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Molecular high-harmonic generation spectroscopy with two-colour bicircular fields: a theoretical chemist's point of view

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We present here our recent work on the development of ab initio time-domain methods for studying the contribution of inner molecular orbitals to the HHG spectrum [1] of aligned or non-aligned molecules [2-4]. First, we show how, in the presence of a linearly polarised pulse, the selection rules for harmonic generation can be different depending on the molecular orbital considered: an example is given by ammonia [5], with a specific pulse polarisation. As a second house, we show how to modulate the selection rules in molecules such as methane and fluoromethane [6], interacting with two-colour bicircular (BCR) fields, by changing the relative orientation and geometry of the spectroscopic target. In conclusion, results on HHG spectra of a chiral molecule, such as methyloxirane, with BCR pulses [6] are shown and discussed. The work on BCR fields is in collaboration with Vozzi's experimental group.

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