Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

SUPPORTING INFORMATION

Ionization Dynamics of Water Dimer : Specific Reaction Selectivity

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1. Ionization dynamics of $(H_2O)_2$: total, potential and kinetic energies.

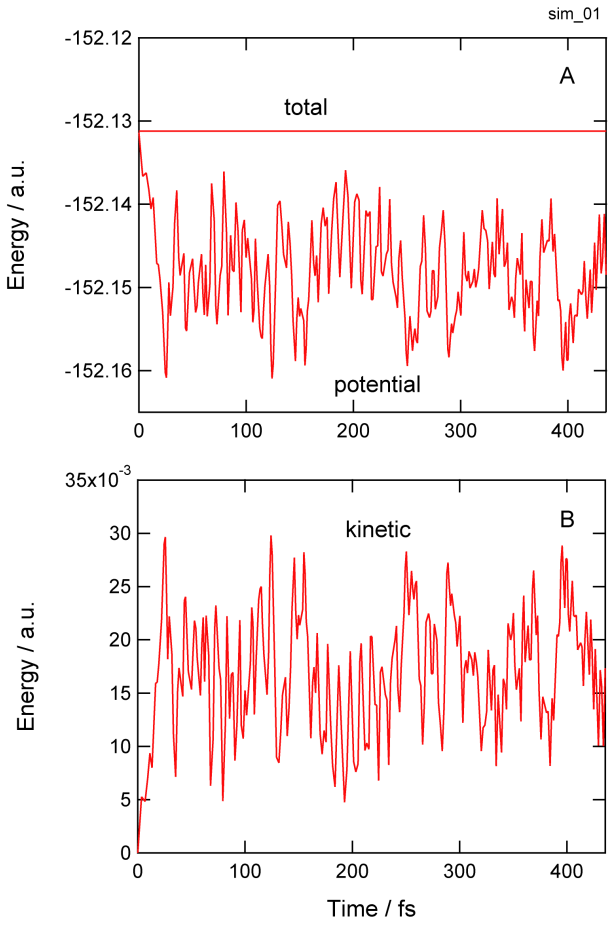

Figure S1. Time propagation of total, potential, and kinetic energies of the ionization reaction of water dimer obtained by direct ab-initio MD calculation. Total energy is expressed by summation of potential and kinetics energies. The total energy is constant

during simulation.

2. Optimized Structure of $(H_2O)_2$

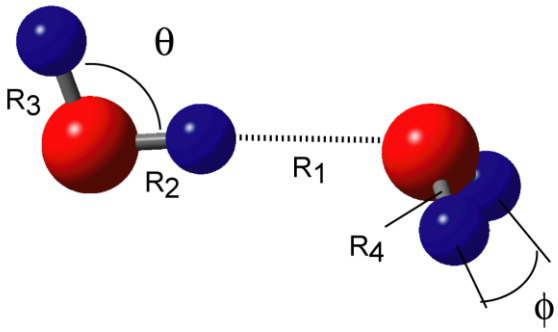

Figure S2. Optimized structure and definition of geometrical parameters of water dimer system.

Table S1. Optimized geometrical parameters of water dimer calculated several methods with a 6-311++G(d,p) basis set. Bond lengths and angles are in A and in degrees, respectively.

parameter	M2	MP4SDQ	QCISD	CCSD
R(O-O)[a]	2.914	2.936	2.938	2.938
R1	1.95	1.975	1.977	1.977
R2	0.966	0.963	0.963	0.963
R3	0.959	0.958	0.957	0.957
R4	0.961	0.959	0.96	0.959
q	103.5	103.7	103.8	103.8
f	104	104.2	104.2	104.2

[a] Experimetal value of R(O-O) is 2.976 A [Odutola, J.A.; Dyke, T.R., J. Chem. Phys., **1980**, 72, 5062].

3. Energy diagram of ionization of water dimer

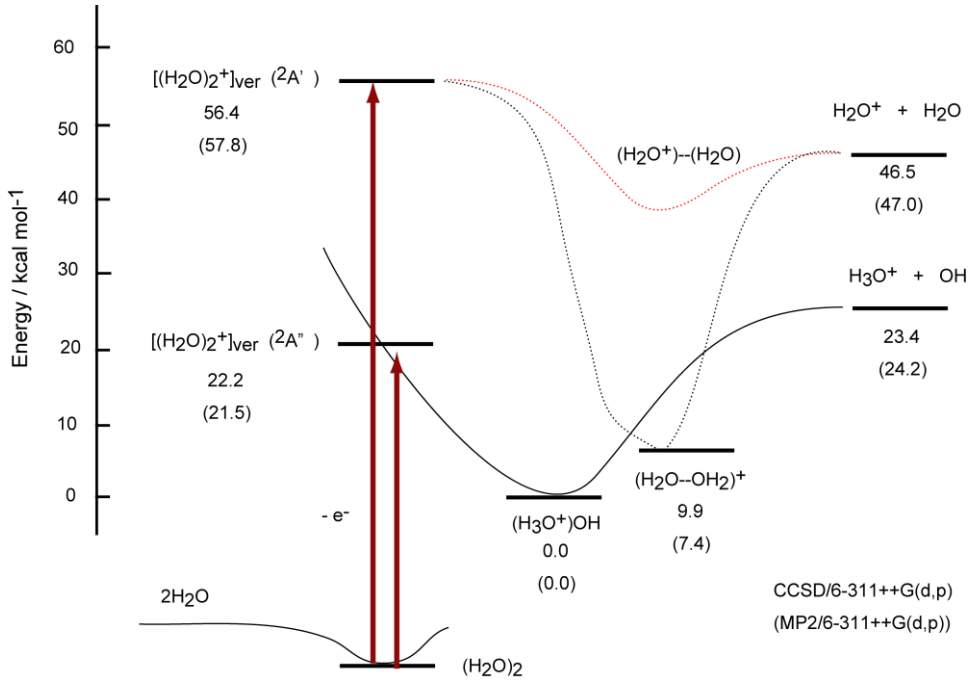

Figure S3. Energy diagram of ionization of water dimer. The values were calculated at the CCSD/6-311++G(d,p)//CCSD/6-311++G(d,p) level (in kcal/mol). The M2/6-311++G(d,p) values are given in parenthesis (in kcal/mol).

4. Initial configuration dependence on the dynamics

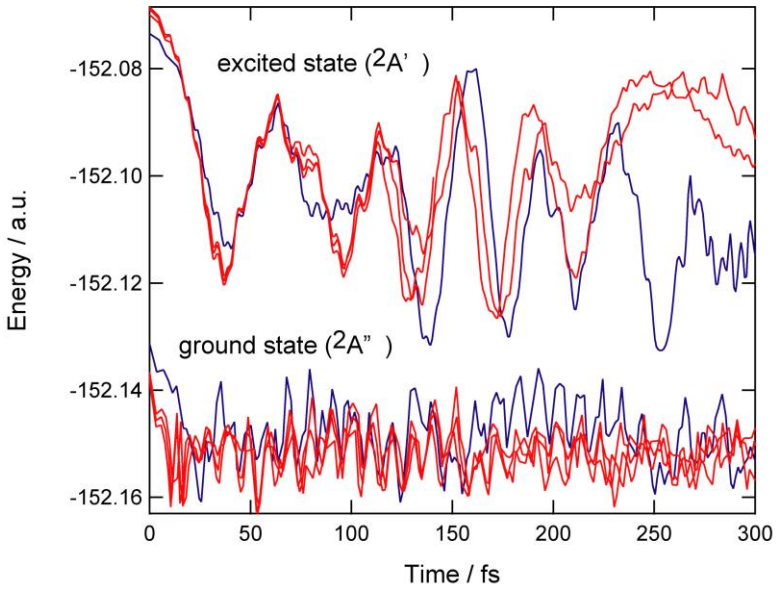

Figure S4. Dependence of initial configuration in the ionization dynamics.

5. Direct ab-initio MD calculation of $(H_2O)_2$ with zero point energy.

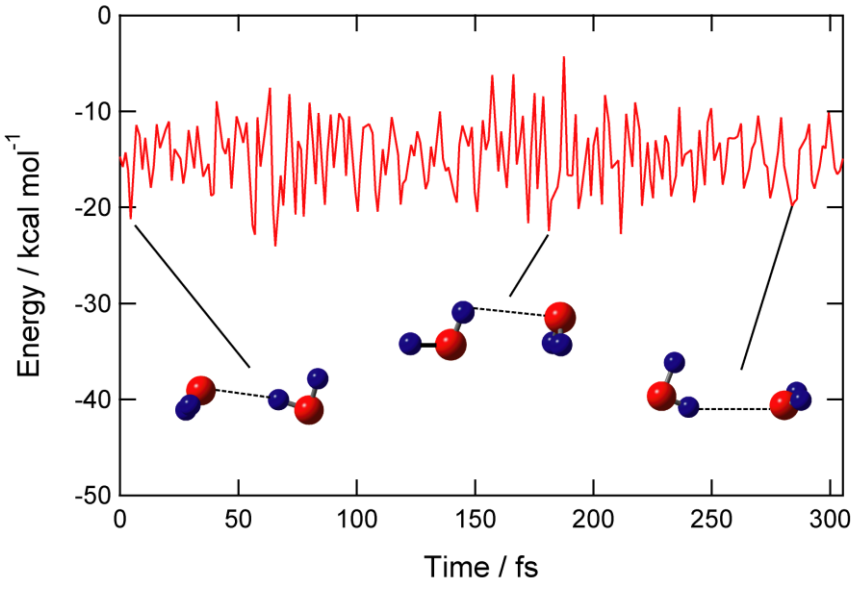

Figure S5. Potential energy of water dimer $(H_2O)_2$ with zero point energy (ZPE) obtained by direct ab-initio MD calculation at the MP2/6-311++G(d,p) level.