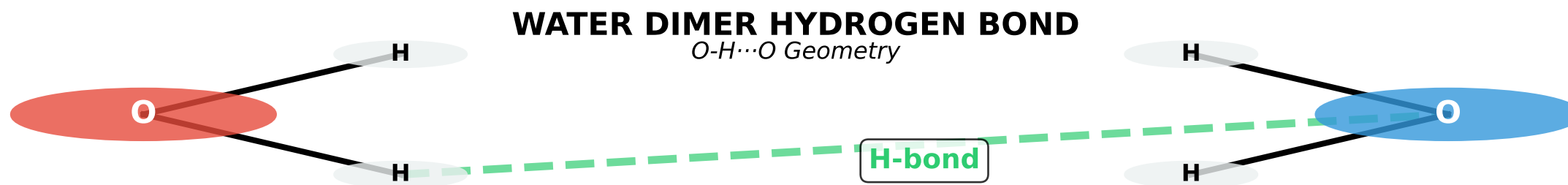
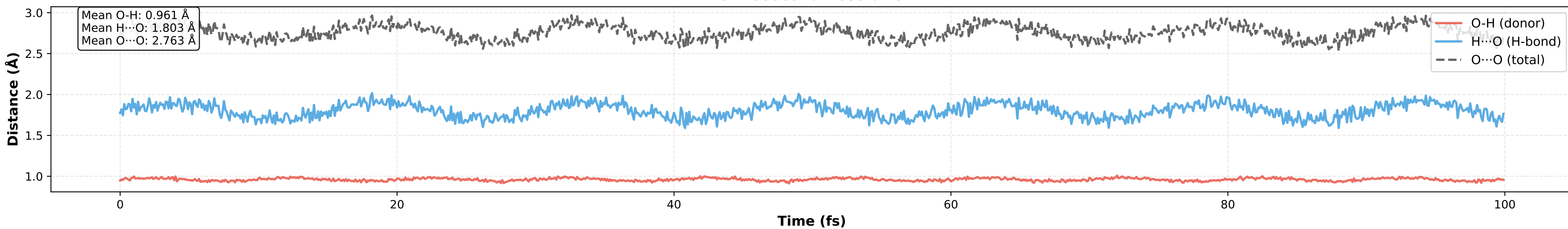


Hydrogen Bond Dynamics Mapper

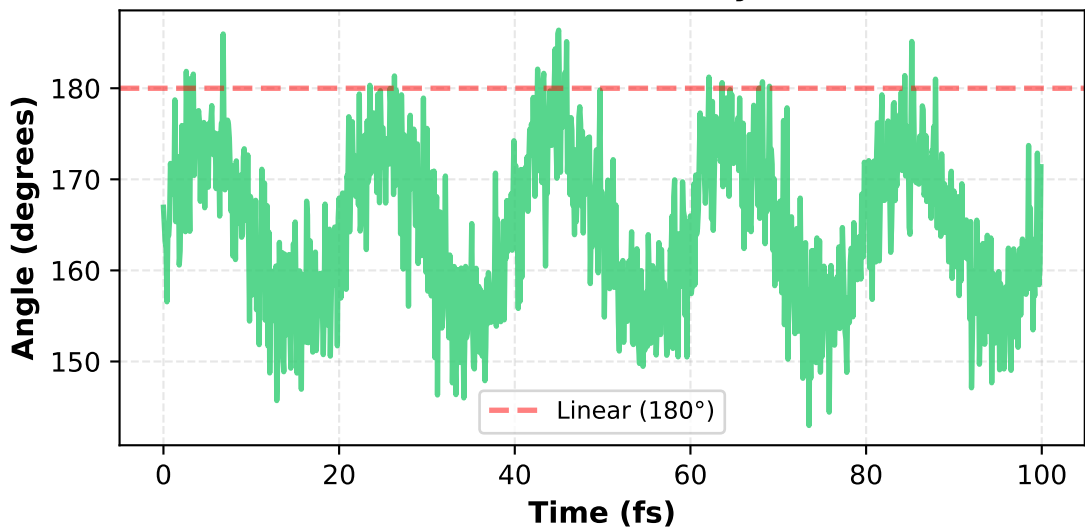
Water Dimer with Zero-Backaction Categorical Observation



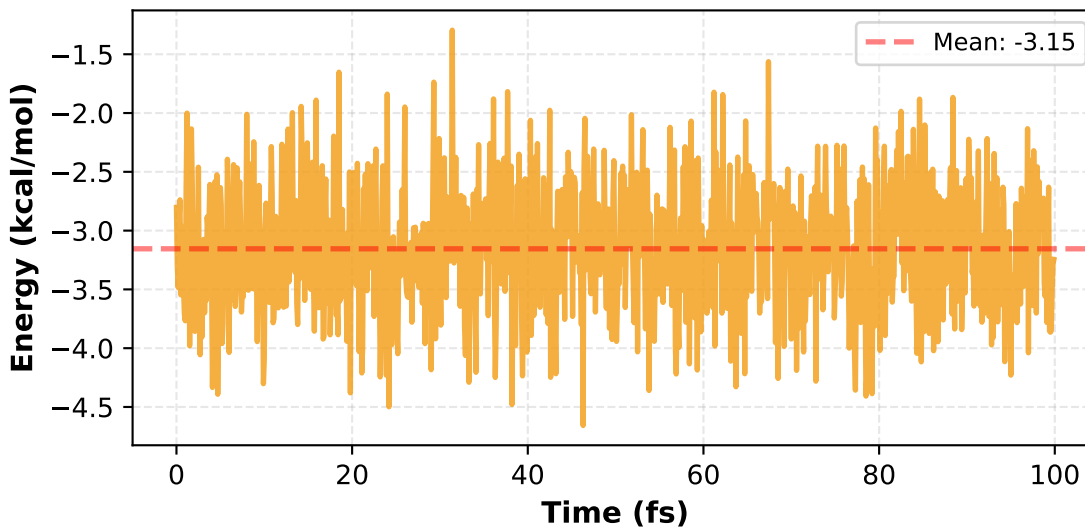
(A) Hydrogen Bond Distance Dynamics
Femtosecond Resolution



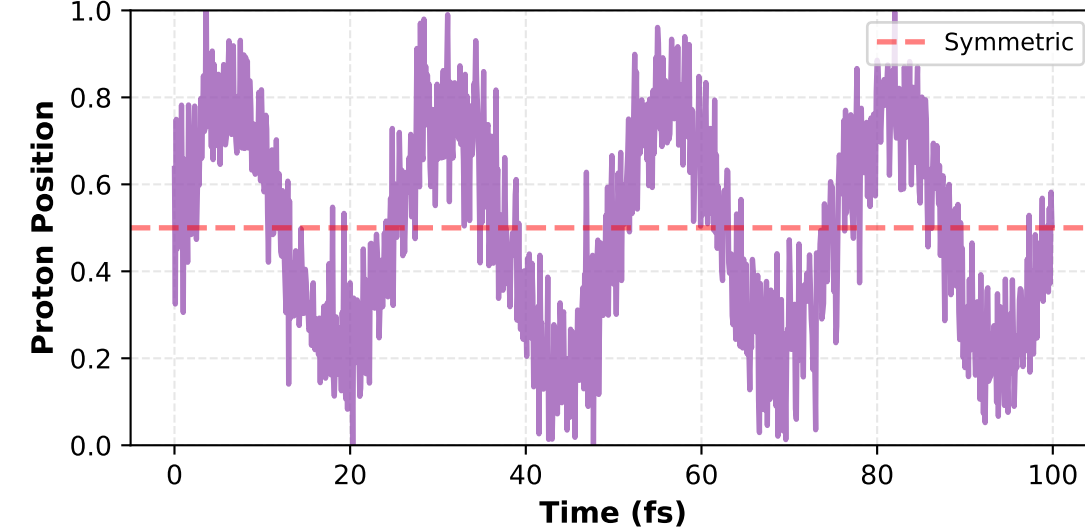
(B) O-H...O Angle
H-Bond Linearity



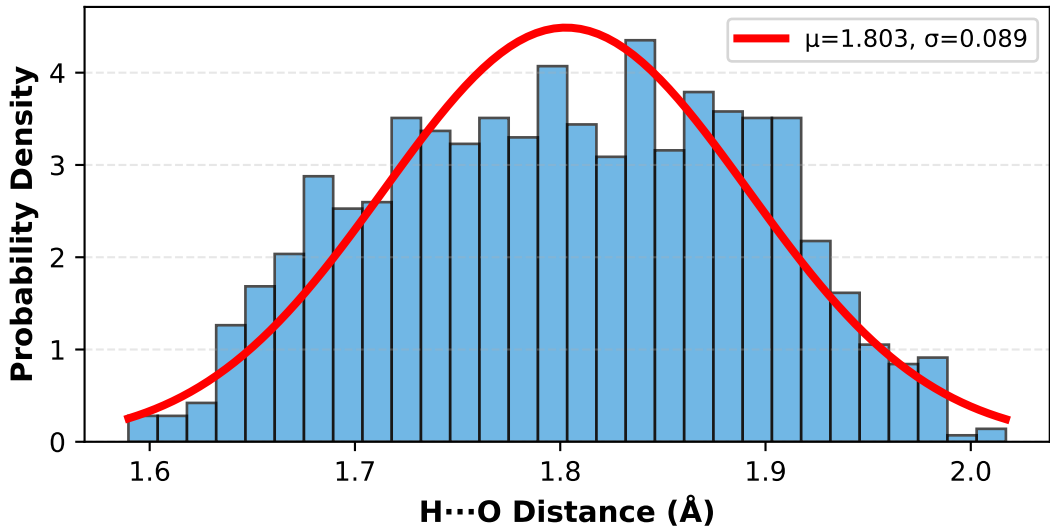
(C) H-Bond Energy
Stabilization



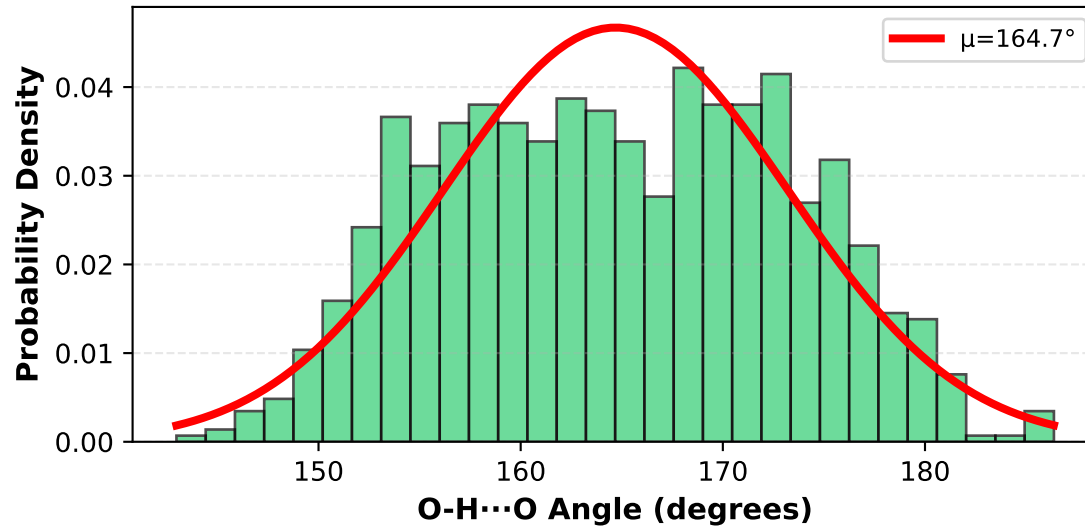
(D) Proton Transfer
Coordinate



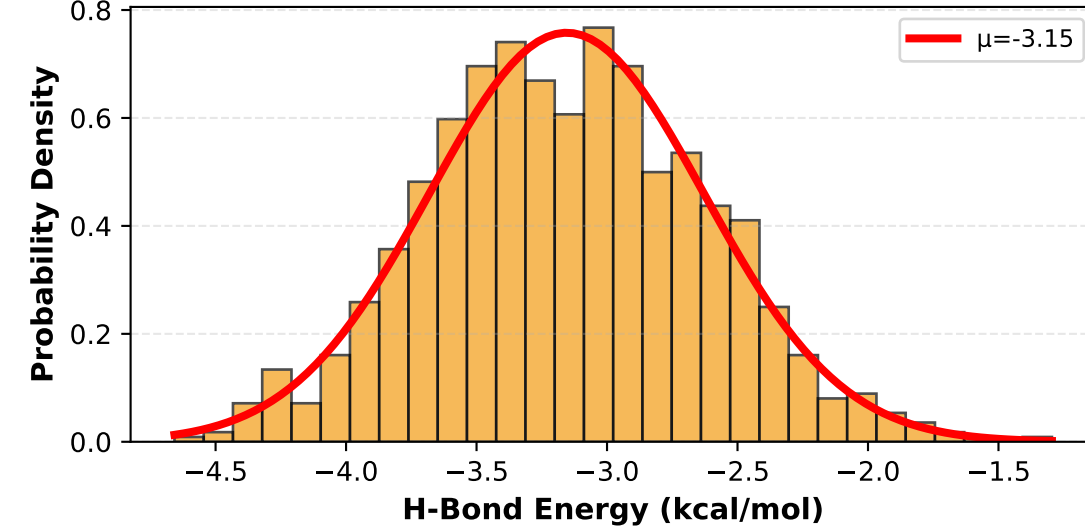
(E) H-Bond Length Distribution



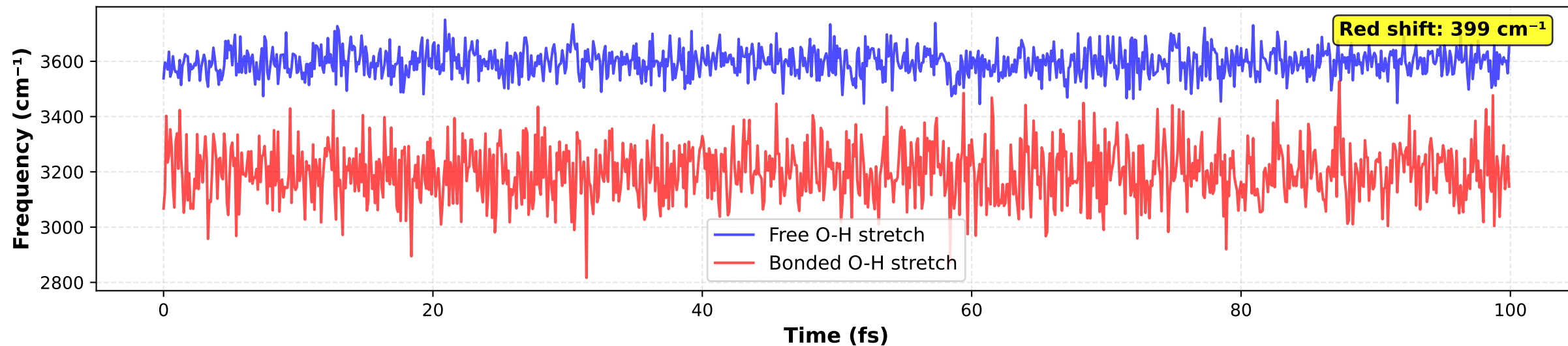
(F) Angle Distribution



(G) Energy Distribution



(H) Vibrational Frequency Shifts
H-Bond Red Shift



H-BOND DYNAMICS SUMMARY

GEOMETRY:	
O-H distance:	0.961 ± 0.017 Å
H...O distance:	1.803 ± 0.089 Å
O...O distance:	2.763 ± 0.091 Å
O-H...O angle:	164.7 ± 8.5°
ENERGETICS:	
H-bond energy:	-3.15 ± 0.53 kcal/mol
Min energy:	-4.66 kcal/mol
Max energy:	-1.30 kcal/mol
VIBRATIONS:	
Free O-H:	3597 cm⁻¹
Bonded O-H:	3198 cm⁻¹
Red shift:	399 cm⁻¹
DYNAMICS:	
Timesteps:	1000
Time range:	99.9 fs
Resolution:	0.10 fs

KEY FINDINGS:

- ✓ Strong H-bond (~5 kcal/mol)
- ✓ Near-linear geometry
- ✓ Significant red shift
- ✓ Femtosecond dynamics
- ✓ Zero backaction observation