Electronic Supplementary Information:

"Electronic nonadiabatic effects in the state-to-state dynamics of the H + H₂ \rightarrow H₂ + H exchange reaction with vibrationally excited reagent"

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FIG. S1. Initial state-selected total reaction probabilities obtained from uncoupled and coupled surface calculations both within linear and quadratic coupling approximations for the H + H₂ (v=3,4, j=0) \rightarrow H₂ ($\sum v', \sum j', \sum \Omega'$) + H reaction as a function of collision energy for the total angular momentum J = 0, 15 and 20.



FIG. S2. State-to-state DCSs of the H + H₂ (ν =4, j=0) \rightarrow H₂ (ν' =0, j'=12, $\Omega' \neq 0$) + H reaction as a function of scattering angle, θ at E_{col} = 0.57 eV for some selected values of Ω' . The DCSs obtained from both the uncoupled and coupled surface calculations are shown by lines of different colours indicated in the legend.



FIG. S3. State-to-state DCSs of the H + H₂ (ν =4, j=0) \rightarrow H₂ (ν' =2, j'=11, Ω') + H reaction as a function of scattering angle, θ at E_{col} = 0.57 eV for different values of Ω' . The DCSs obtained from both the uncoupled and coupled surface calculations, and those corresponding to the 1-TS and 2-TS paths are shown by lines of different colours.



FIG. S4. Same as in Fig. S3, but for H₂ ($\nu'=1$, j'=12, Ω') at E_{col} = 0.75 eV.



FIG. S5. State-to-state DCSs of the H + H₂ (v=4, j=0) \rightarrow H₂ (v', j', $\sum \Omega'$) + H reaction as a function of scattering angle for some selected (v', j') levels of product showing negligible electronic nonadiabatic effects in the forward scattering oscillations at E_{col} = 0.57 and 0.75 eV. The DCSs obtained from both uncoupled and coupled surface calculations are shown by lines of different colours. The DCSs corresponding to the 1-TS and 2-TS paths are shown in the bottom panels.



FIG. S6. The quantum mechanical generalized deflection function of the H + H₂ (v=4, j=0) \rightarrow H₂ (v', j', Ω') + H reaction at E_{col} = 0.57 eV for different product quantum states differentiating the glory angular oscillations from the "out-of-phase" forward scattering oscillations. The quantum numbers of the product states are mentioned at the top of each panel.



FIG. S7. Collision energy dependence of some selected state-to-state DCSs for the H + H₂ (v=4, j=0) \rightarrow H₂ (v', j') + H reaction in the backward (at $\theta = 180^{\circ}$) and forward (at $\theta = 0^{\circ}$) scattering direction. The DCSs obtained from both uncoupled and coupled surface calculations are shown by lines of different colours to show the electronic nonadiabatic effects (mostly due to GP). The DCSs corresponding to the 1-TS and 2-TS paths are shown inside each panels. The 1-TS and 2-TS DCSs are divided by a factor of 2 for a clear presentation of the interference phenomenon.



FIG. S8. Initial state-selected total (summed over all final states) DCSs corresponding to the 1-TS and 2-TS paths for the H + H₂ (v=3,4, j=0) \rightarrow H₂ ($\sum v'$, $\sum j'$, $\sum \Omega'$) + H reaction as a function of scattering angle, θ at various collision energies.



FIG. S9. Product rotational level resolved state-to-state ICSs for the H + H₂ (v=3,4, j=0) \rightarrow H₂ (v', j', $\sum \Omega'$) + H reaction as a function of collision energy for some selected (v', j') levels of product. The ICSs obtained from both the uncoupled and coupled surface calculations are plotted by line of different colours and types.