

Electronic Supplementary Information (ESI) for: Electron-driven proton transfer enables nonradiative photodeactivation in microhydrated 2-aminoimidazole

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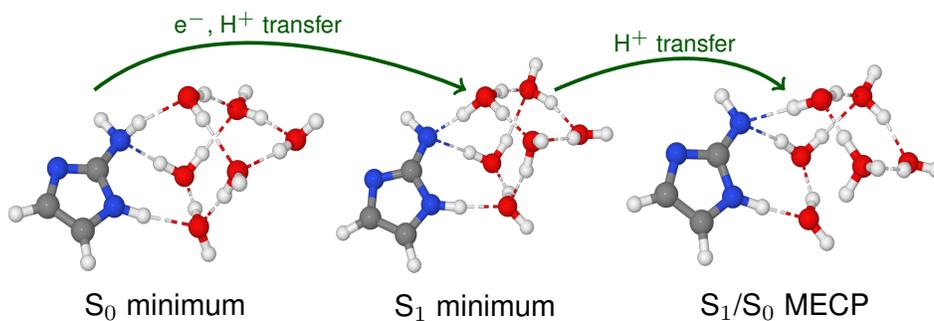


Fig. S1 The presented 2-AIM-(H₂O)₆ structures correspond to the ground-state and the S₁ ($\pi\sigma^*$) minimum-energy geometries, and the S₁/S₀ minimum-energy crossing point (MECP), respectively. The S₁ stationary point was reached after the N–H proton transfer towards the water cluster, indicating that the solvated electron is located far enough to observe a proton transfer in the cluster of six water molecules. The successive N–H proton transfer leads to the formation of $\pi\sigma^*/S_0$ conical intersection. All structures were obtained at the MP2/ADC(2)/aug-cc-pVDZ level.

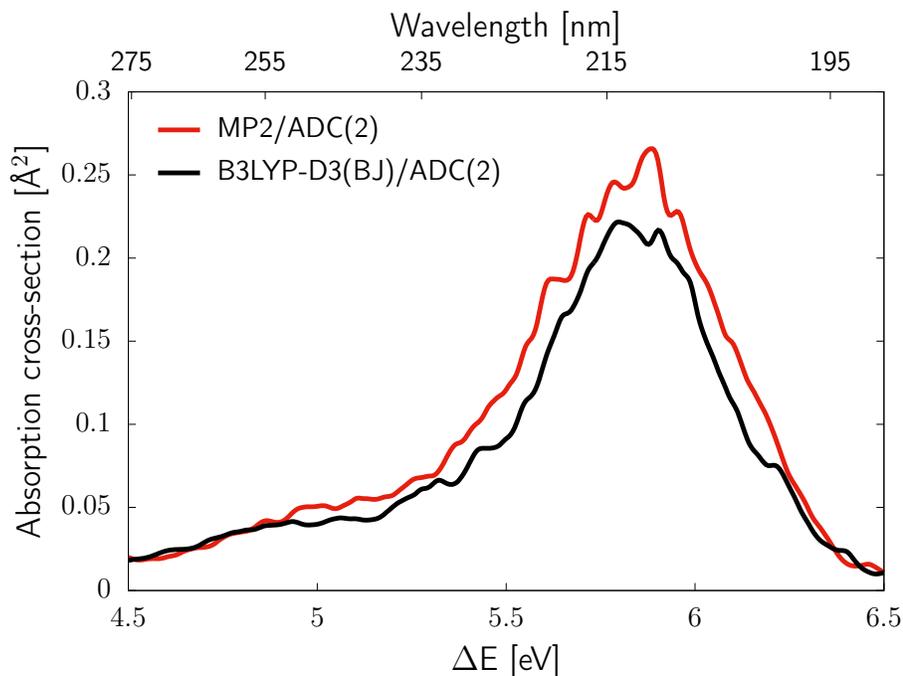


Fig. S2 The presented UV-absorption spectra of 2-AIM-(H₂O)₅ were simulated with nuclear ensemble method assuming the ground-state structures optimized using either the B3LYP-(D3)/def2-TZVPP or the MP2/aug-cc-pVDZ approach and utilizing the corresponding harmonic vibrational frequencies. The UV spectra were obtained using the same approach as the one described in Methodology section of the main article. The only exception is the number of points generated from a Wigner distribution for the MP2/aug-cc-pVDZ approach which was equal to 500. The presented UV spectra suggest that the ground-state minimum-energy structures obtained at the B3LYP-D3(BJ) and MP2 levels are consistent and without any significant discrepancies which could be important for non-adiabatic molecular dynamics simulations.

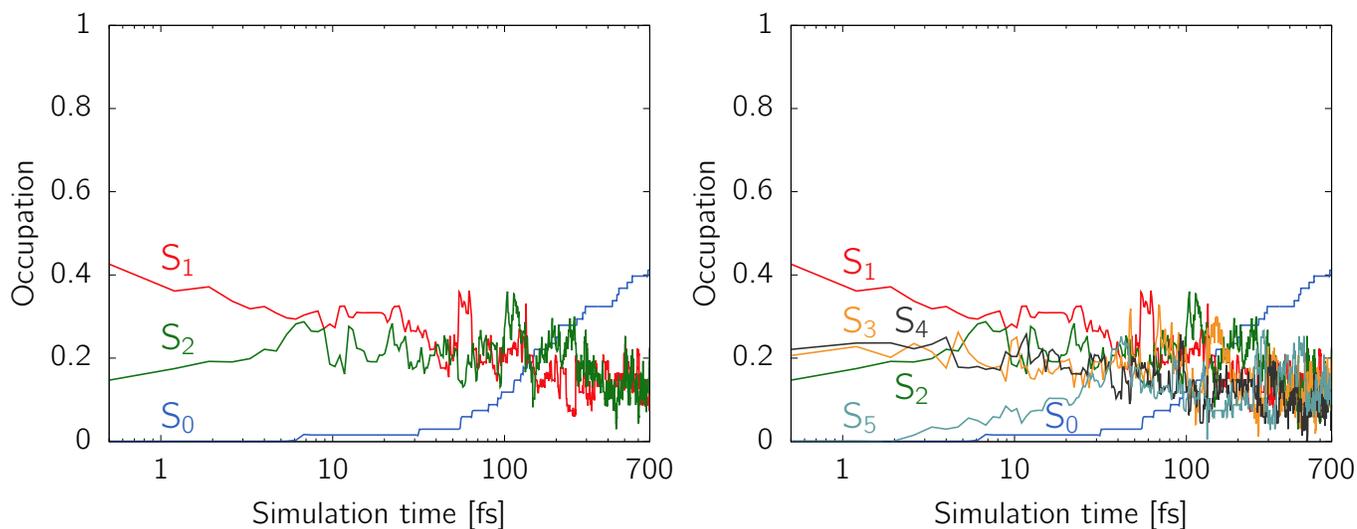


Fig. S3 Time evolution of the five lowest-lying excited states and the ground state populations of 2-AIM-(H₂O)₅ from the ADC(2) NAMD simulations.

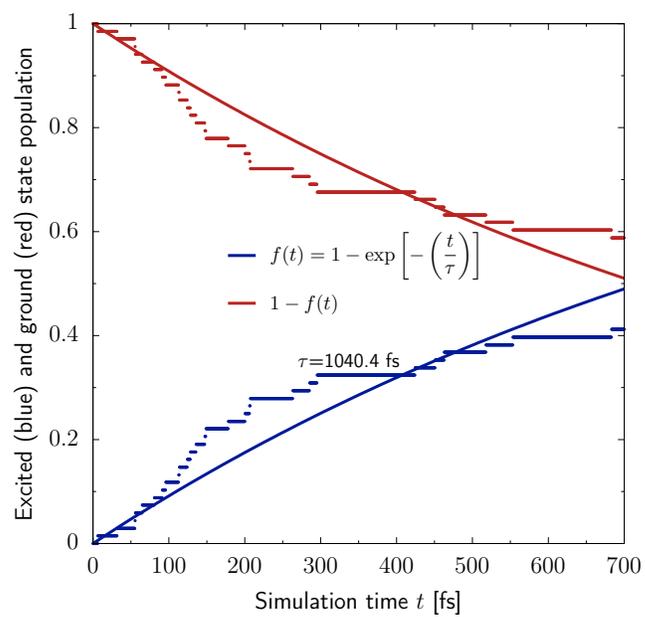


Fig. S4 Fitting of exponential function to either ground state or total excited states population.