SUPPORTING INFORMATION

Electron Detachment Dynamics of $O_2^-(H_2O)$:

Direct Ab initio Molecular Dynamics (AIMD) Approach

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1. Electron detachment dynamics of $O_2^-(H_2O)$ with C$_{2v}$ symmetry.

**Figure S1.** Electron detachment dynamics of $O_2^-(H_2O)$ with C$_{2v}$ on *triplet* and *singlet* potential energy surfaces. The values indicate intermolecular distances (in Å). Dynamics calculation were carried out at the MP2/6-311++G(d,p) level. The trajectory was started from the optimized geometry of $O_2^-(H_2O)$ with C$_{2v}$ structure.
**Figure S2.** Time evolutions of potential energies of $\text{O}_2(\text{H}_2\text{O})$ on singlet and triplet state PESs.
2. Effects of initial structures on the reaction dynamics.

*Figure 3.* Effects of initial configurations on the time evolutions of potential energies of $\text{O}_2(\text{H}_2\text{O})$ on singlet state PES.