

Submitted to PCCP, October/19/2019, revised, November/22/2019

**An Accurate Potential Energy Surface and Ring Polymer Molecular
Dynamics Study of the $\text{Cl} + \text{CH}_4 \rightarrow \text{HCl} + \text{CH}_3$ Reaction**

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Supporting Information

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Figure S1. Tests on the time steps, 0.1 or 0.3 fs, used in the PMF, $W(\xi)$, and the transmission coefficient, $\kappa(t)$, for Cl + CH₄ at $T = 400$ K with 32 beads. The numbers of the “childTrajectories” were also tested for Cl + CH₄ at $T = 1000$ K with 1 bead. In the current work, the time step was set as 0.3 fs and the number of “childTrajectories” was set as 100000.

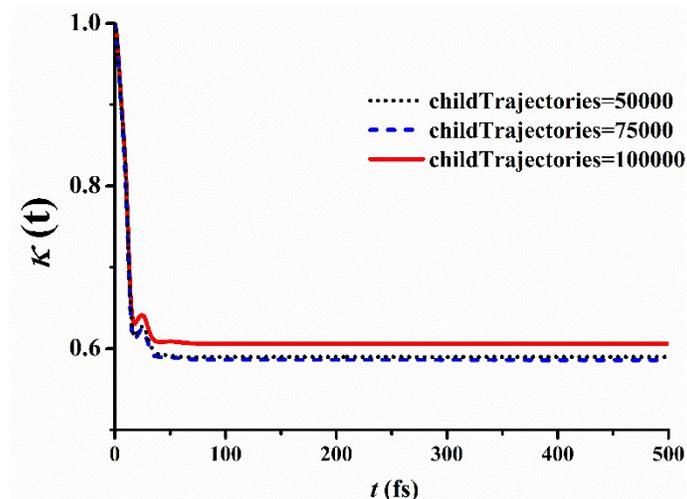
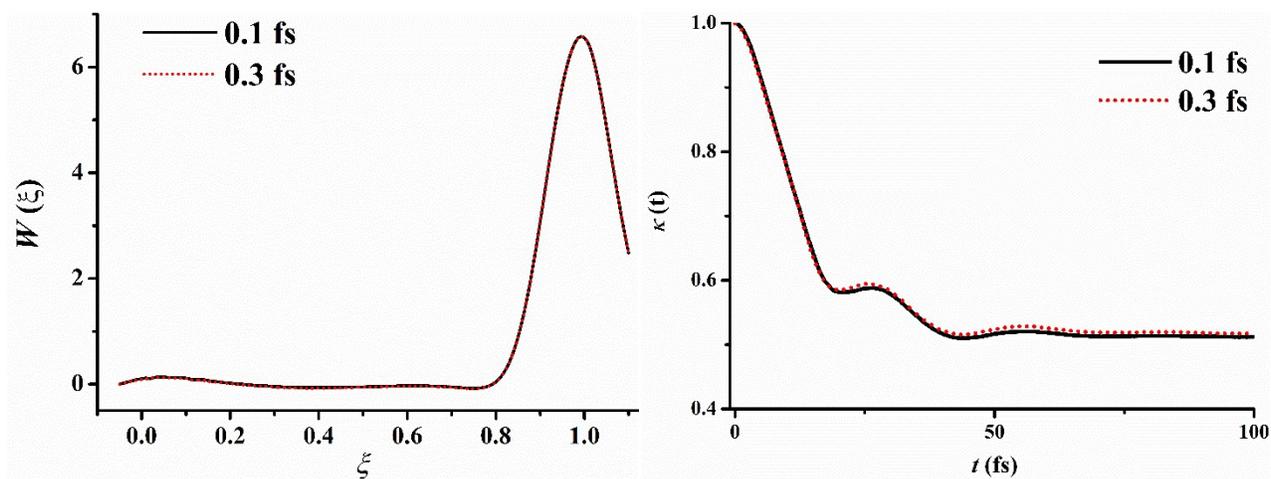


Figure S2. PMFs, transmission coefficients, and the overlaps between windows with different numbers of beads for Cl + CH₄ at $T = 200$ K. If the overlaps are not sufficiently large, the errors might be increased.

The overlaps can be adjusted by the force constants and the intervals.

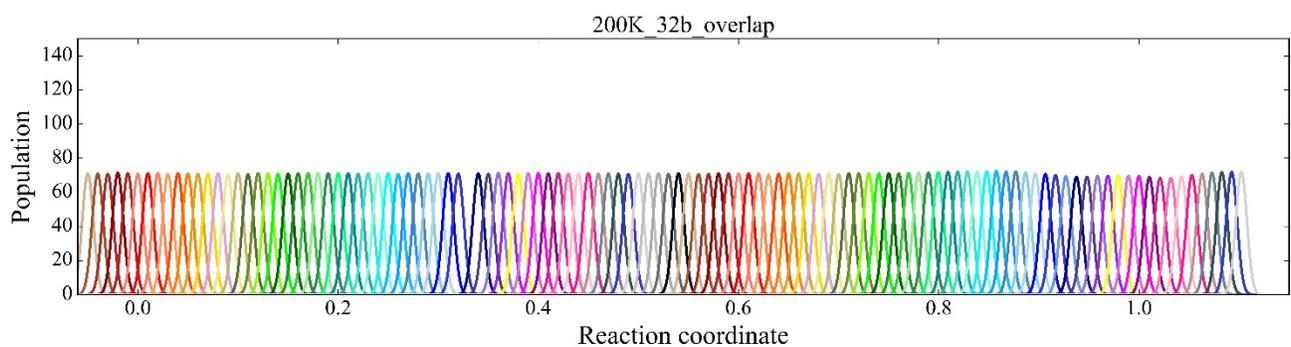
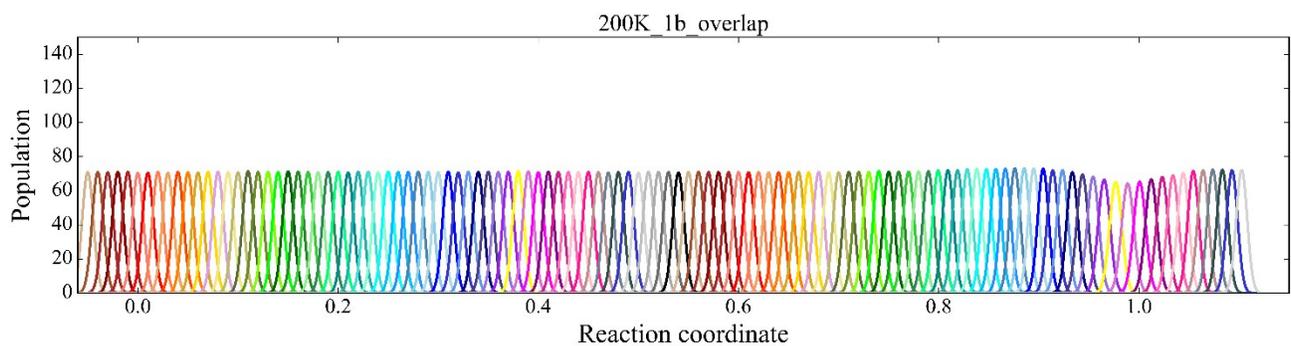
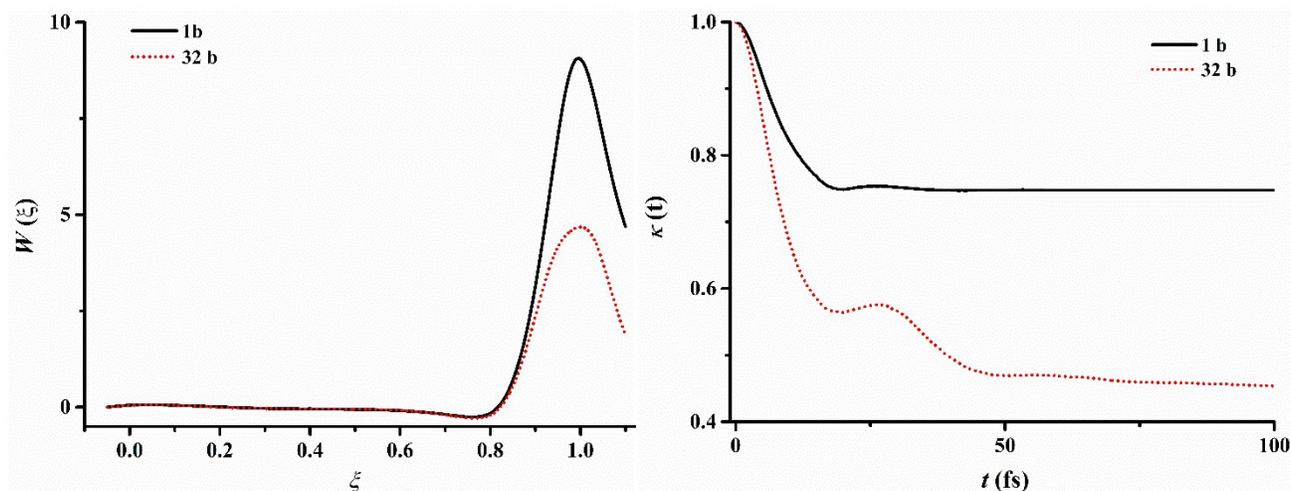


Figure S3. PMFs, transmission coefficients, and the overlaps between intervals with different numbers of beads for Cl + CH₄ at $T = 300$ K.

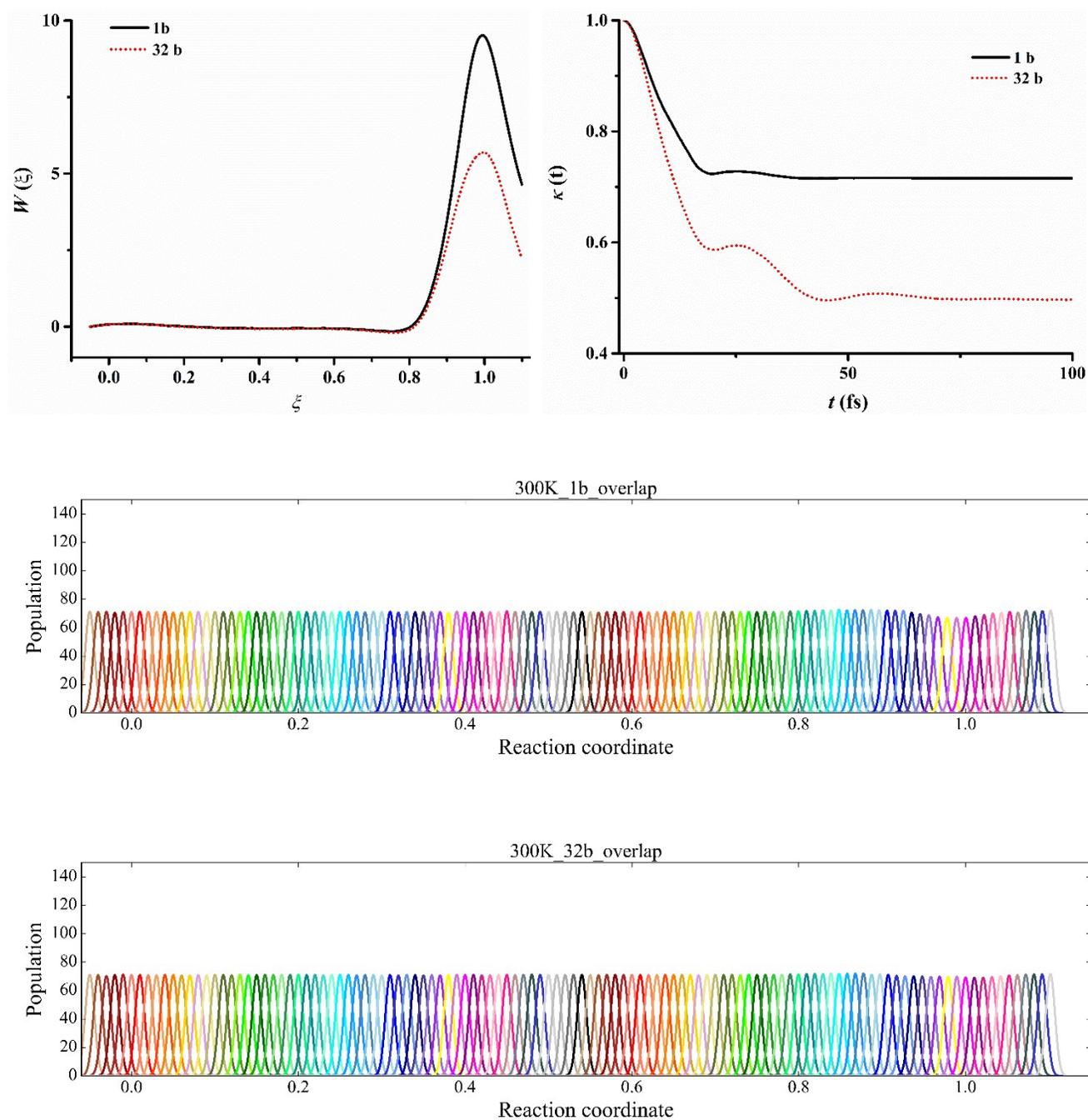


Figure S4. PMFs, transmission coefficients, and the overlaps between intervals with different numbers of beads for Cl + CH₄ at $T = 400$ K.

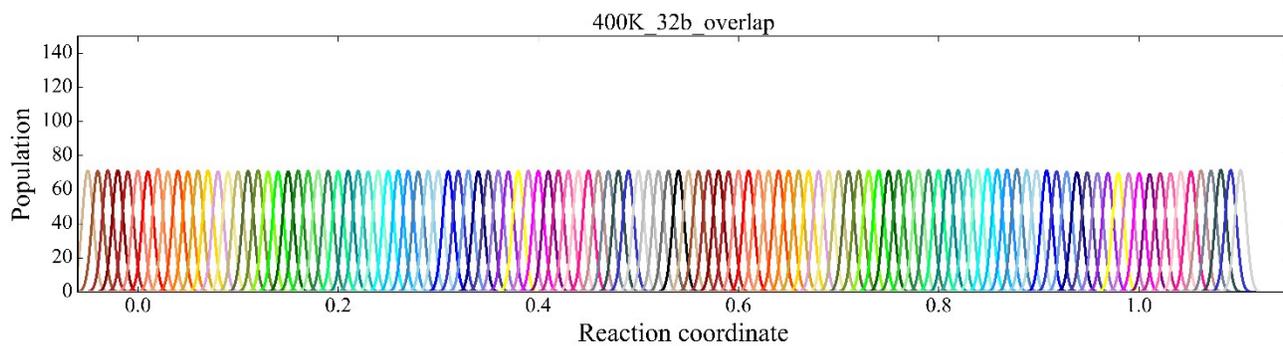
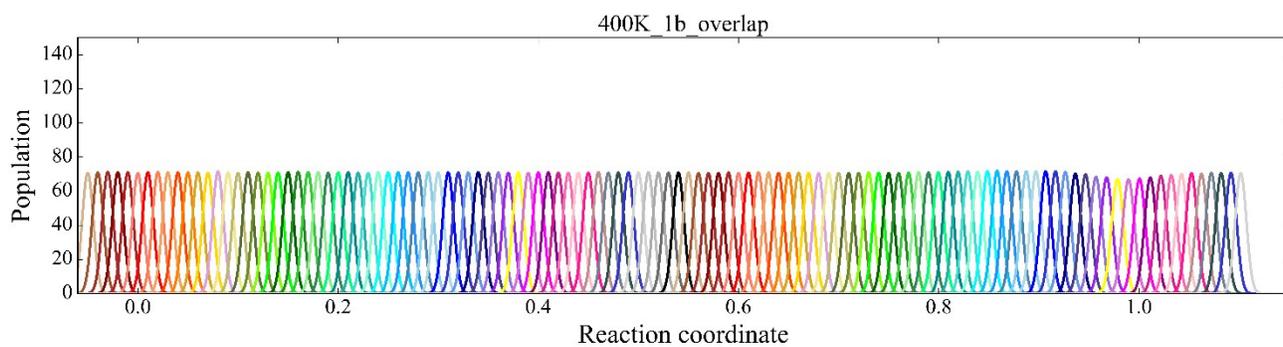
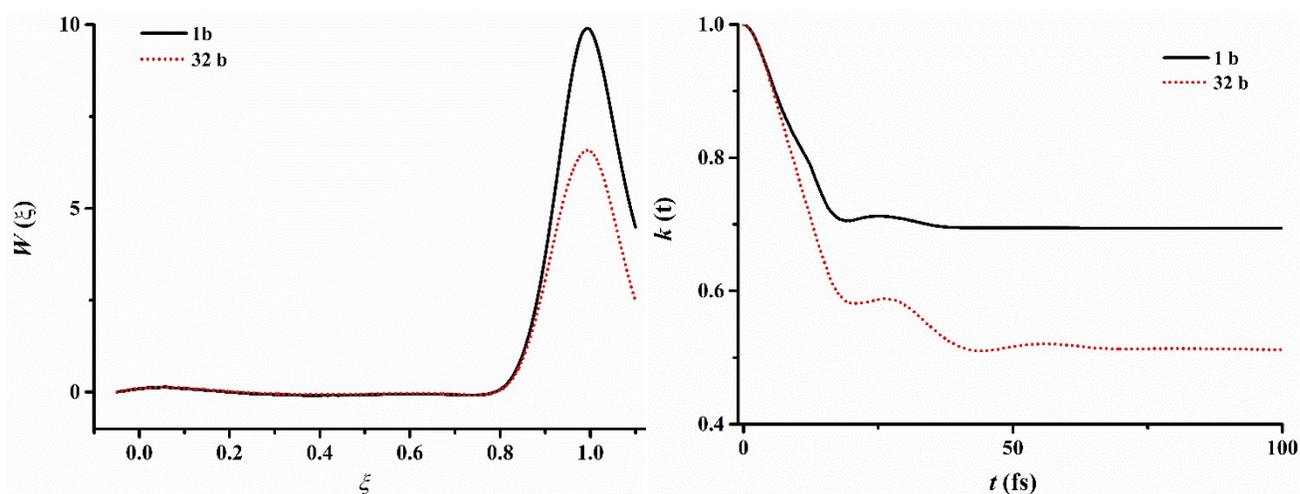


Figure S5. PMFs, transmission coefficients, and the overlaps between intervals with different numbers of beads for Cl + CH₄ at $T = 600$ K.

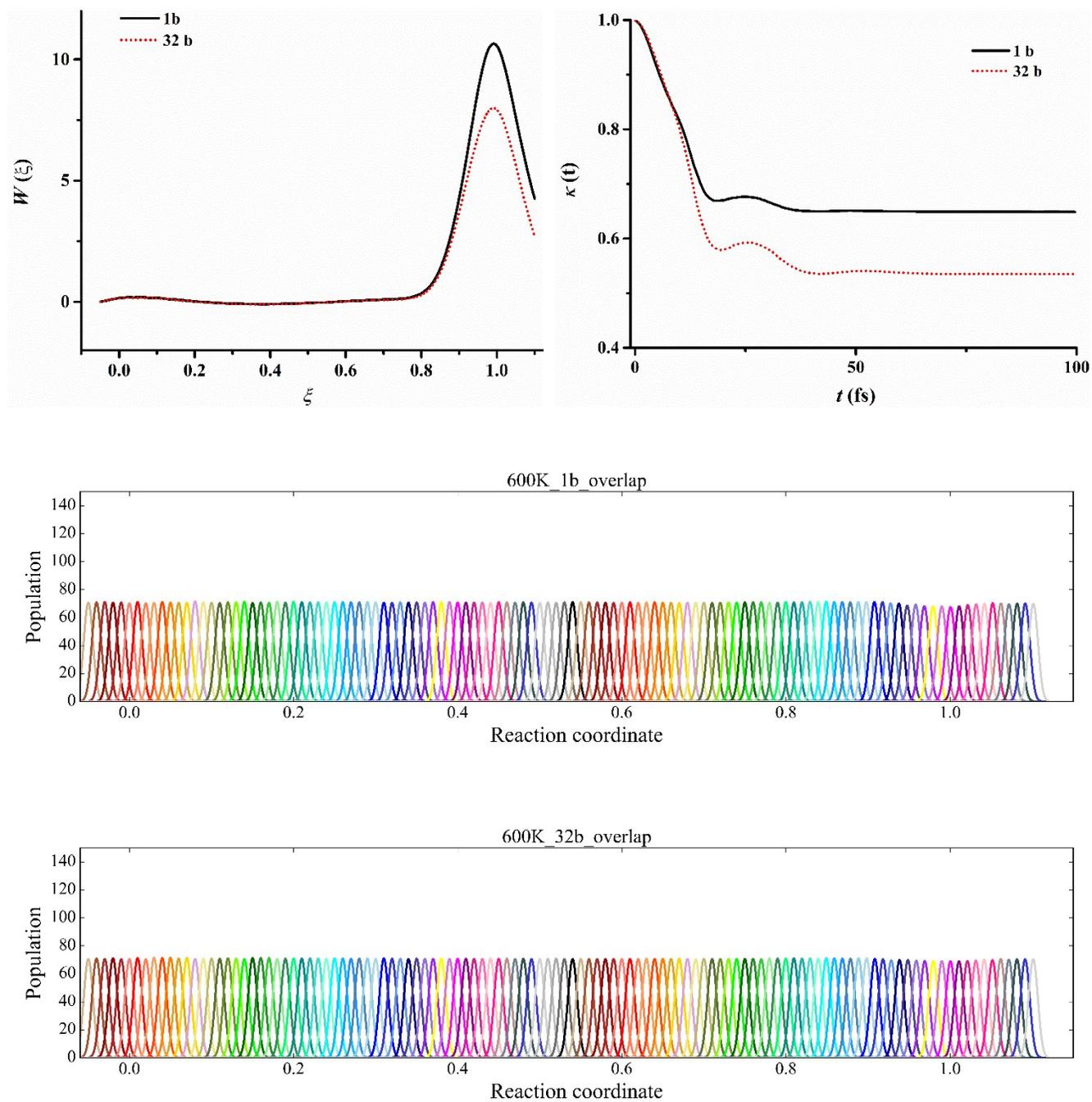


Figure S6. PMFs, transmission coefficients, and the overlaps between intervals with different numbers of beads for Cl + CH₄ at $T = 800$ K.

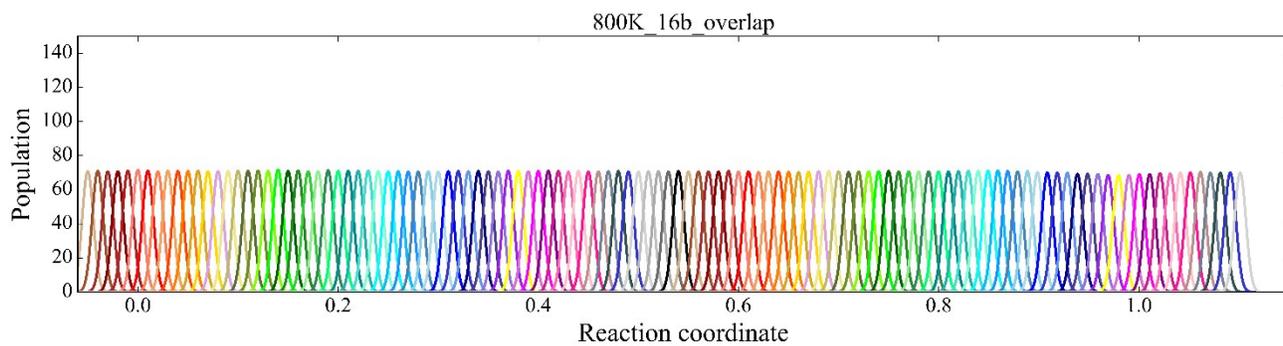
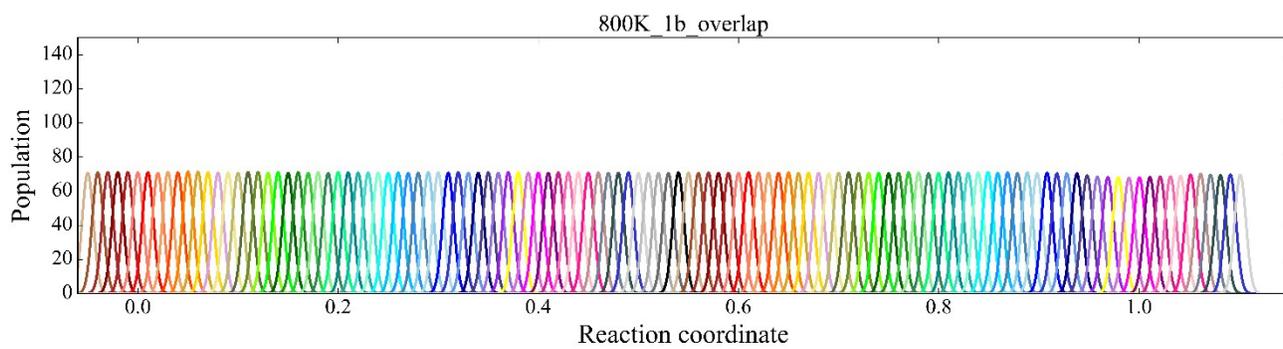
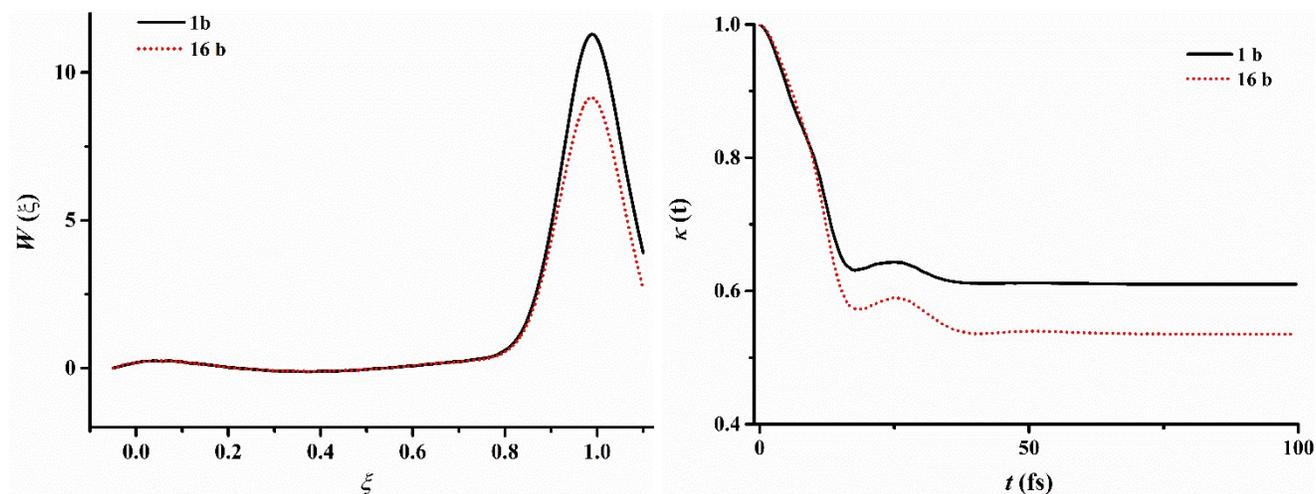


Figure S7. PMFs, transmission coefficients, and the overlaps between intervals with different numbers of beads for Cl + CH₄ at $T = 1000$ K.

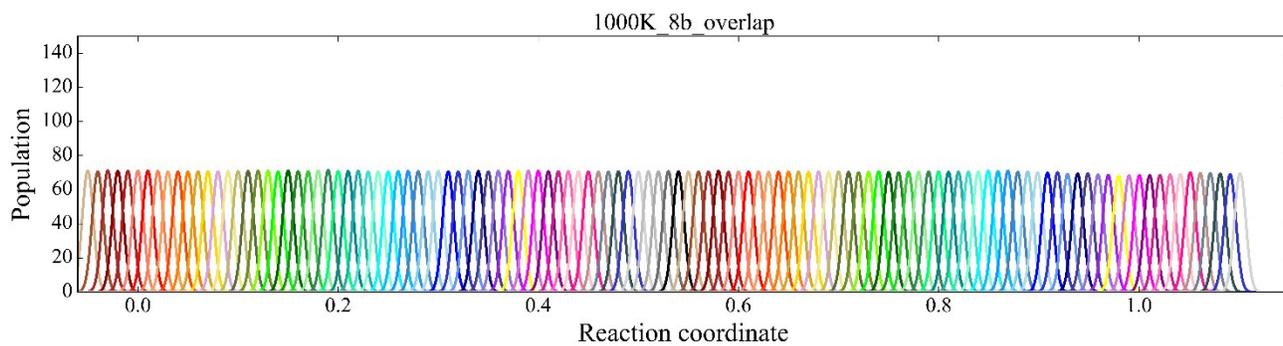
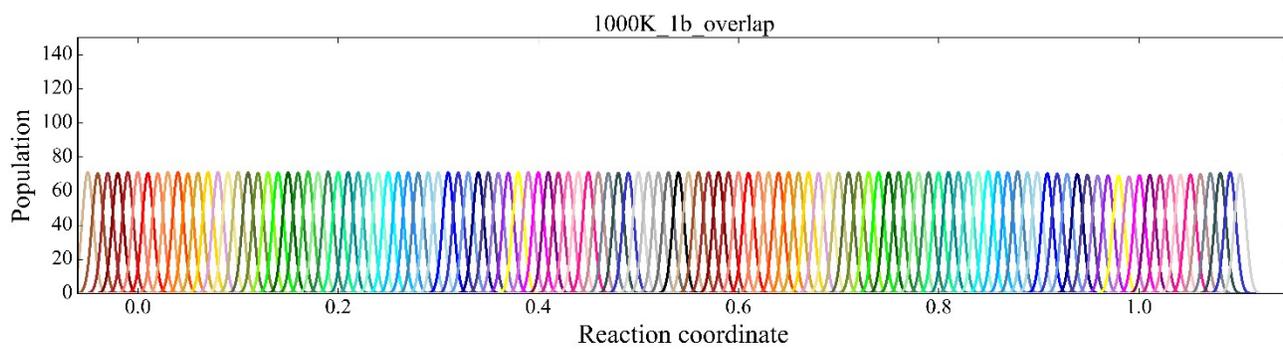
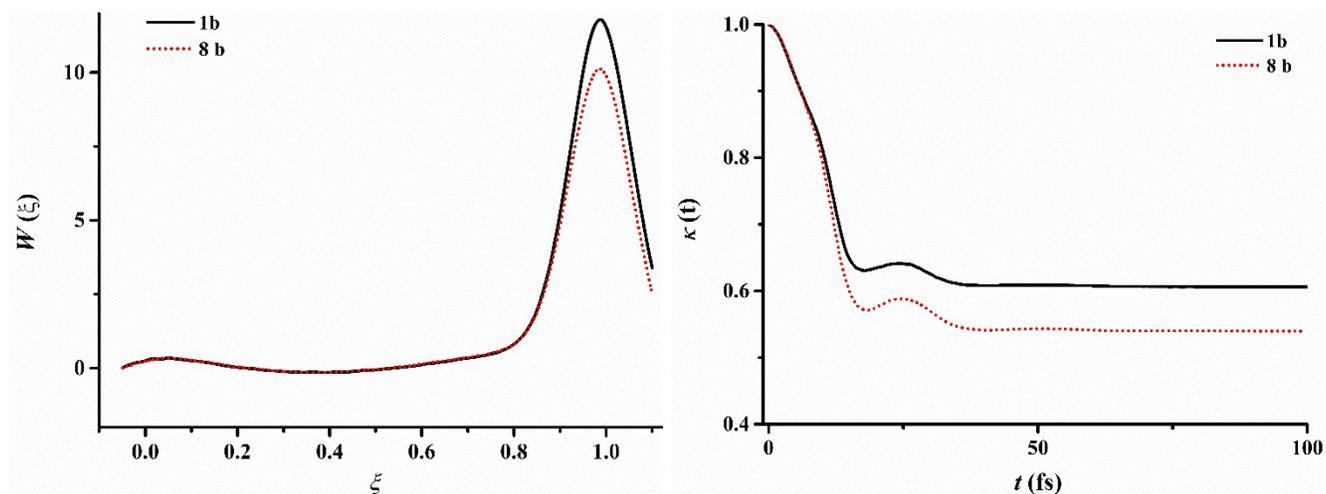


Figure S8. PMFs, transmission coefficients, and the overlaps between intervals with different numbers of beads for Cl + CH₄ at $T = 1100$ K.

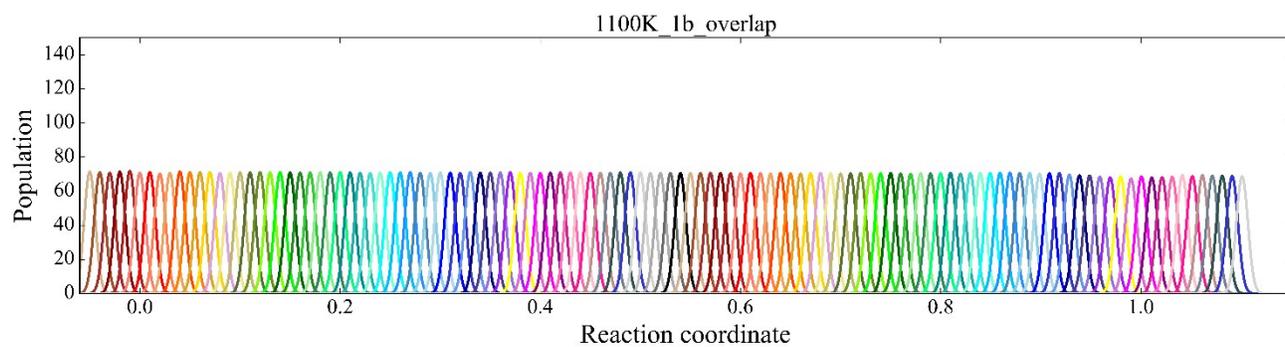
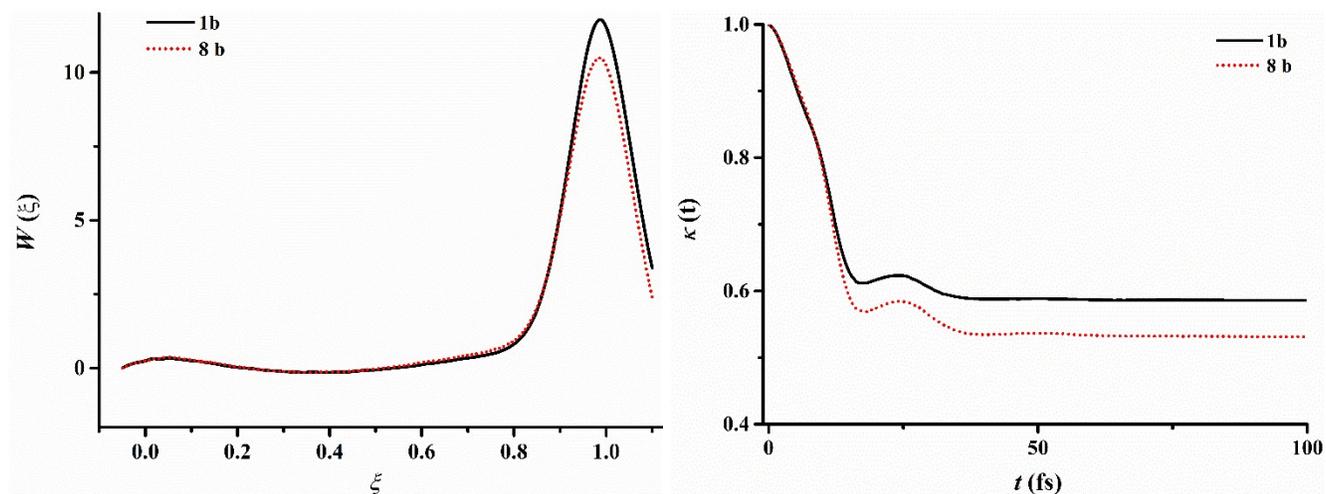


Figure S9. PMFs, transmission coefficients, and the overlaps between intervals with different numbers of beads for Cl + CH₄ at $T = 1500$ K.

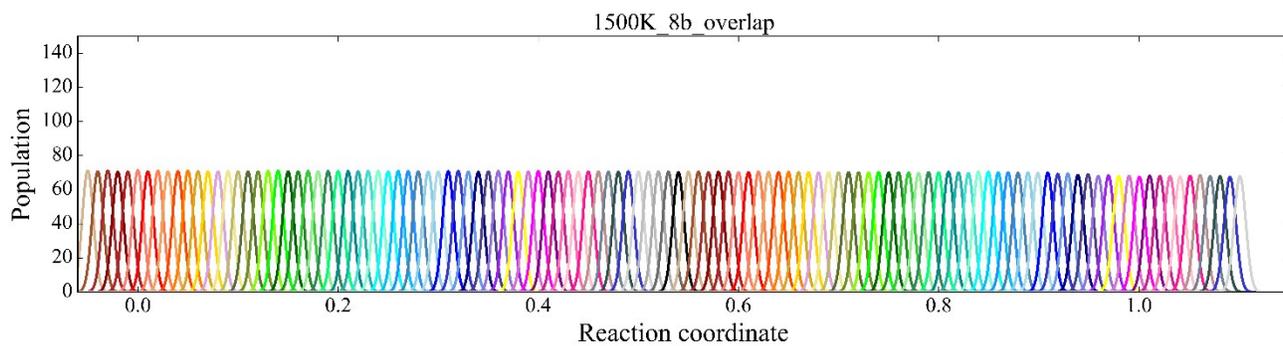
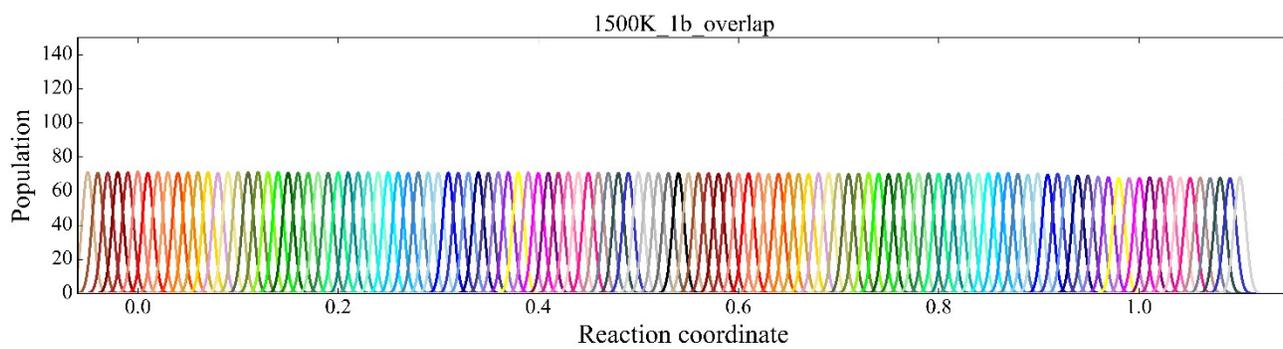
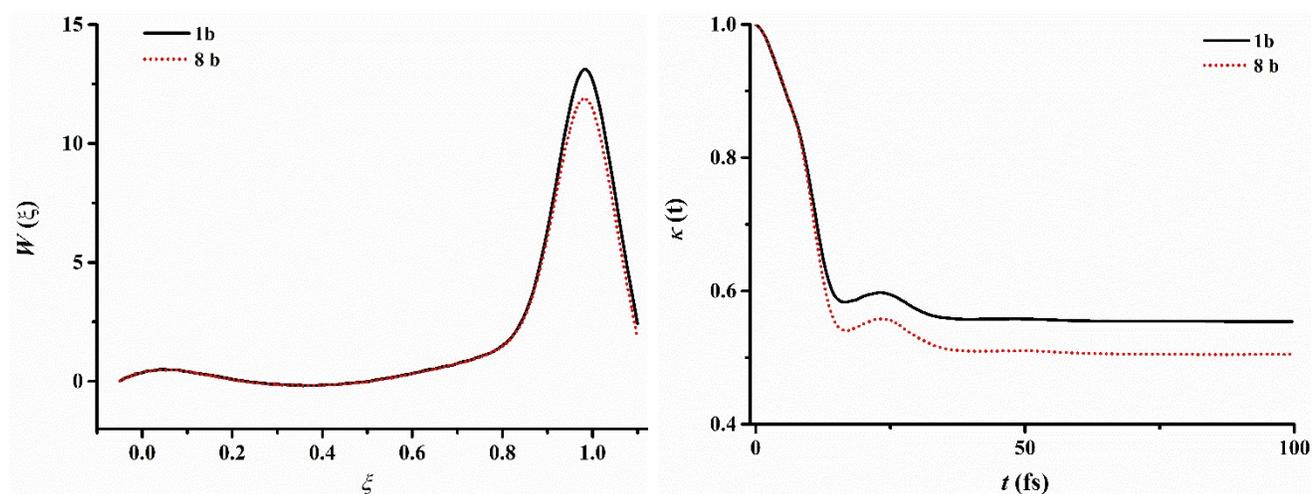


Figure S10. PMFs, transmission coefficients, and the overlaps between intervals with different numbers of beads for Cl + CH₄ at $T = 2000$ K.

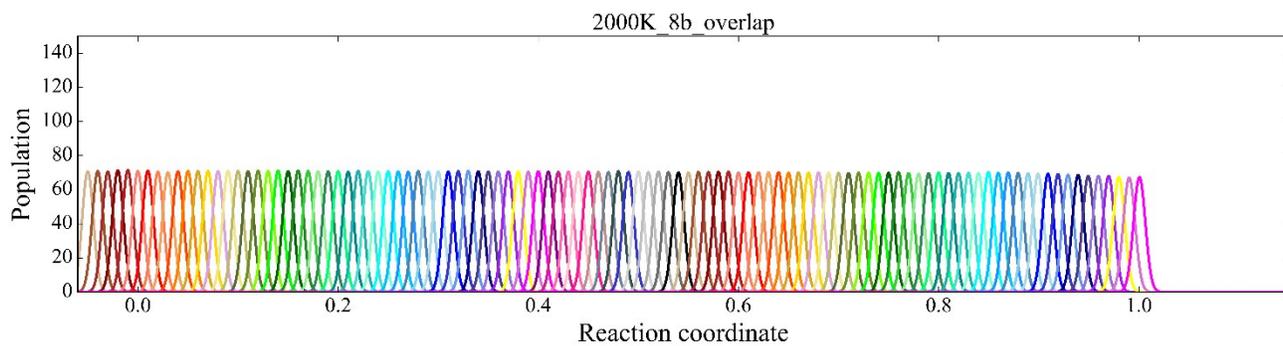
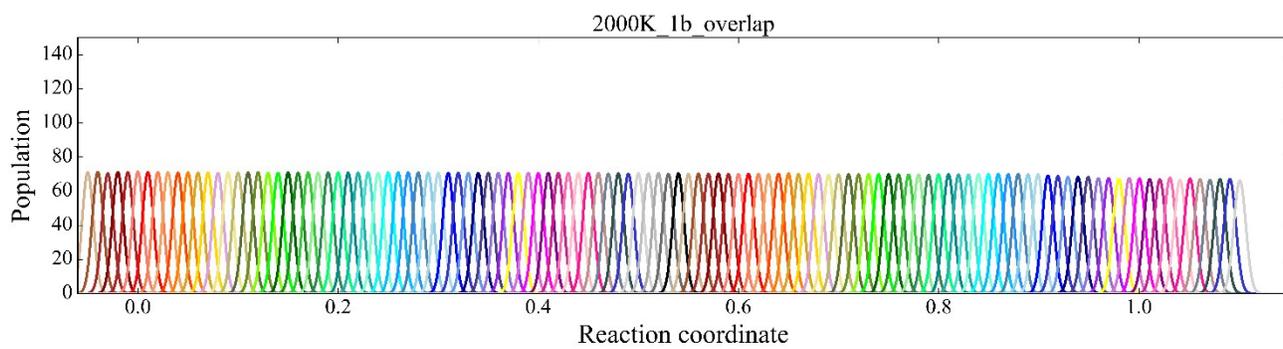
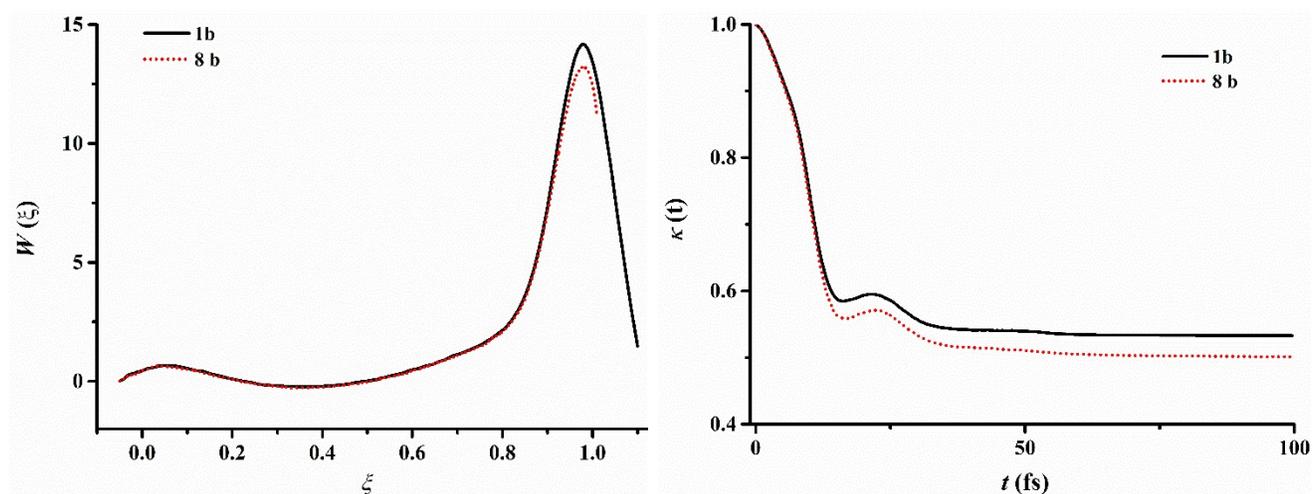


Figure S11. PMFs, transmission coefficients, and the overlaps between intervals with different numbers of beads for Cl + CD₄ at $T = 300$ K.

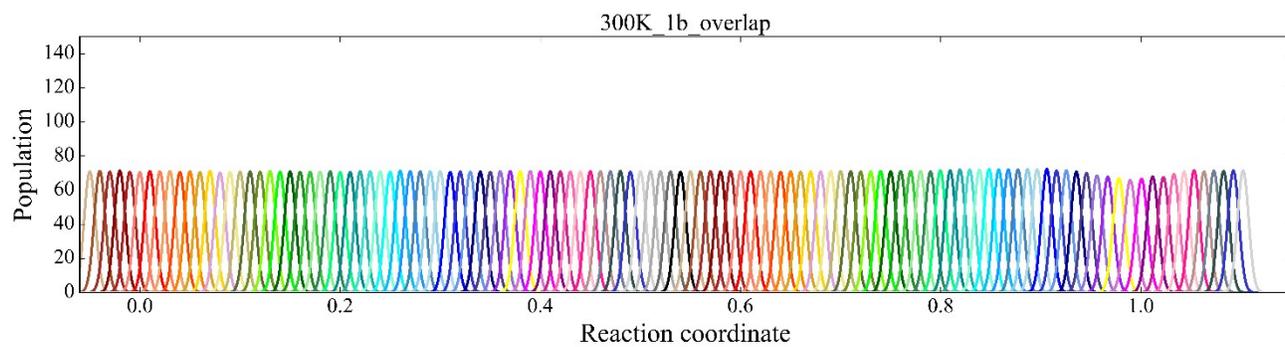
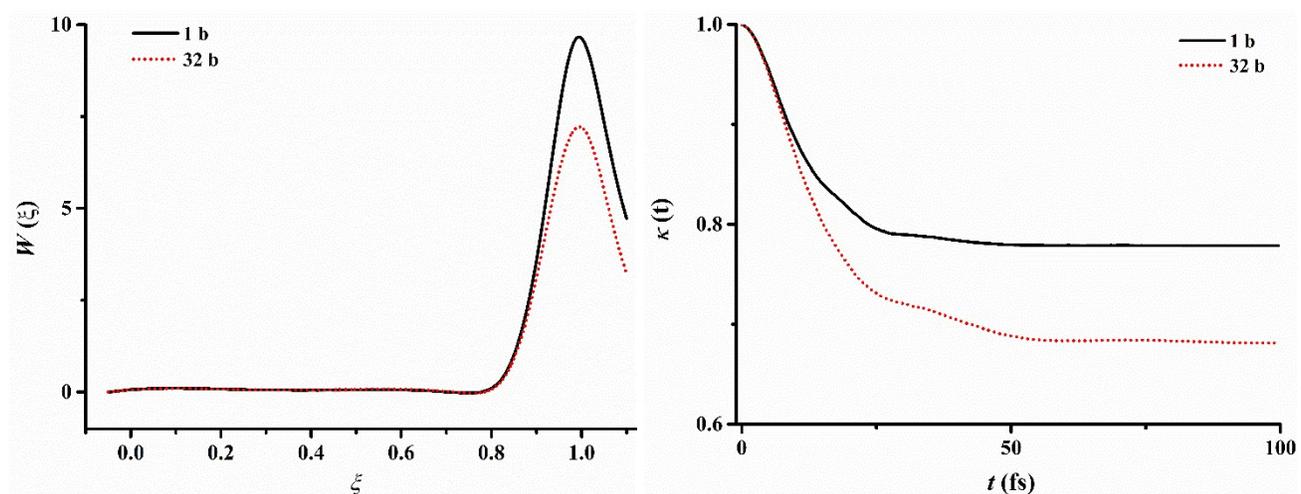


Figure S12. PMFs, transmission coefficients, and the overlaps between intervals with different numbers of beads for Cl + CD₄ at $T = 400$ K.

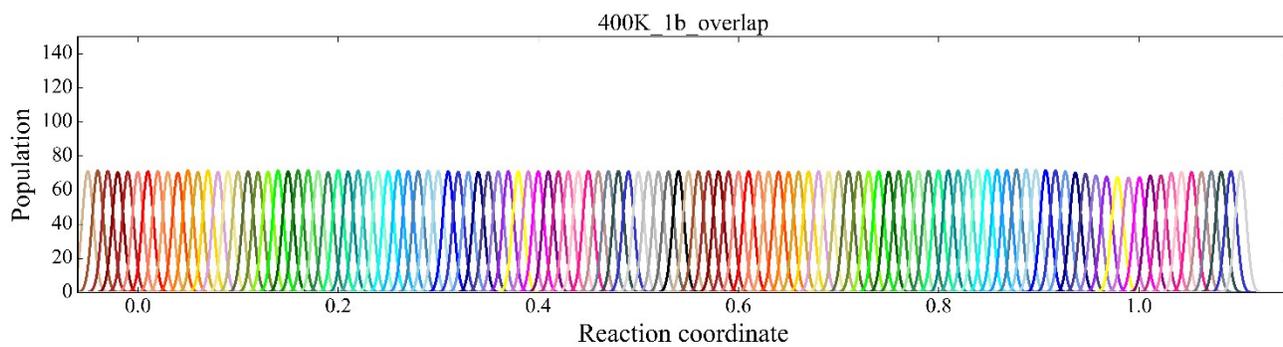
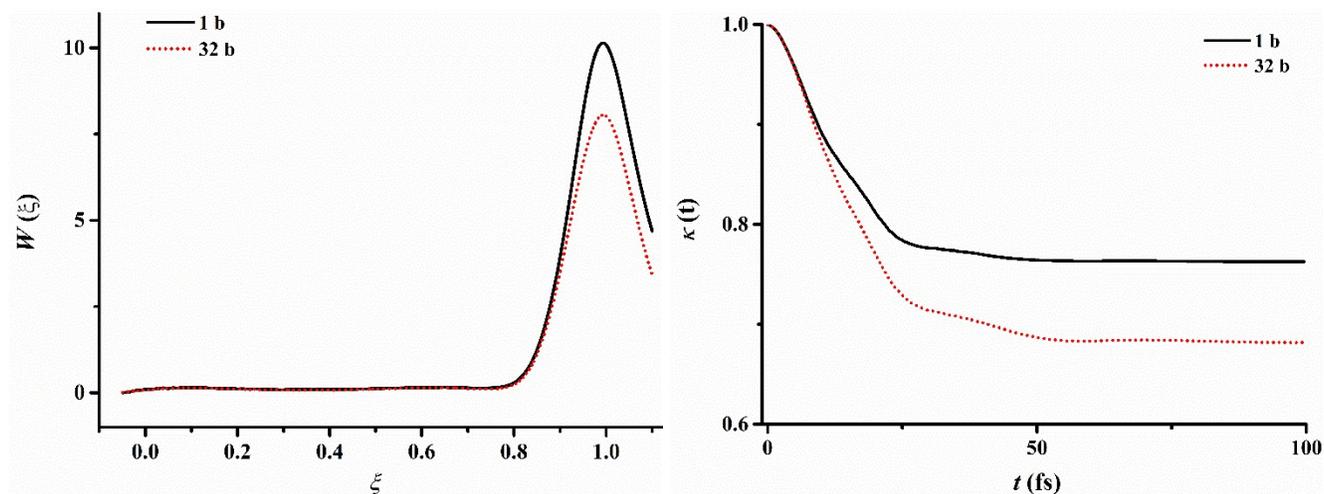


Figure S13. PMFs, transmission coefficients, and the overlaps between intervals with different numbers of beads for Cl + CD₄ at $T = 600$ K.

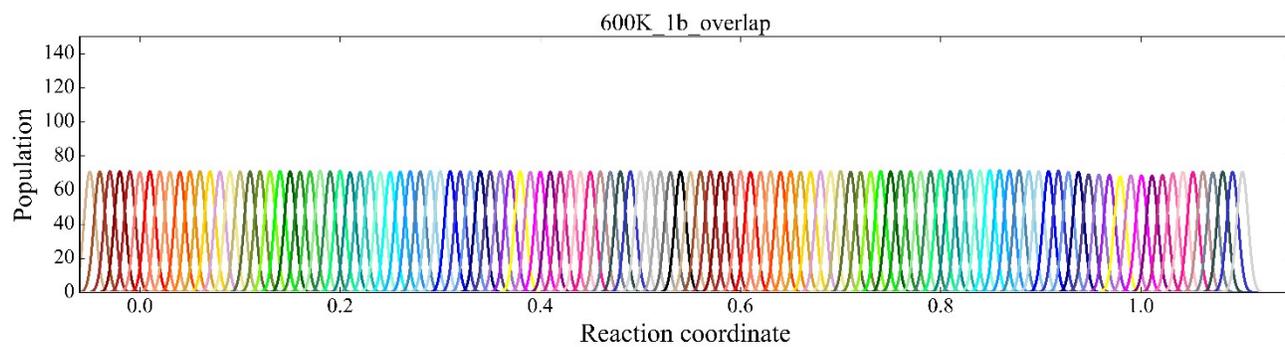
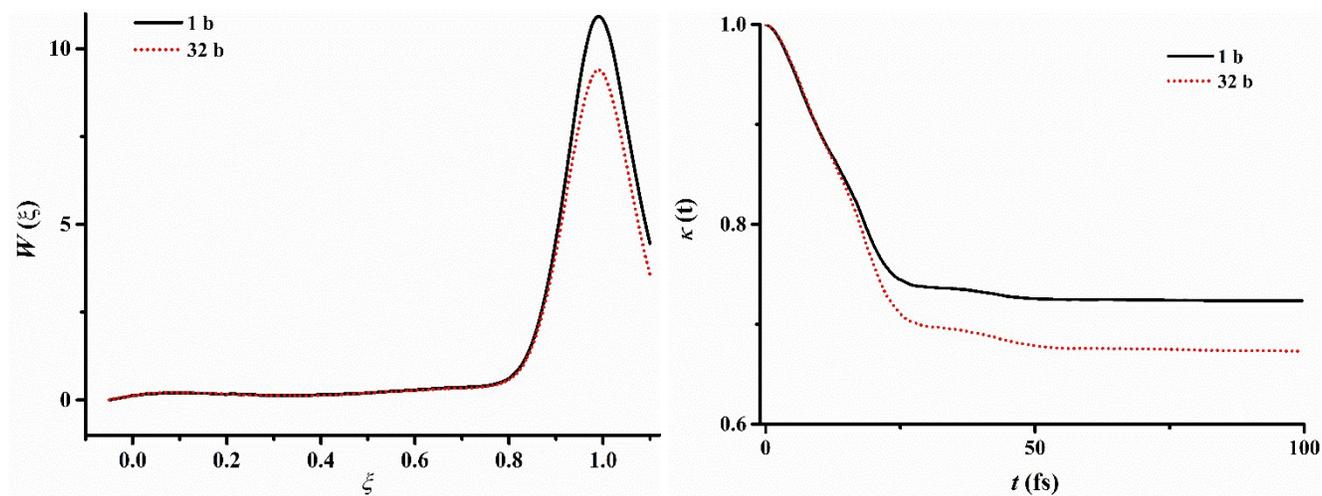


Figure S14. PMFs, transmission coefficients, and the overlaps between intervals with different numbers of beads for Cl + CD₄ at $T = 800$ K.

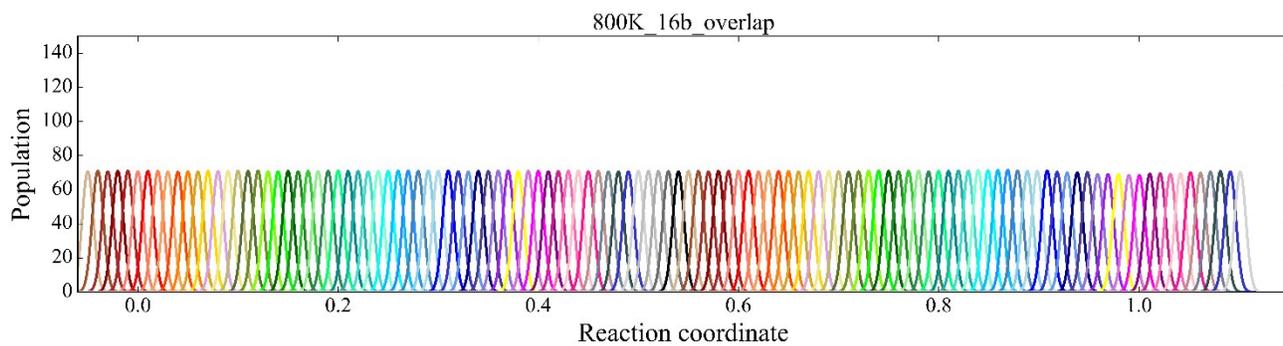
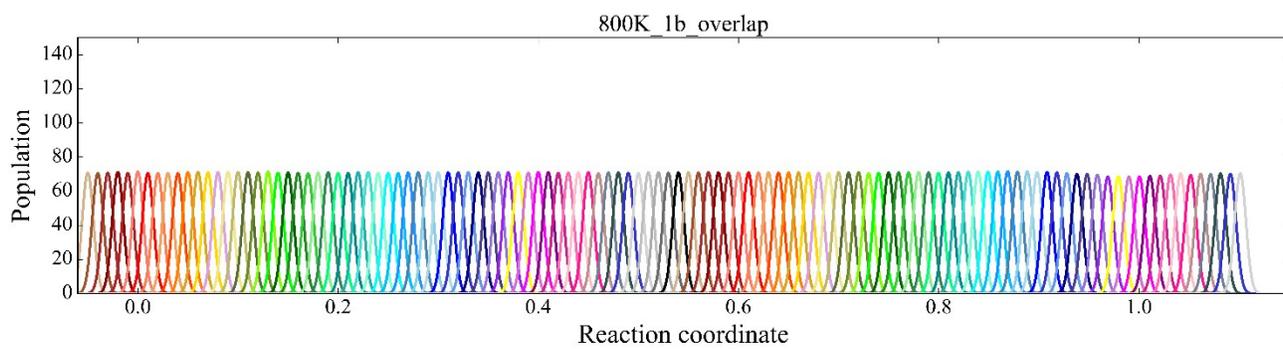
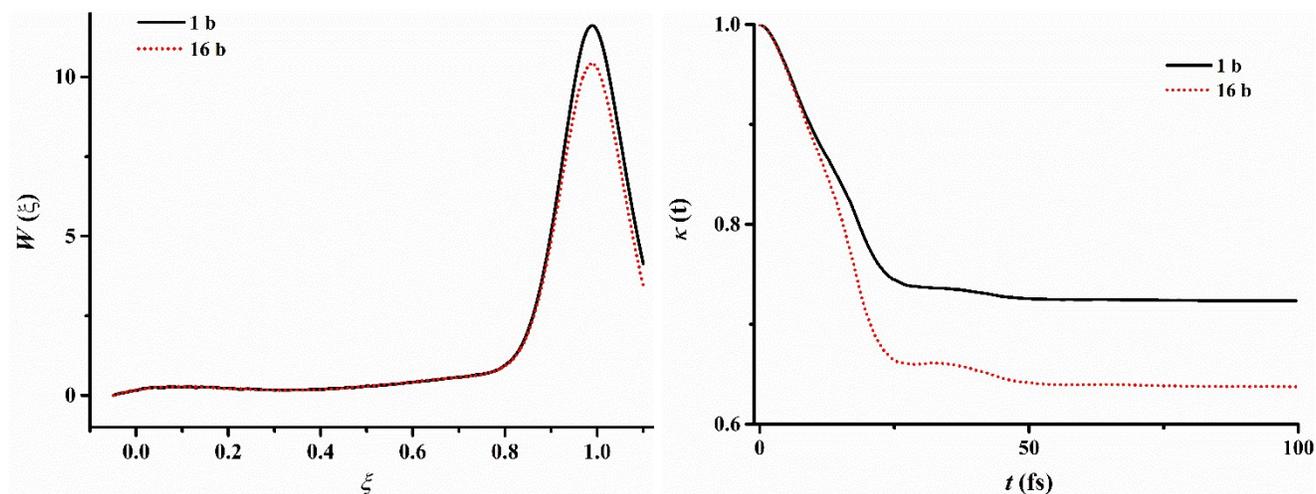


Figure S15. PMFs, transmission coefficients, and the overlaps between intervals with different numbers of beads for Cl + CD₄ at $T = 1000$ K.

