

## Trajectory Surface Hopping Study of Photocatalyzed H<sub>2</sub> Dissociation on a Gold Cluster

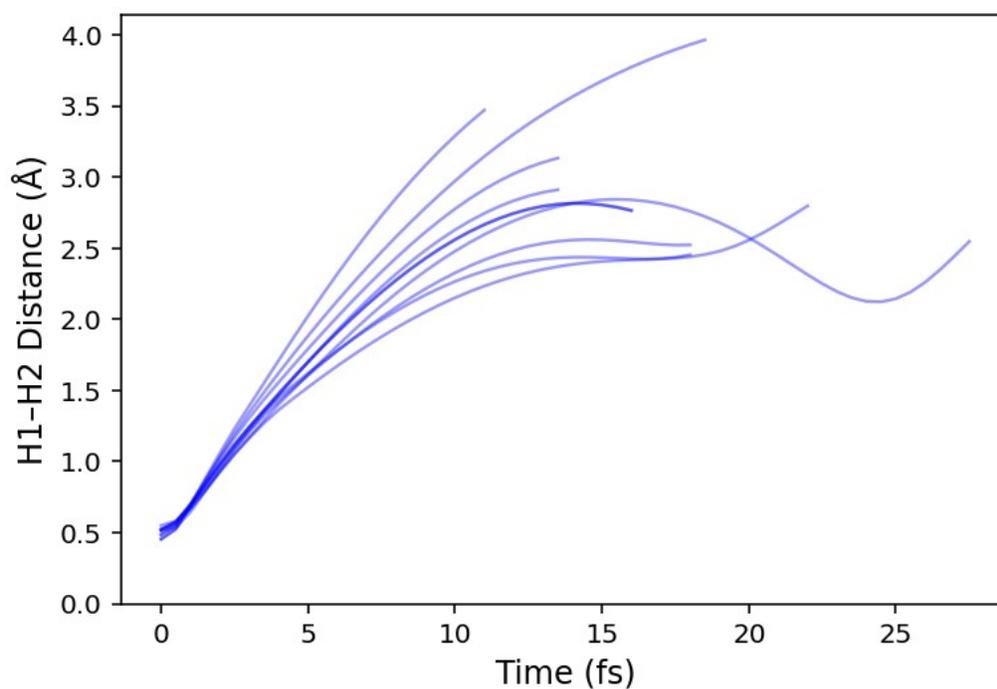
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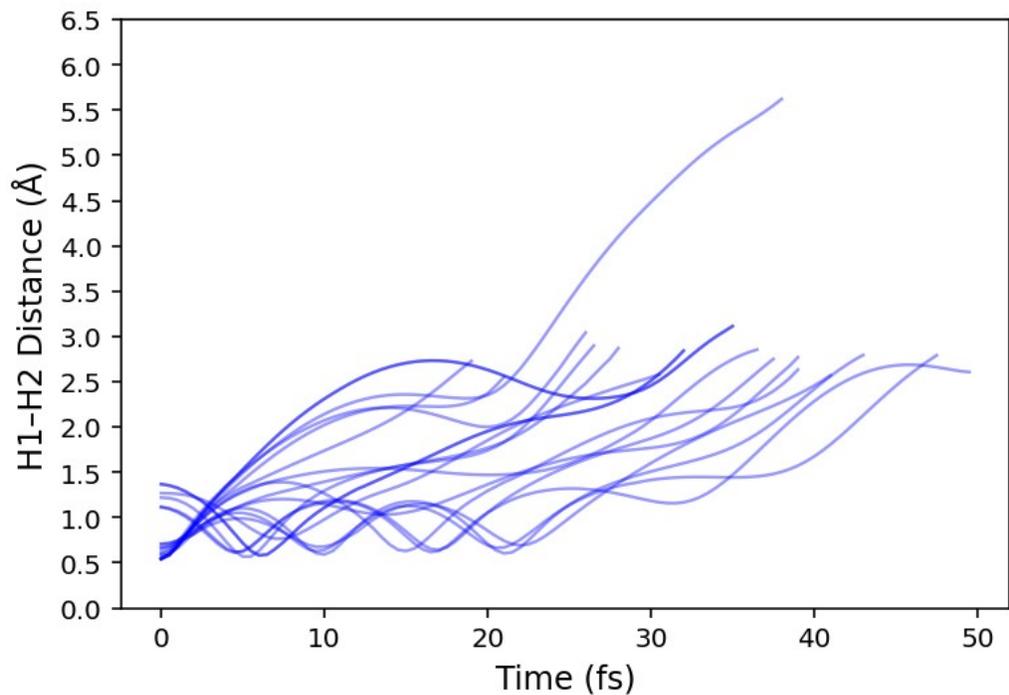
### SUPPLEMENTARY INFORMATION

**Figure S1. Adiabatic fast H<sub>2</sub> dissociation.**



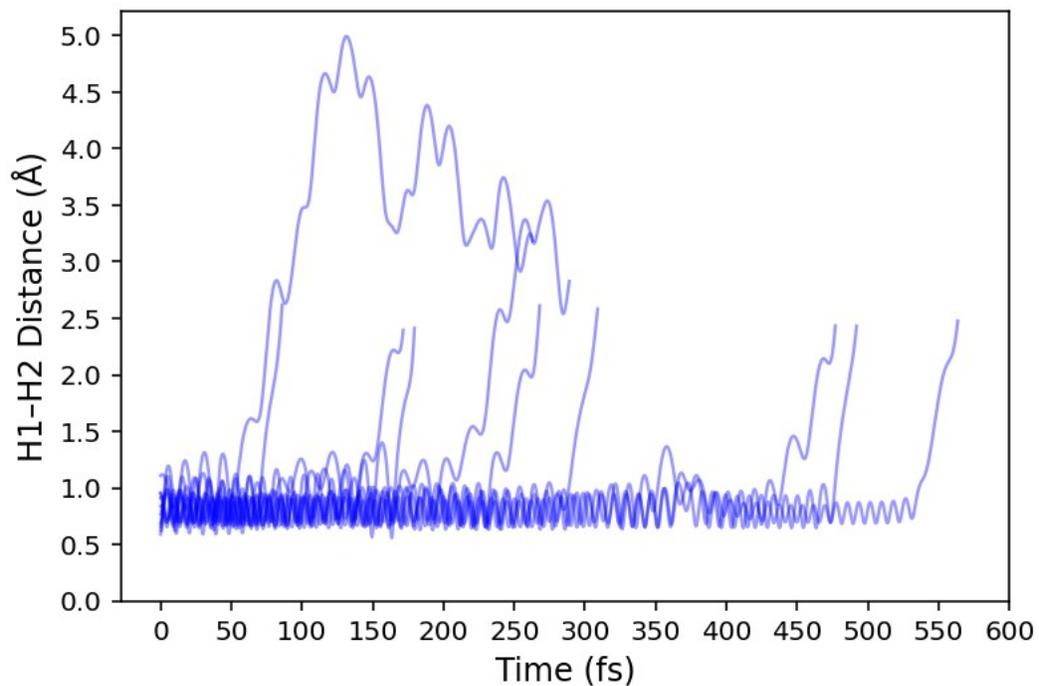
Internuclear H1-H2 distances over time for swarm of trajectories.

**Figure S2. Nonadiabatic fast H<sub>2</sub> dissociation.**



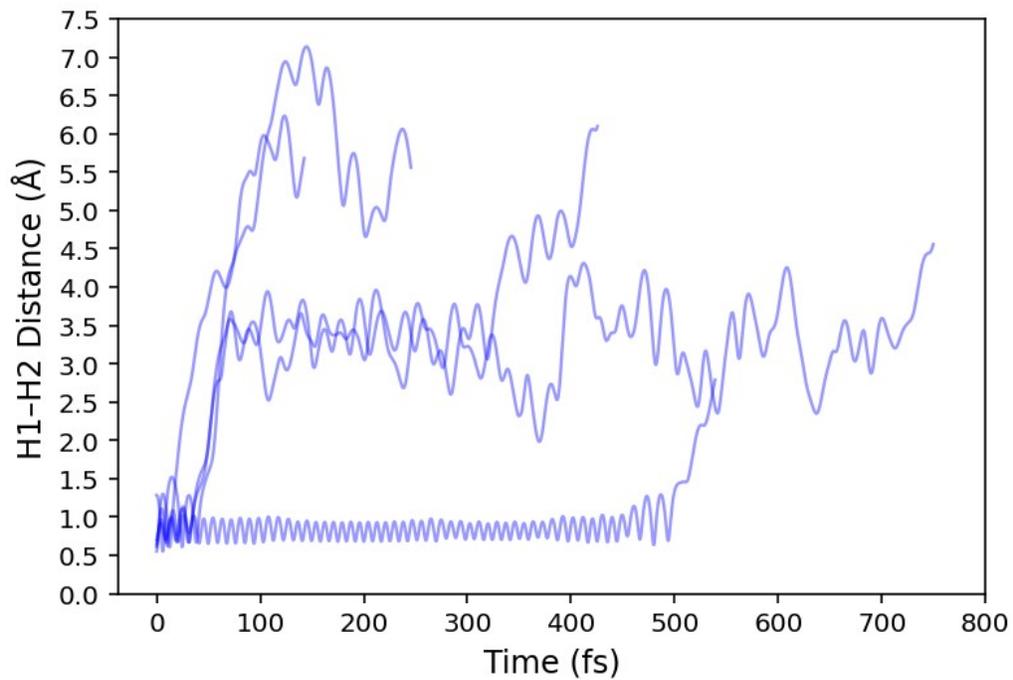
Internuclear H1-H2 distances over time for swarm of trajectories.

**Figure S3. Nonadiabatic slow H<sub>2</sub> dissociation.**



Internuclear H1-H2 distances over time for swarm of trajectories.

**Figure S4. The H<sub>2</sub> dissociation with H's ending up on two different Au atoms.**



Internuclear H1-H2 distances over time for swarm of trajectories