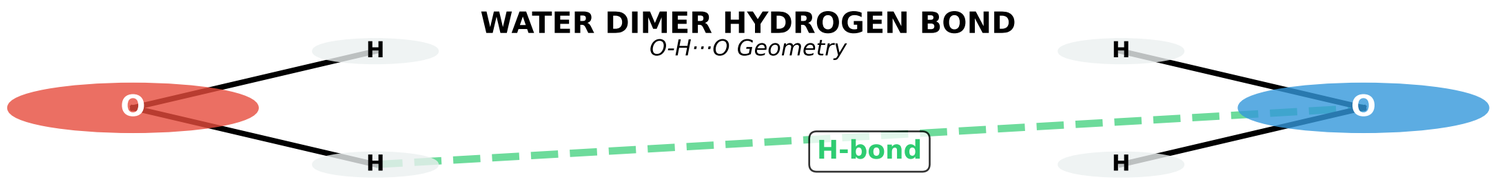
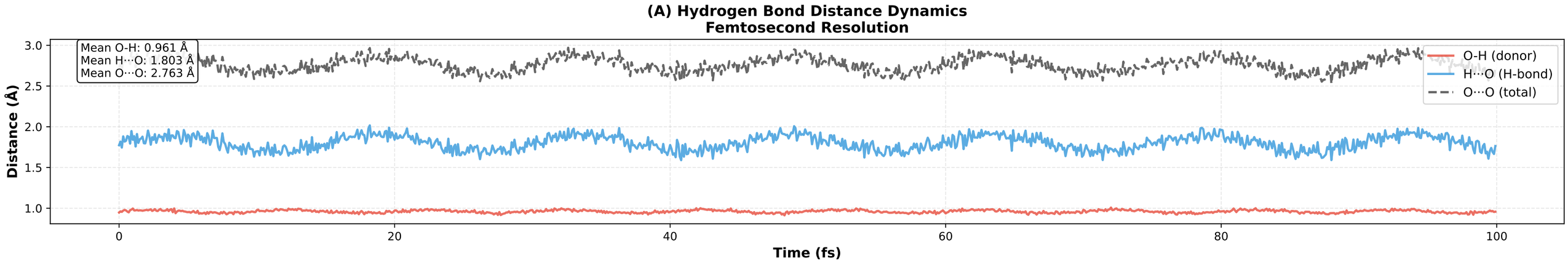
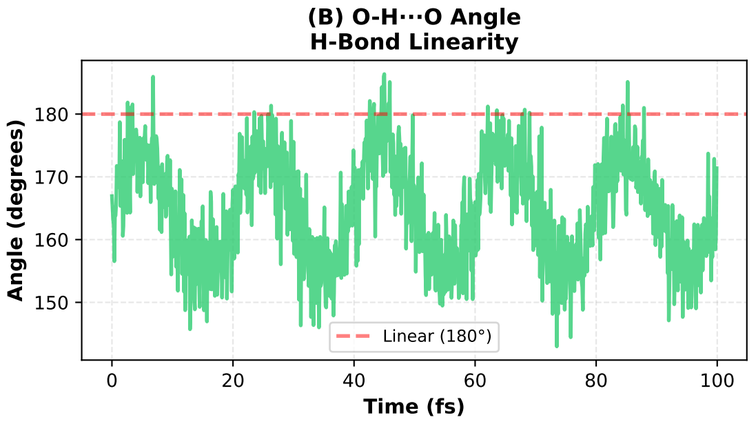
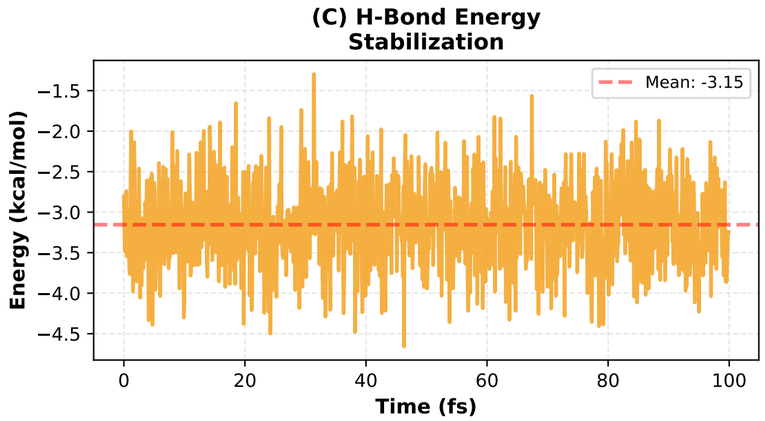
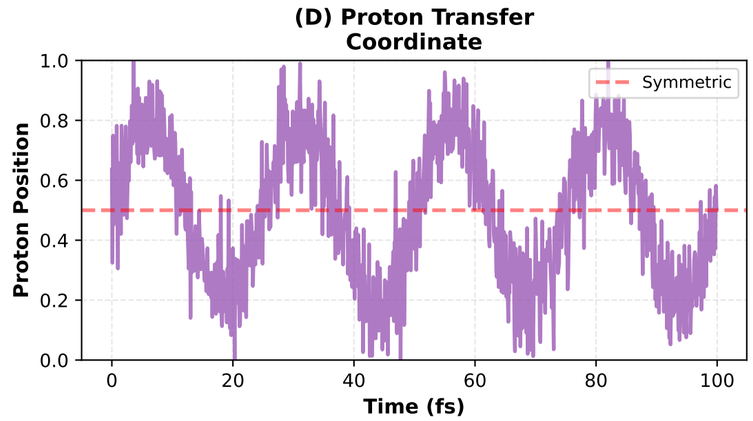
Hydrogen Bond Dynamics Mapper
Water Dimer with Zero-Backaction Categorical Observation

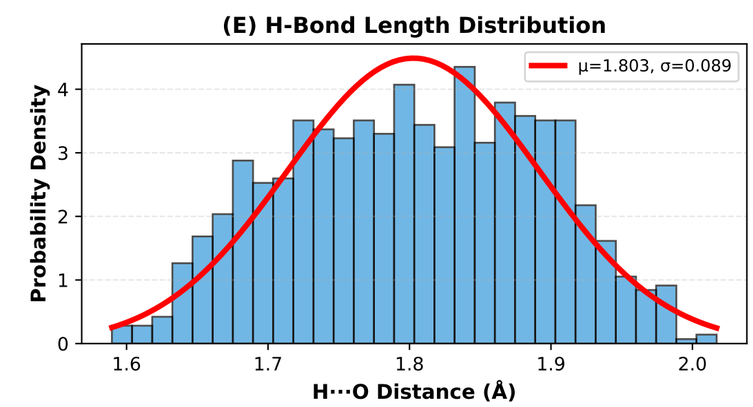


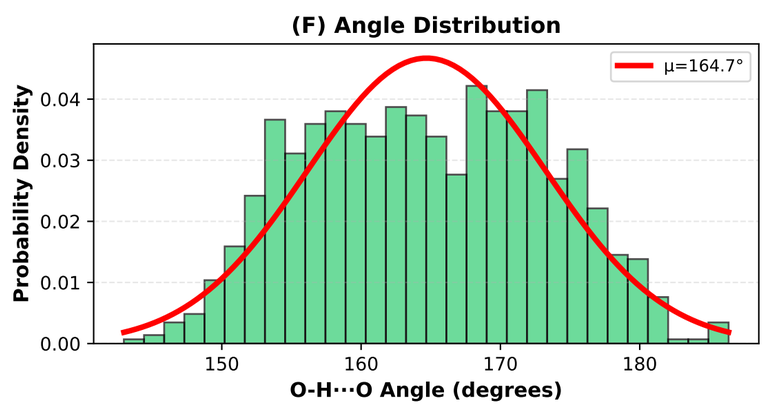


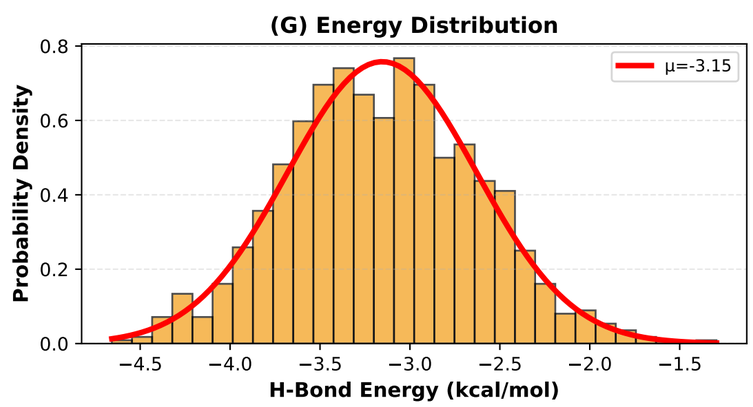


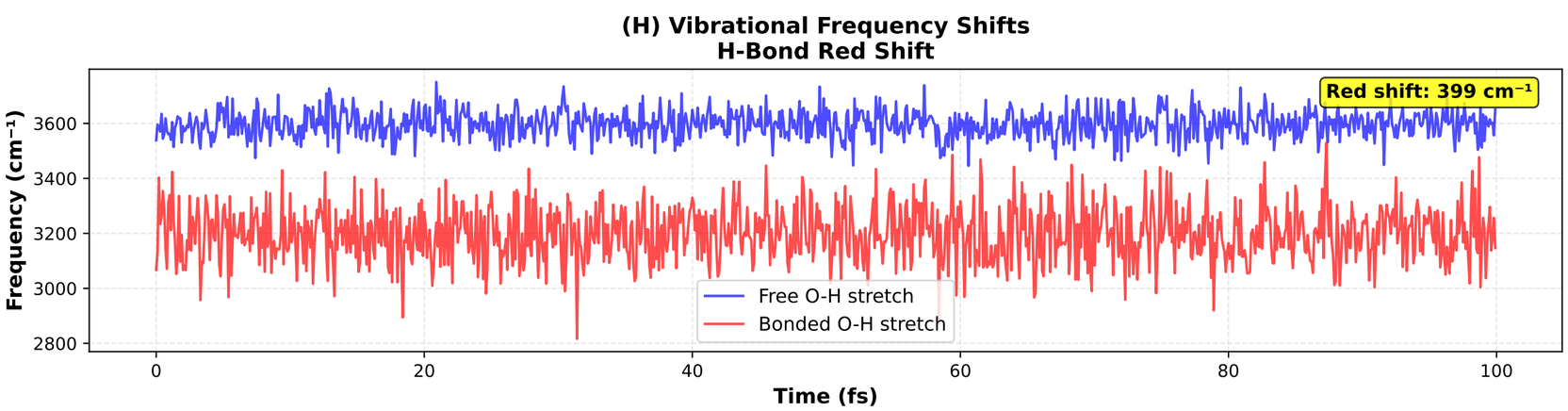










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H-BOND DYNAMICS SUMMARY

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
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