

## Supplementary Videos

### I. SMALLER HYDROGEN CHAINS

Both FCI and eigenvector continuation trajectories are plotted side by side, including their comparison for energies, populations and atomic distances. The trajectory for the 4-atom hydrogen chain is given under H4/traj\_H4\_S1.mp4 and for the 8-atom hydrogen chain under H8/traj\_H8\_S3\_sym.mp4. The training wavefunctions used for eigenvector continuation and details of the electronic and FSSH calculations are given in the main text.

### II. 28-ATOM HYDROGEN CHAIN DYNAMICS

Some exemplary trajectories for the different configurations of the nonadiabatic 28-atom hydrogen chain dynamics are given in the H28 folder. H28/traj\_idealdimer.gif shows one the trajectories that was identified to form ideal H<sub>2</sub> dimers, whereas a trimer formation is demonstrated in H28/traj\_trimer567.gif between the 5<sup>th</sup>, 6<sup>th</sup> and 7<sup>th</sup> hydrogen atoms. Finally, a rare free hydrogen case is shown in H28/traj\_free12.gif where H<sub>10</sub>-H<sub>11</sub> and H<sub>13</sub>-H<sub>14</sub> form dimers leaving the 12<sup>th</sup> hydrogen free.