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Author(s)	Takada, Tomoya; Tachikawa, Hiroto
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Supplementary Material

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

Tomoya Takada[1] and Hiroto Tachikawa[2]

[1] Department of Applied Chemistry and Bioscience, Chitose Institute of Science and Technology, Chitose 066-8655, Japan

[2] Division of Applied Chemistry, Faculty of Engineering, Hokkaido University, Sapporo 060-8628, Japan

Corresponding Author: Tomoya Takada

E-mail: t-takada@photon.chitose.ac.jp

Table S1. Optimized geometrical parameters of $(H_2O)_2$ and $H_3O^+(OH)$ 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**
$(H_2O)_2$	ROO	2.914	2.863
	r1	1.950	1.897
	r2	0.966	0.969
	r3	0.959	0.959
$H_3O^+(OH)$	ROO	2.493	2.488
	r1	1.050	1.060
	r2	1.447	1.433
	r3	0.976	0.982

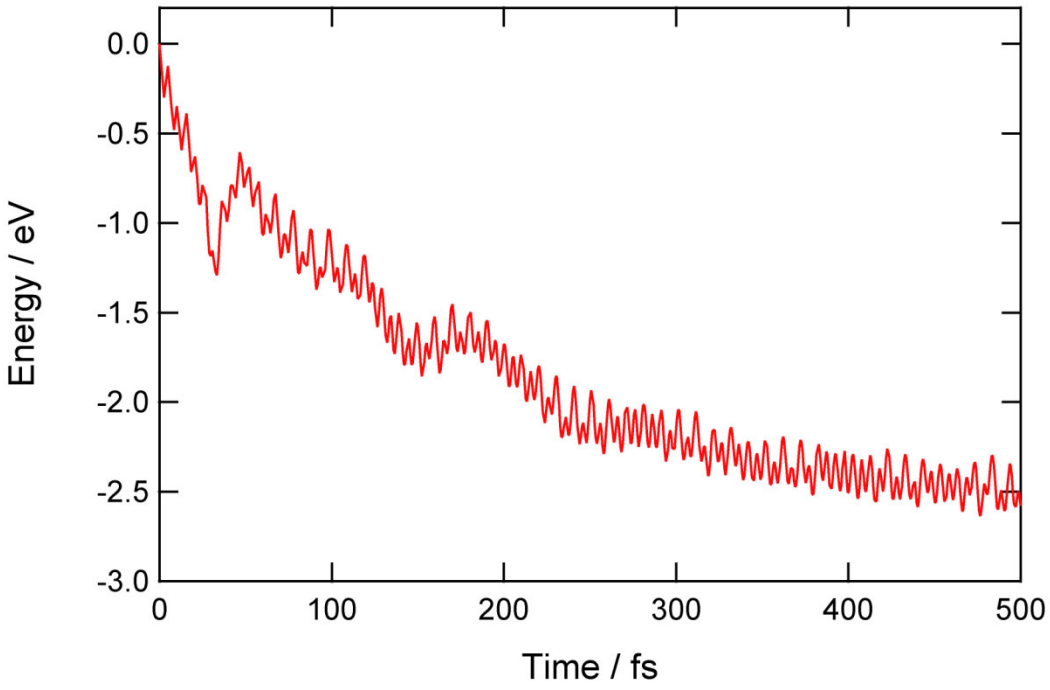

Figure S1. Potential energy curve of $(H_2O)_2^{2+}$ (in eV) following the vertical two-electron ionization from neutral water dimer. Direct AIMD calculations were carried out at the CAM-B3LYP/6-311++G(d,p) level. The MP2/6-311++G(d,p) optimized structure of the neutral water dimer was chosen as the initial structure at time zero.

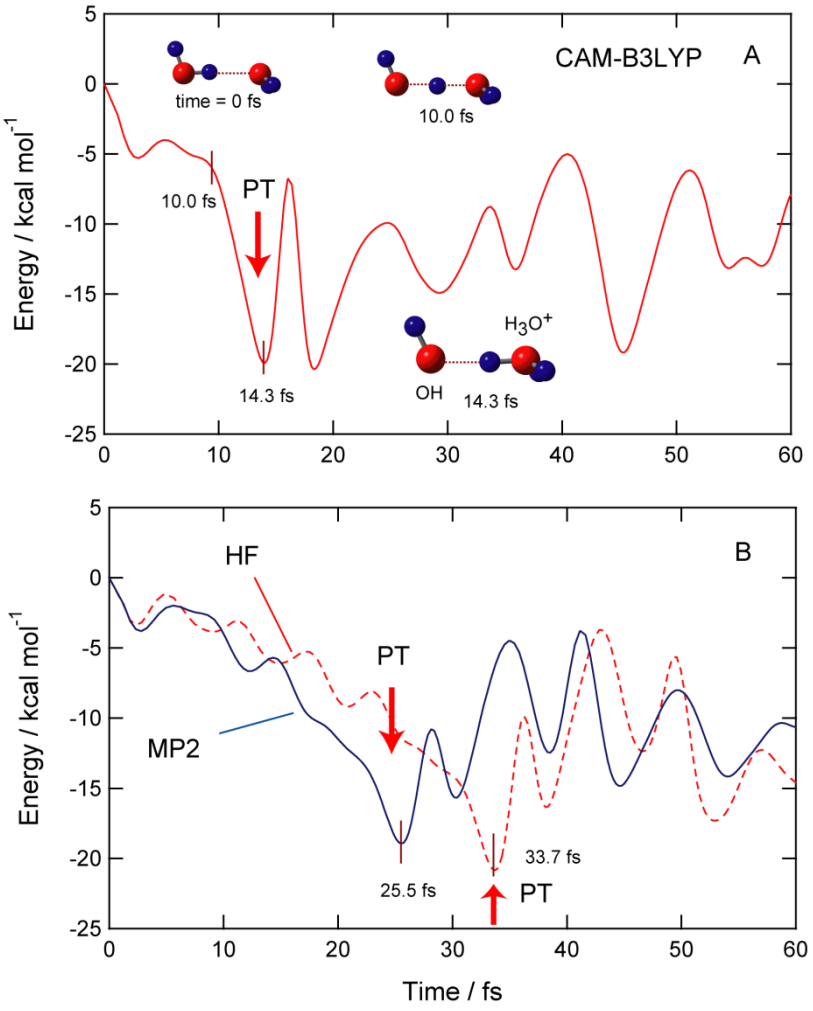

Figure S2. (A) Time evolution of potential energy and snapshots of $(H_2O)_2^+$, following the single electron ionization of neutral water dimer, calculated at the CAM-B3LYP/6-311++G(d,p) level. (B) Time evolution of potential energies of $(H_2O)_2^+$ calculated at the MP2 and HF(Hartree-Fock)/6-311++G(d,p) level.

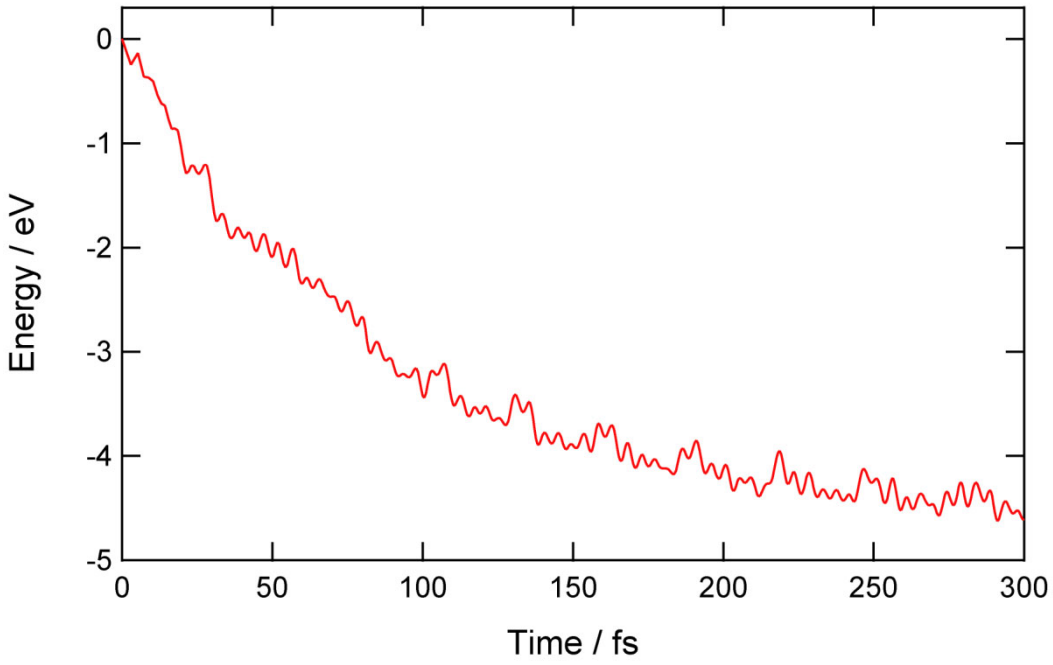

Figure S3. Potential energy curve of $(H_2O)_2^{2+}$ (in eV) following the vertical one-electron ionization from proton-transferred radical-ion pair (H_3O^+...OH). Direct AIMD calculations were carried out at the CAM-B3LYP/6-311++G(d,p) level. The MP2/6-311++G(d,p) optimized structure of H_3O^+...OH was chosen as initial structure at time zero.

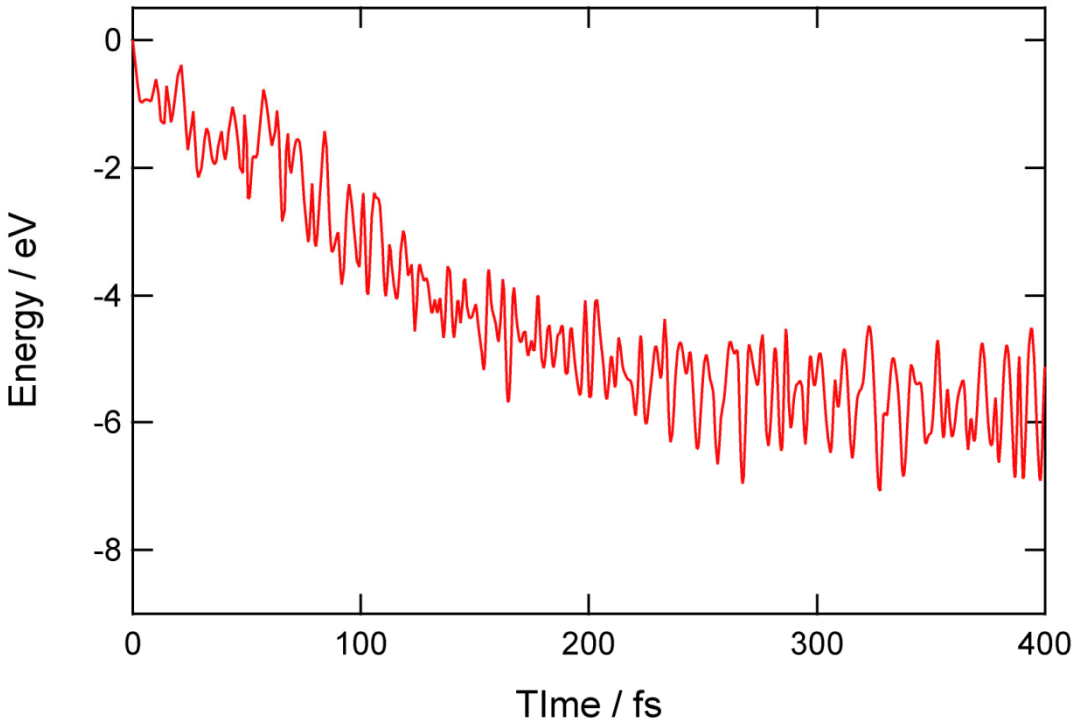

Figure S4. Potential energy curve (in eV) of $(H_2O)_2^{2+*}$ at first excited state following the vertical two-electron ionization from neutral water dimer. Direct AIMD calculations were carried out at the CAM-B3LYP/6-311++G(d,p) level. The MP2/6-311++G(d,p) optimized structure of neutral water dimer was chosen as initial structure at time zero.