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Imaging an isolated water molecule with an attosecond electron wave packet

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Synopsis We use laser-induced electron diffraction (LIED) to self-image the molecular structure of an isolated water molecular ion using its own retuning attosecond electron wave packet (EWP). Using LIED's sub-femtosecond and picometre spatio-temporal resolution imaging capabilities, we observe the symmetric stretching of the O-H and H-H internuclear distances with increasing laser field strength.

Many biologically important processes, such as protein folding dynamics in a water solvation shell [1], are strongly influenced by the geometric structure of water. In fact, the geometry of water molecules can be altered using electric fields on the order of 0.2 V/Å [2]. Here, we investigate the structural changes that a single water molecule undergoes in an intense (10^{13} – 10^{14} Wcm⁻²), 97 fs (FWHM) 3.2 μm linearly laser pulse, corresponding to an electric field with field strengths of around 2 – 3 V/Å which mimics liquid water in its natural conditions. We use laser-induced electron diffraction [3] by Fourier Transform (FT-LIED) [4] to directly retrieve the geometric structure of isolated water molecules with attosecond and picometre spatio-temporal resolution. The LIED imaging process can be explained by the laser-induced electron recollision model [4]: an attosecond EWP is emitted by tunnel ionization, accelerated and returned by the driving laser field before elastically scattering against the parent ion. We employ the Reaction Microscope's electron-ion coincidence detection capabilities to isolate the high-energy LIED electrons that are detected in coincidence with H₂O⁺ ions. Structural information, which is embedded within the high-energy electron momentum distribution, is directly retrieved without any prior knowledge nor the use of retrieval algorithms and *ab initio*

calculations. We directly retrieve a symmetric with the ground electronic state structure of H₂O⁺. We also observe that increasing the field strength of the laser pulse leads to a further stretched H₂O⁺ structure. The observed increase in bond length could be related to the coupling between the molecular dipole and the electric field of the laser, thus permitting the simultaneous modification and measurement of the O-H bond length with LIED in field-dressed H₂O.

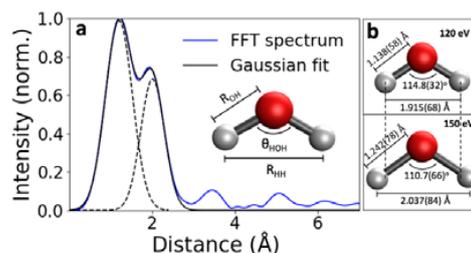


Figure 1. (a) Fourier spectrum (blue) from LIED data with Gaussian fits (black). The O-H and H-H internuclear distances are extracted using a sum of two Gaussians (black solid) along with the individual Gaussian fits (black dashed). (b) Experimentally retrieved molecular structures for laser intensities equivalent to a ponderomotive energy, U_p , of 120 and 150 eV.

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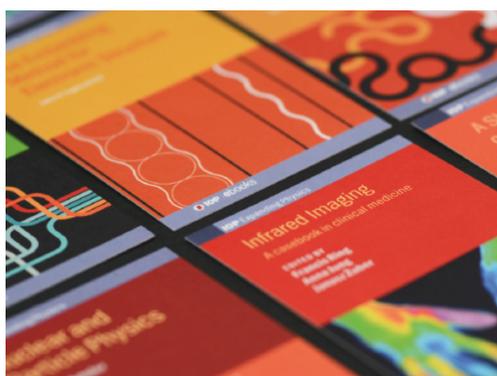


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