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High-harmonic generation in aligned water molecules¹ SONG WANG, JULIEN DEVIN, Stanford PULSE Institute, MATTHIAS HOFFMANN, SLAC, JAMES CRYAN, ANDREAS KALDUN, PHILIP BUCKSBAUM, Stanford PULSE Institute — In recent years, the use of high harmonic generation (HHG) in aligned molecular vapors has become a powerful tool to study ultrafast dynamics of electronic and nuclear wave packets. In our new experimental setup, we are able to orient H_2O and D_2O molecules using a single cycle terahertz (THz) pulse. Aligning water is especially interesting as the highest occupied molecular orbital (HOMO) of water contains a node in the xz plane of the molecular frame, allowing us to perform HHG from second highest occupied molecular orbital (HOMO-1) only, by setting the polarization of the fundamental laser along the z-axis of the aligned water molecules. We are particularly interested in the HOMO-1 state, as there is fast motion of the H-O-H angle leading to sub-wavelength dynamics. On this poster we present our all-optical alignment setup where HHG and single-cycle THz generation take place in high-vacuum, where measurements with arbitrary polarization angles between the two are possible. In addition, we discuss the effects of the molecular orientation on HHG, including symmetry breaking that could produce even harmonics and isotope effects between H₂O and D₂O due to different vibrational energies.

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