Supporting Information for

Kinetic Study of the OH + HO_2 → H_2O + O_2 Reaction using Ring Polymer Molecular Dynamics and Quantum Dynamics

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To get proper overlap between neighboring windows, suitable force constant k_{ufc} and interval should be selected in the umbrella sampling. In the asymptotic and product regions, the neighboring windows overlap well by choosing k_{ufc} as 2.72 (T/K) eV. However, the overlap is not sufficiently large in the region near the barrier when the same k_{ufc} = 2.72 (T/K) eV is used, especially at low temperatures. Consequently, larger k_{ufc} and smaller interval are used to make the overlap sufficiently large.

At T = 300 K, in the asymptotic region ($\xi \in$ [-0.05, 0.97]) and the product region ($\xi \in$ [0.99, 1.1]), the intervals are both 0.01 and the force constants are chosen to be 2.72 and 4.08 (T/K) eV, respectively. However, in the region near the barrier (ξ = 0.98 and 0.985), the force constants are selected to be 5.44 (T/K) eV. At T = 400, 500, 1000 and 1300 K, the intervals are 0.01 for the whole region, but different force constants are used for different regions. At T = 400 K, the force constant of 2.72 (T/K) eV is used in the region ($\xi \in$ [-0.05, 0.97]). For the region near the barrier (ξ = 0.99), k_{ufc} = 4.08 (T/K) eV. But, in the product region, the force constants are 4.90 and 4.08 (T/K) eV at $\xi \in$ [1.00, 1.03] and [1.03, 1.10], respectively. At T = 500 K, the force constant is 2.72 (T/K) eV for $\xi \in$ [-0.05, 0.98] and [1.04, 1.1]. While in the rest region ($\xi \in$ [0.99, 1.03]), larger k_{ufc} (1.2 ~ 1.8 times) values are used. At T = 1000 K, for $\xi \in$ [-0.05, 0.99] and [1.03, 1.1], the force constant is 2.72 (T/K) eV. While in the rest region, it becomes lager (3.26 (T/K) eV at ξ = 1.00 and 1.02 and 4.08 (T/K) eV at ξ = 1.01). For T = 1300 K, k_{ufc} = 2.72 (T/K) eV is used for the whole region ($\xi \in$[-0.05, 1.1]).

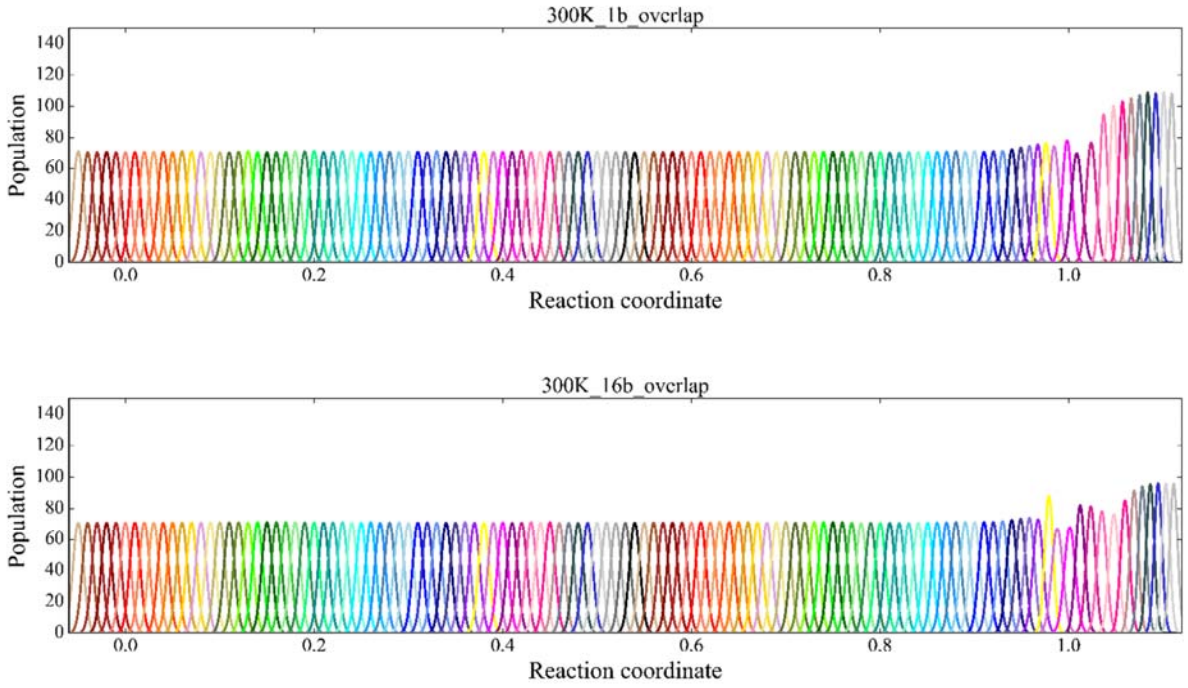

Figure S1. The overlaps between windows with different numbers of beads for the OH + HO_2 → H_2O + O_2 at 300 K.

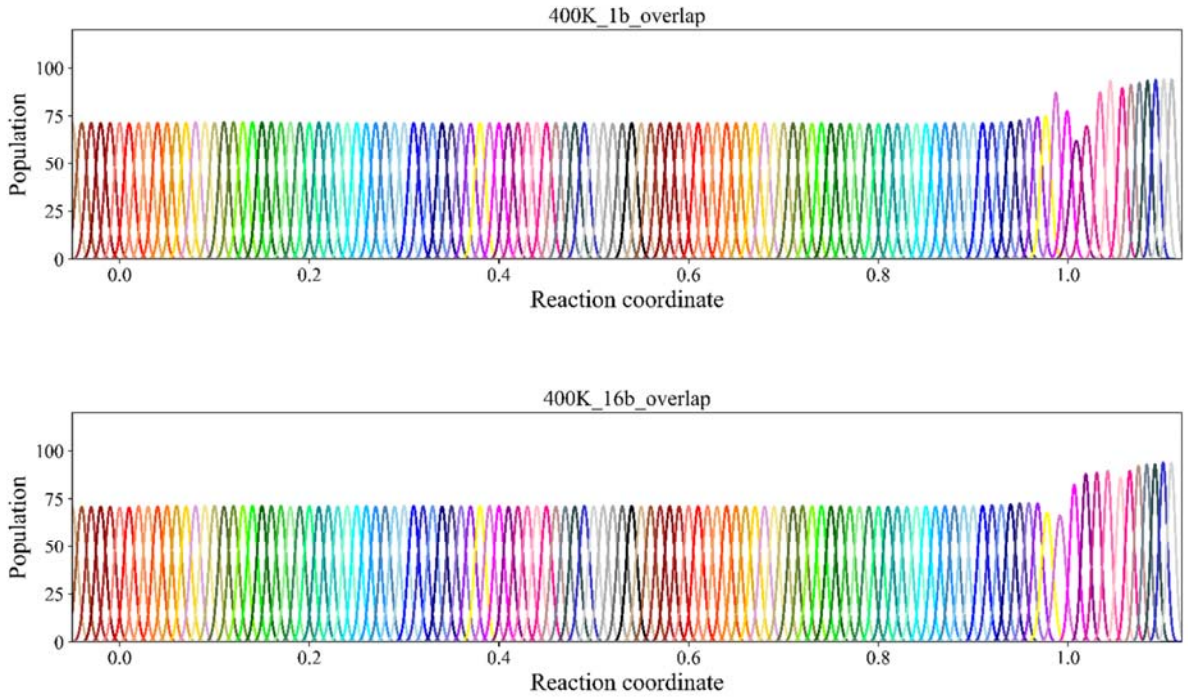

Figure S2. The overlaps between windows with different numbers of beads for the OH + HO_2 → H_2O + O_2 at 400 K.

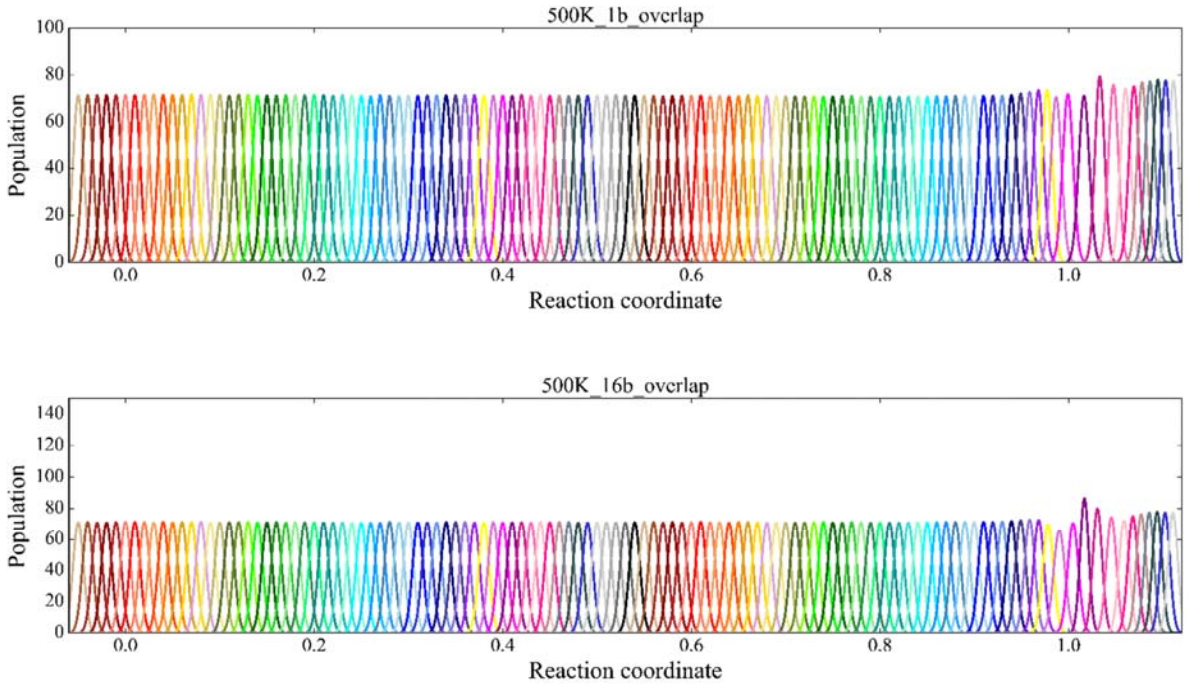

Figure S3. The overlaps between windows with different numbers of beads for the OH + HO_2 → H_2O + O_2 at 500 K.

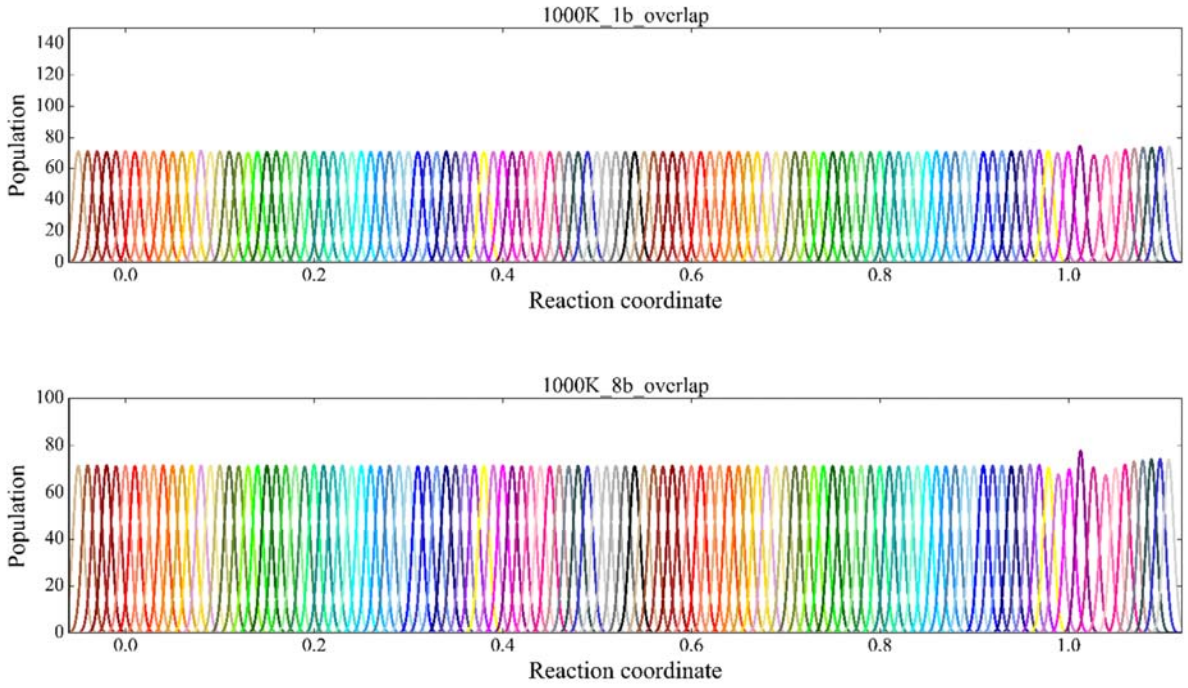

Figure S4. The overlaps between windows with different numbers of beads for the OH + HO_2 → H_2O + O_2 at 1000 K.

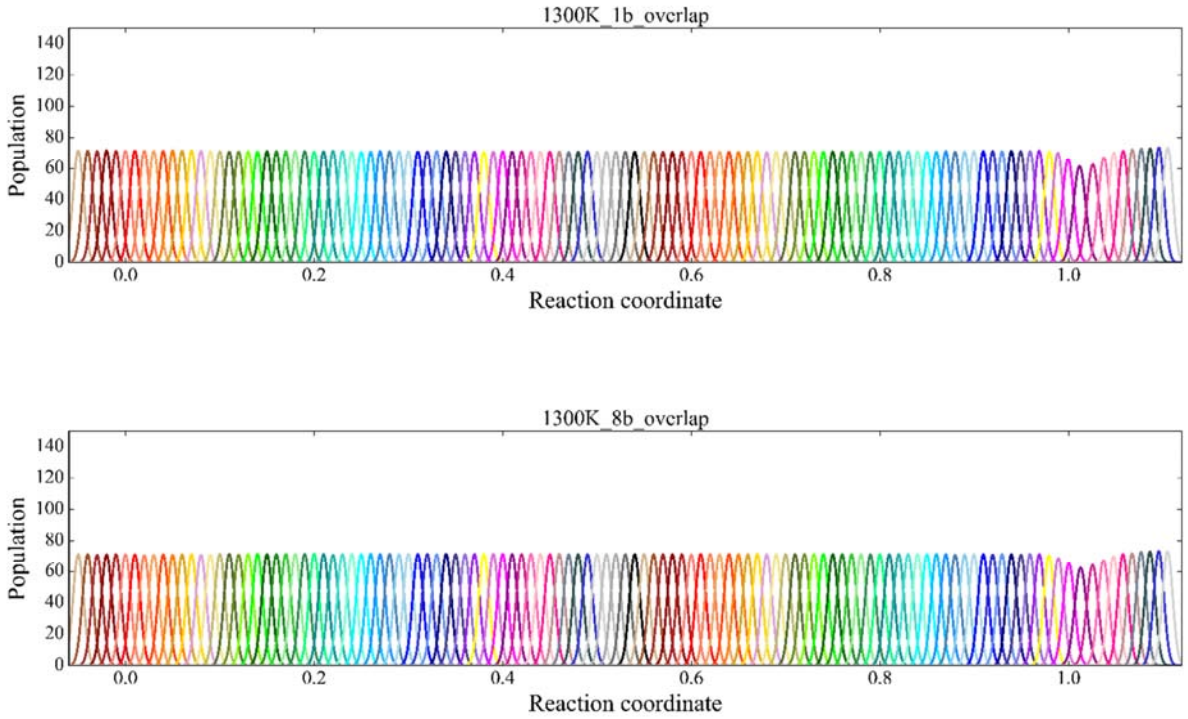

Figure S5. The overlaps between windows with different numbers of beads for the OH + HO_2 → H_2O + O_2 at 1300 K.

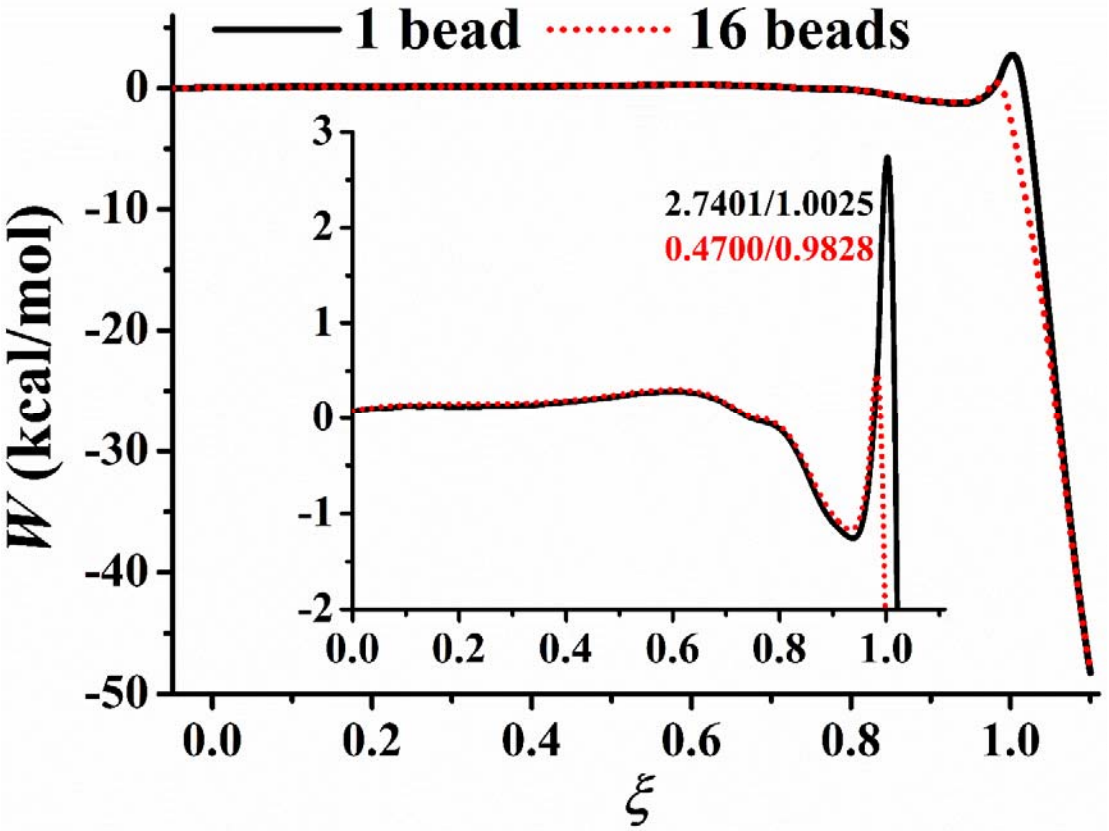

Figure S6. Potential of mean force (PMF, in kcal mol^{-1}, relative to the reactant asymptote OH + HO_2) along the reaction coordinate at T = 300 K.

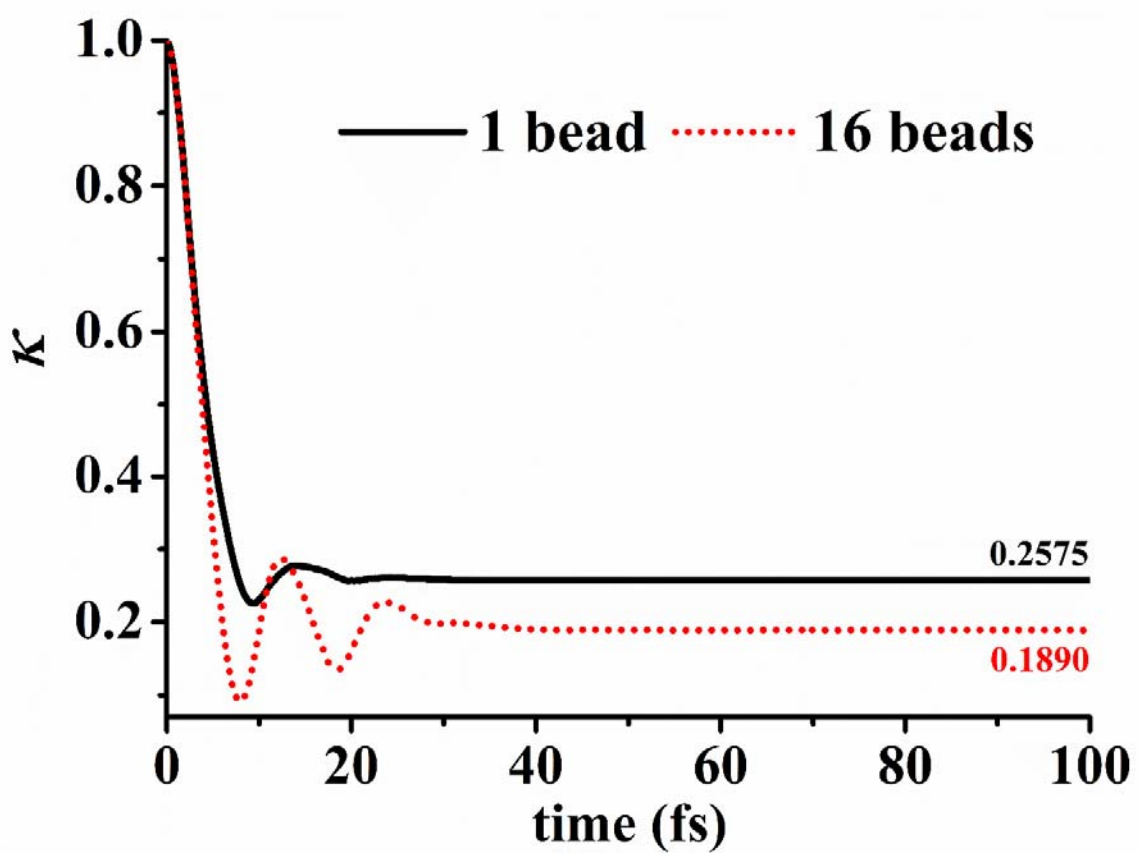

Figure S7. Transmission coefficients at 300 K.