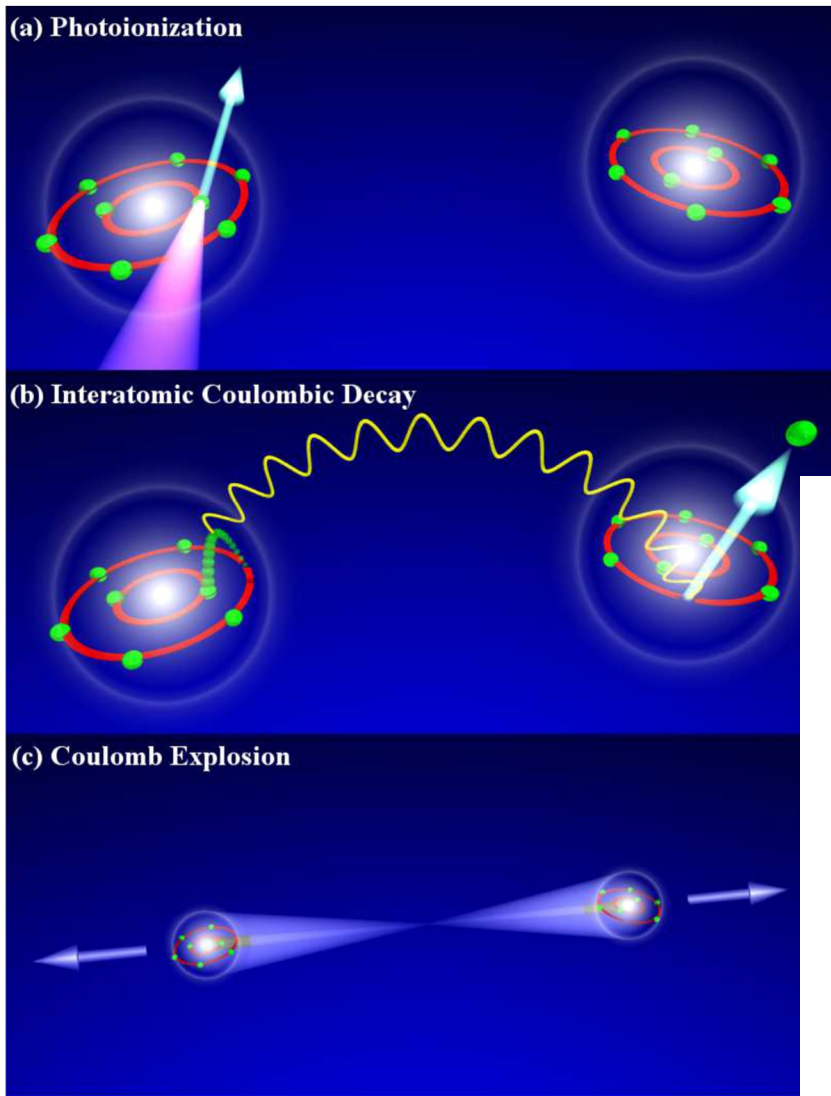
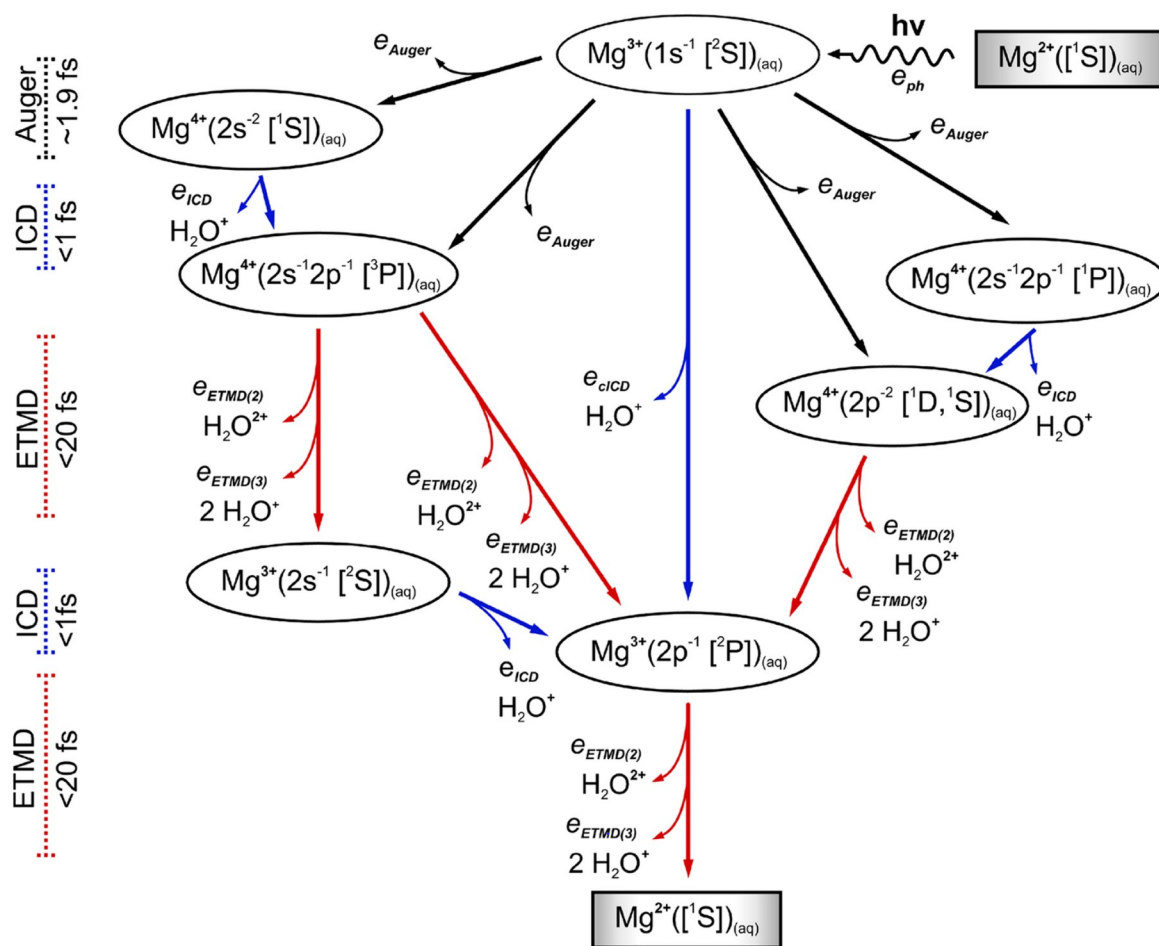




ICD – Interatomic Coulombic Decay



Intermolecular Coulombic decay in liquid water competes with proton transfer and non-adiabatic relaxation

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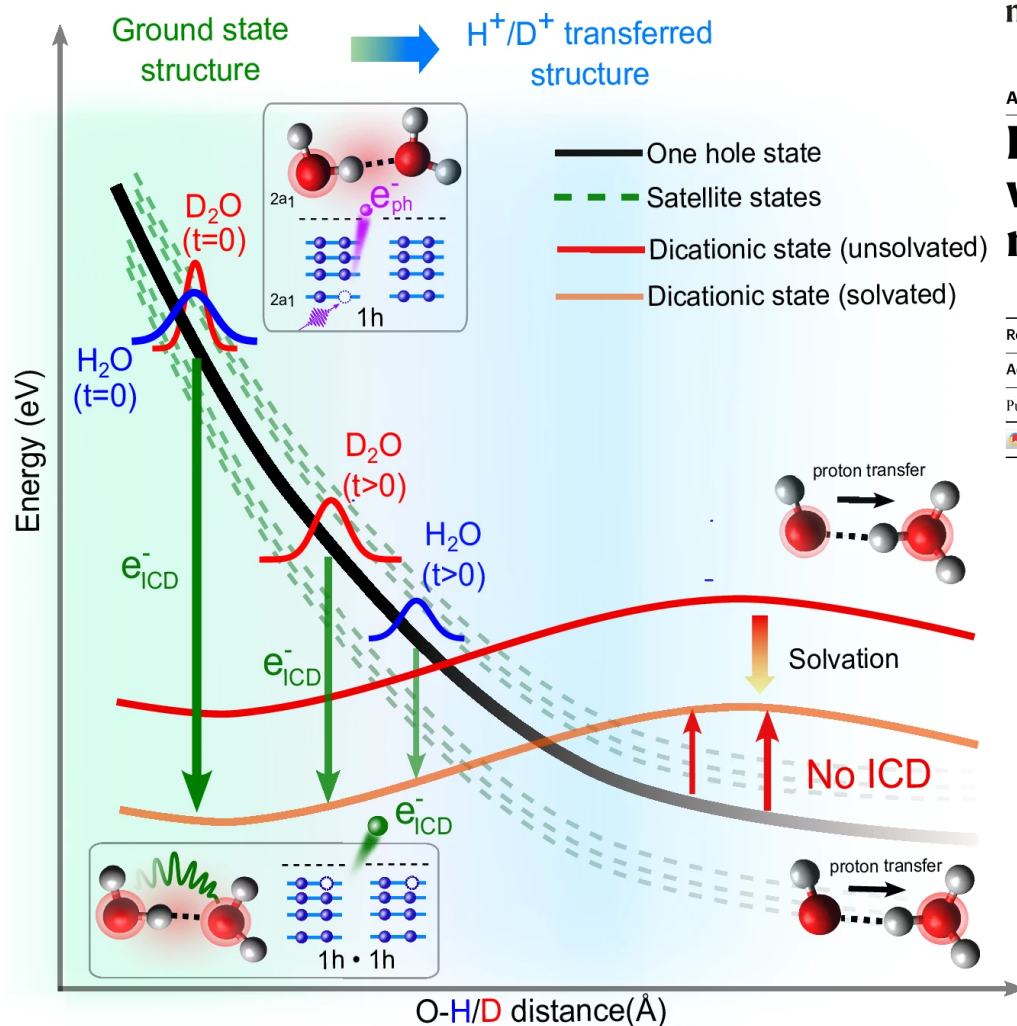
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Pengju Zhang^{1,2}✉, Joel Trester², Jakub Dubský³, Přemysl Kolorenc⁴, Petr Slaviček³✉ & Hans Jakob Wörner²✉

Despite decades of research, our understanding of radiation damage in aqueous systems remains limited. The recent discovery of Intermolecular Coulombic Decay (ICD) following inner-valence ionization of liquid water raises interesting questions about its efficiency as a major source of low-energy electrons responsible for radiation damage. To investigate, we performed electron-electron coincidence measurements on liquid H₂O and D₂O using a monochromatized high-harmonic-generation light source, detecting ICD electrons in coincidence with photoelectrons from the 2a₁ shell. We find that the ICD efficiency γ is below unity in both liquids and that $\gamma(\text{H}_2\text{O})/\gamma(\text{D}_2\text{O}) = 0.86 \pm 0.03$. Ab initio calculations reveal that ICD competes with proton transfer and non-adiabatic relaxation, which can close the ICD channel. A multi-scale stochastic model incorporating solvent effects reproduces these efficiencies. Our combined experimental and theoretical results suggest that the higher ICD efficiency in D₂O arises from slower proton transfer and non-adiabatic transitions, highlighting the crucial role of nuclear motion in liquid-phase ICD and advancing the understanding of radiation damage.



Intermolecular Coulombic decay in liquid water competes with proton transfer and non-adiabatic relaxation

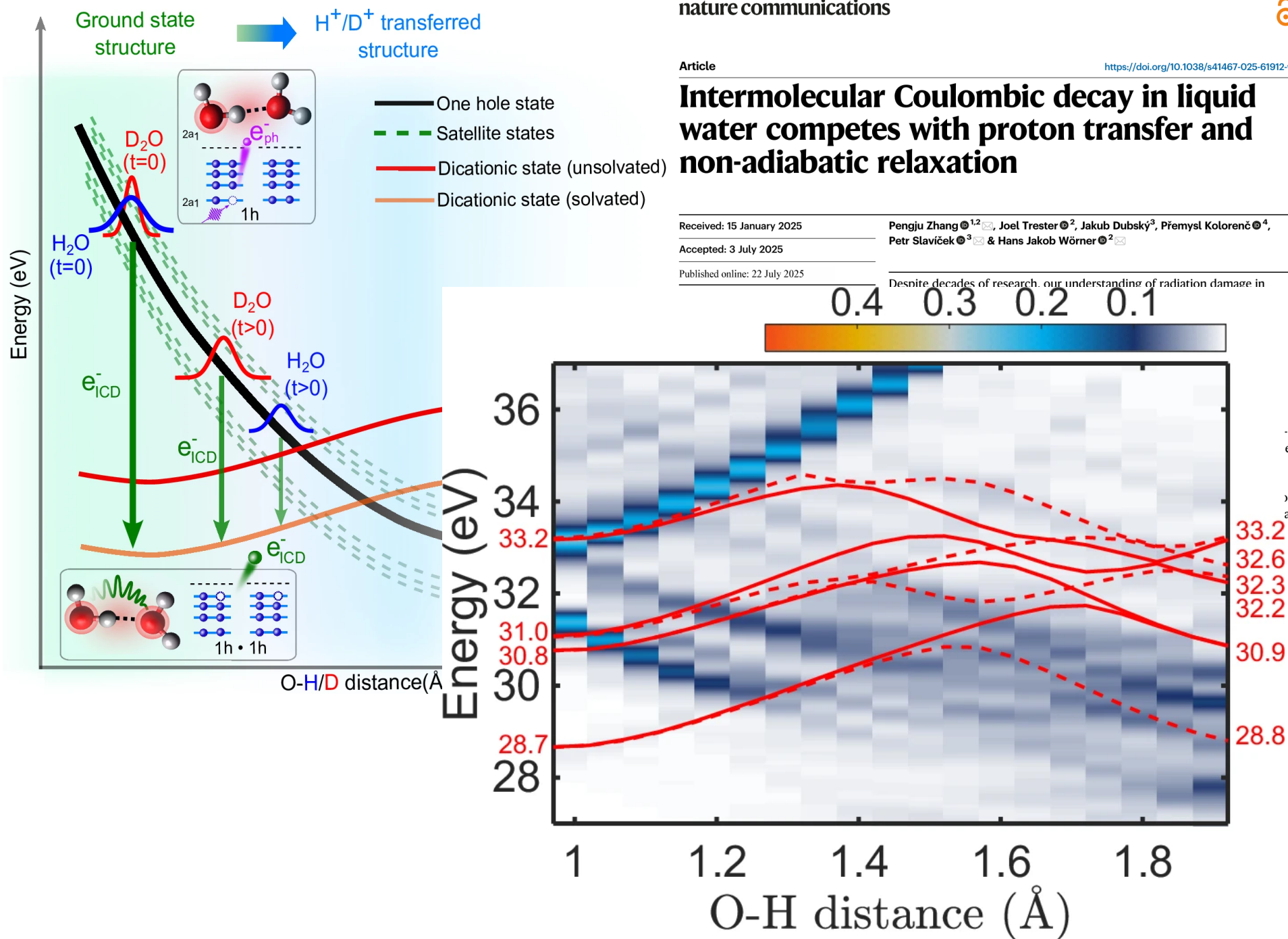
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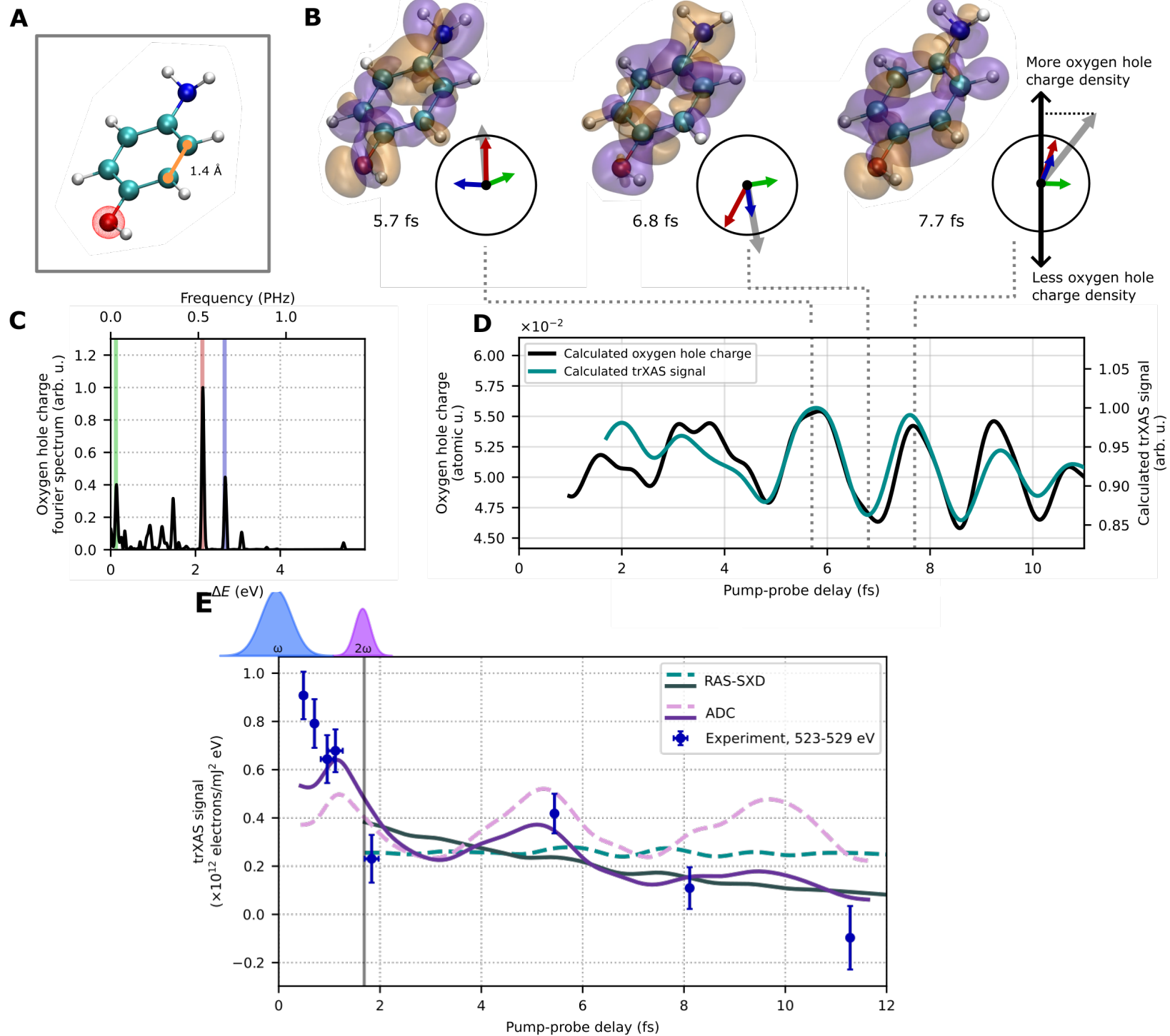
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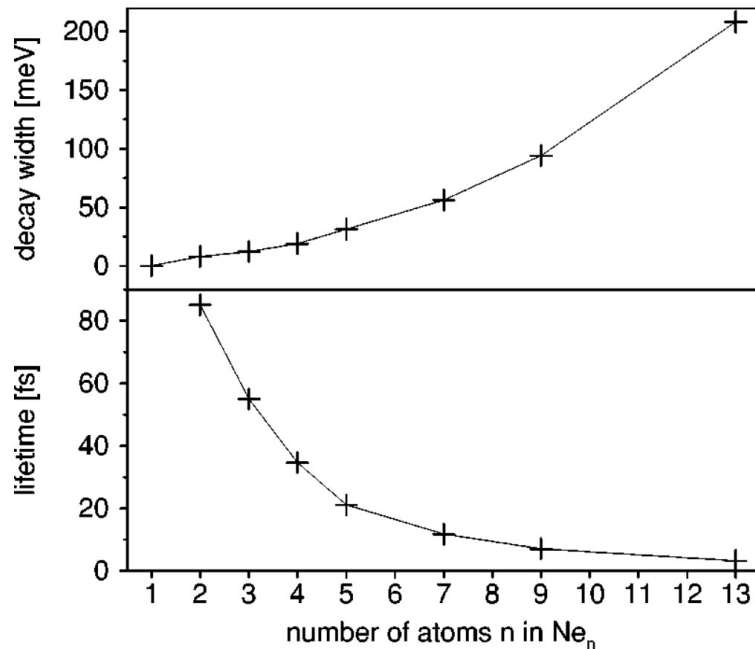
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Electronic decay of valence holes in clusters and condensed matter

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