the laser pulse is over. We theoretically investigate whether this impulsive molecular alignment technique may be exploited for experiments using x-ray pulses from a third-generation synchrotron radiation facility. Using a linear rigid rotor model, the alignment dynamics of model molecular systems with systematically increasing size is calculated utilizing both a quantum density matrix formalism and a classical ensemble method. For each system, the alignment dynamics obtained for a 95-ps laser is compared to that obtained for a 10-ps laser pulse. The average degree of alignment after the laser pulse, as calculated quantum mechanically, increases with the size of the molecule. This effect is quantitatively reproduced by the classical calculations. The average degree of impulsive alignment is high enough to induce a pronounced linear dichroism in resonant x-ray absorption using the intense 100-ps x-ray pulses currently available. However, for structural studies based on elastic x-ray scattering, bright x-ray pulses with a duration of 1 ps or shorter will be required in order to make full use of impulsive molecular alignment.

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