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Supplementary Material

Direct *ab initio* molecular dynamics study on the reactions of multi-valence ionized states of water dimer

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Table S1. Optimized geometrical parameters of (H₂O)₂ and H₃O⁺(OH) calculated at the MP2/6-311++G(d,p) and CAM-B3LYP/6-311++G(d,p) levels of theory. Bond lengths are in Å.

		MP2	CAM-B3LYP
(H₂O)₂	ROO	2.914	2.863
	r1	1.950	1.897
	r2	0.966	0.969
	r3	0.959	0.959
H₃O⁺(OH)	ROO	2.493	2.488
	r1	1.050	1.060
	r2	1.447	1.433
	r3	0.976	0.982

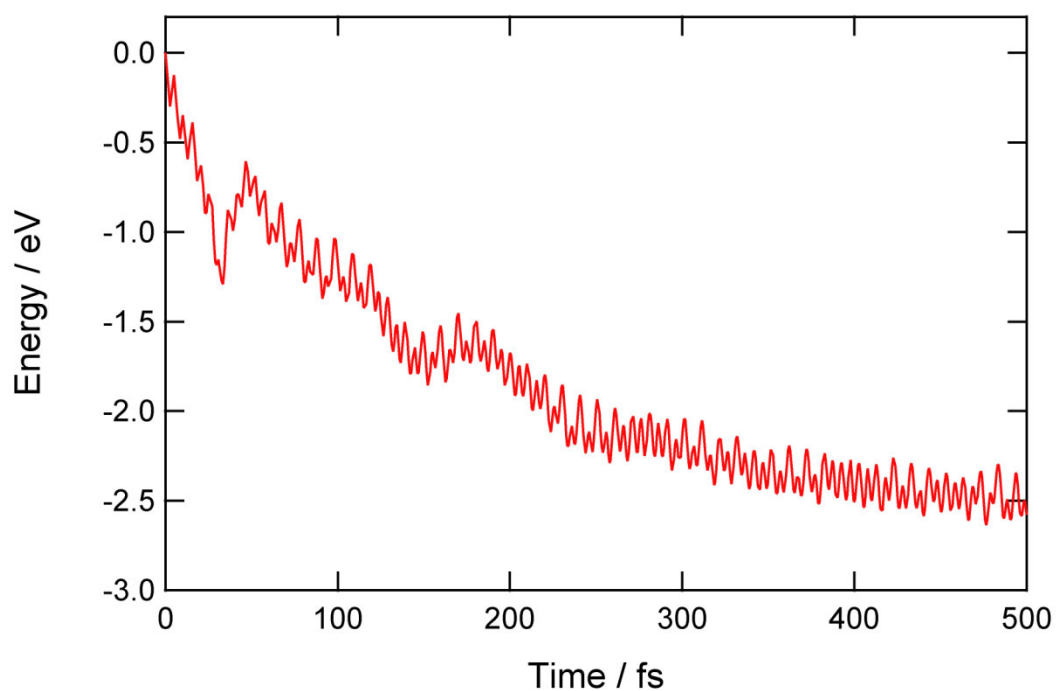


Figure S1. Potential energy curve of $(\text{H}_2\text{O})_2^{2+}$ (in eV) following the vertical two-electron ionization from neutral water dimer. Direct AIMD calculations were carried out at the CAM-B3LYP/6-311++G(d,p) level. The MP2/6-311++G(d,p) optimized structure of the neutral water dimer was chosen as the initial structure at time zero.

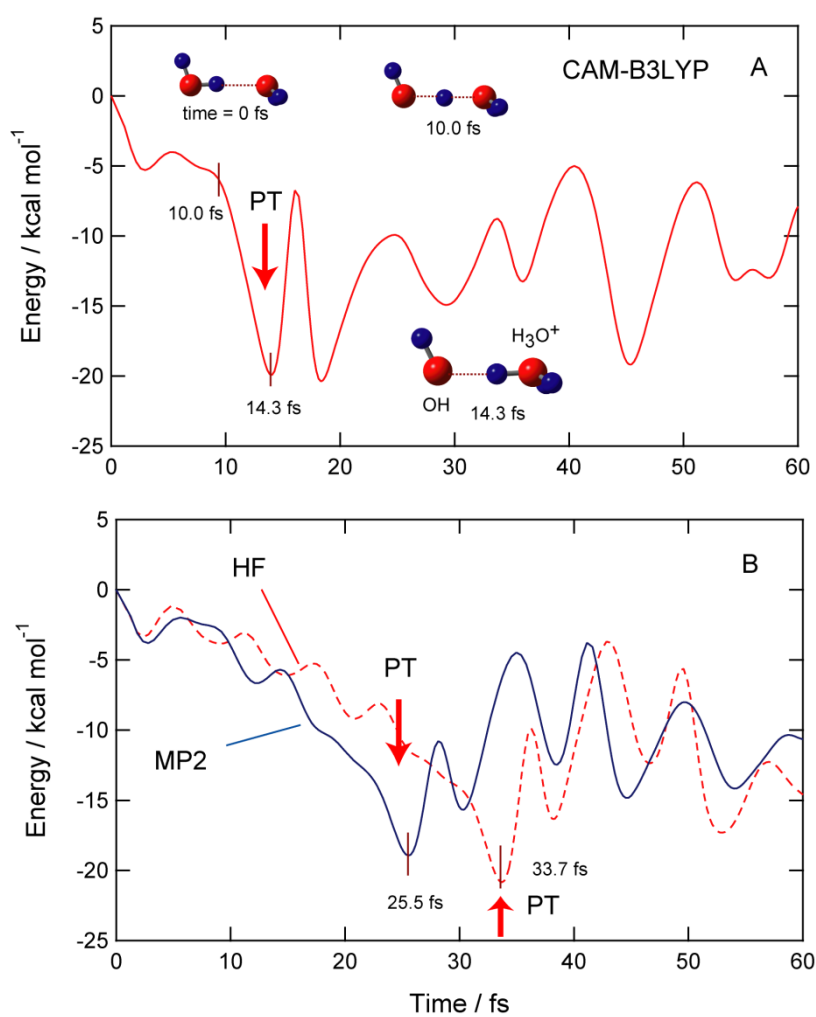


Figure S2. (A) Time evolution of potential energy and snapshots of (H₂O)₂⁺, following the single electron ionization of neutral water dimer, calculated at the CAM-B3LYP/6-311++G(d,p) level. (B) Time evolution of potential energies of (H₂O)₂⁺ calculated at the MP2 and HF(Hartree-Fock)/6-311++G(d,p) level.

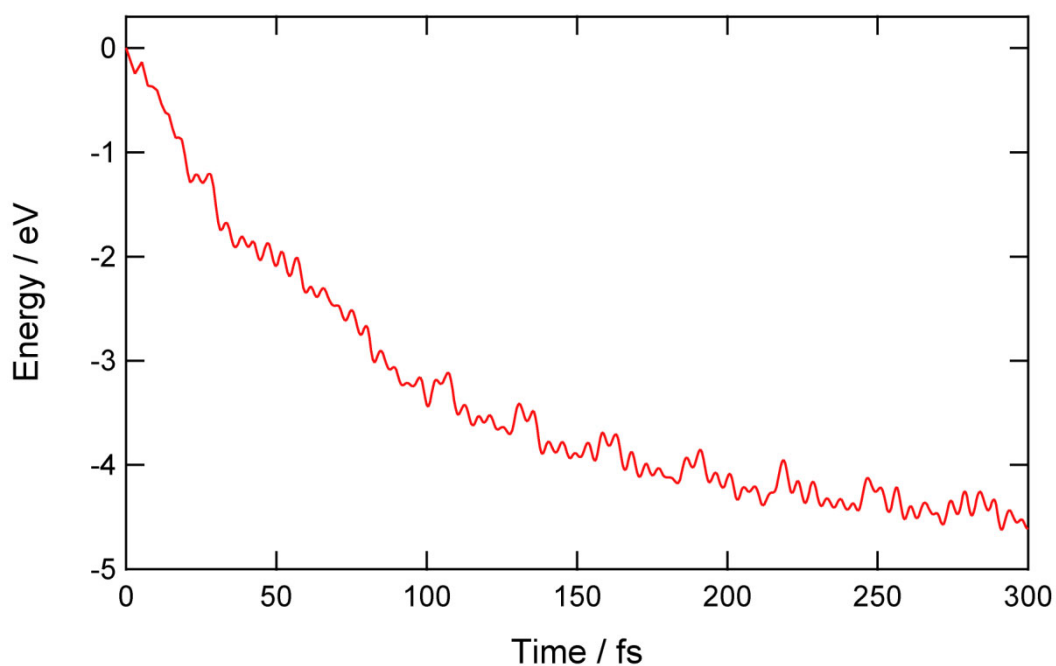


Figure S3. Potential energy curve of $(\text{H}_2\text{O})_2^{2+}$ (in eV) following the vertical one-electron ionization from proton-transferred radical-ion pair ($\text{H}_3\text{O}^+ \dots \text{OH}$). Direct AIMD calculations were carried out at the CAM-B3LYP/6-311++G(d,p) level. The MP2/6-311++G(d,p) optimized structure of $\text{H}_3\text{O}^+ \dots \text{OH}$ was chosen as initial structure at time zero.

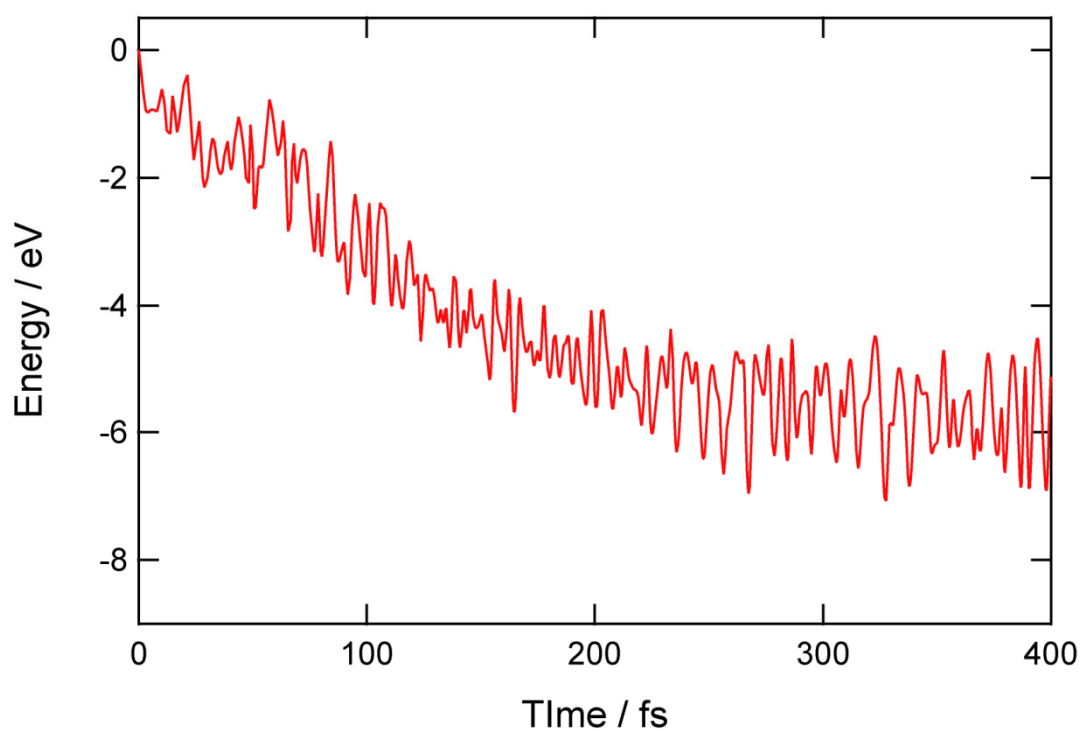


Figure S4. Potential energy curve (in eV) of $(\text{H}_2\text{O})_2^{2+*}$ at first excited state following the vertical two-electron ionization from neutral water dimer. Direct AIMD calculations were carried out at the CAM-B3LYP/6-311++G(d,p) level. The MP2/6-311++G(d,p) optimized structure of neutral water dimer was chosen as initial structure at time zero.