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Computational Study of Orientation-dependent Molecular High Harmonic Spectra ANTHONY DUTOI, TAMAR SEIDEMAN, Northwestern University — Recently, there has been much interest in high harmonic generation (HHG) by aligned molecules [*Phys. Rev. A* **67** 023819, *Nature* **432** 867, *Nature* **435** 470]. During HHG, an electron is ionized and driven back to the cation by a strong, low-frequency field, and radiation is emitted at harmonics of this driving pulse. Because this process is sensitive to the orientation of a molecule, rotational dynamics can be probed on very short time scales. We are working to predict the time-dependent HHG spectra for aligned rotational wavepackets. In conjunction with experiment, these simulations should be valuable for studying the loss of rotational coherence in media such as dense gases. Within the presented formalism, Born-Oppenheimer rotational dynamics are handled exactly, while HHG at any given orientation is estimated by numerical time integration of a one-electron Schrödinger equation. Propagation outside of the integration grid can be handled using an analytical Volkov propagator at the expense of ignoring the cation field at this distance.

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