

Supplementary Material

Signature of the geometric phase in the wave packet dynamics on hypersurfaces

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This Supplementary Material provides the potential energy surfaces (PESs) for the parameter combinations involving a larger intersurface coupling between the two PESs. Moreover, we show the different projections of the wave-packet dynamics except from those on the $|\tilde{e}_1\rangle$ PES which is depicted in Fig. 4 in the main text.

I. POTENTIAL ENERGY SURFACE WITH $\Lambda = 400, 600$ AND 800 CM^{-1}

Here, we show the PESs of the two configurations with a conical intersection (CI) and an avoided crossing (AC) of surfaces for different intersurface electronic coupling strength between two PESs. In Fig. S1, Fig. S2 and Fig. S3, we show the PESs for the electronic coupling between the two surfaces $\Lambda = 400, 600$ and 800 cm^{-1} , respectively.

II. WAVE-PACKET DYNAMICS FOR STRONG INTERSURFACE COUPLING

In this section, we show the dynamics of the wave packet for both the CI and the AC configuration in the regime of stronger intersurface coupling for $\Lambda = 400, 600$ and 800 cm^{-1} . In particular, we show the kinetics of the wave packet on the upper electronic PES $|\tilde{e}_2\rangle$ along the coupling mode Q_c and the tuning mode Q_t and of the wave packet on the lower excited PES $|\tilde{e}_1\rangle$ along the tuning mode Q_t . The results for all values of Λ are qualitatively similar and striking differences between the CI and the AC configurations occur only for the dynamics on the lower excited PES $|\tilde{e}_1\rangle$ along the coupling mode Q_c , which we, thus, show in the main text.

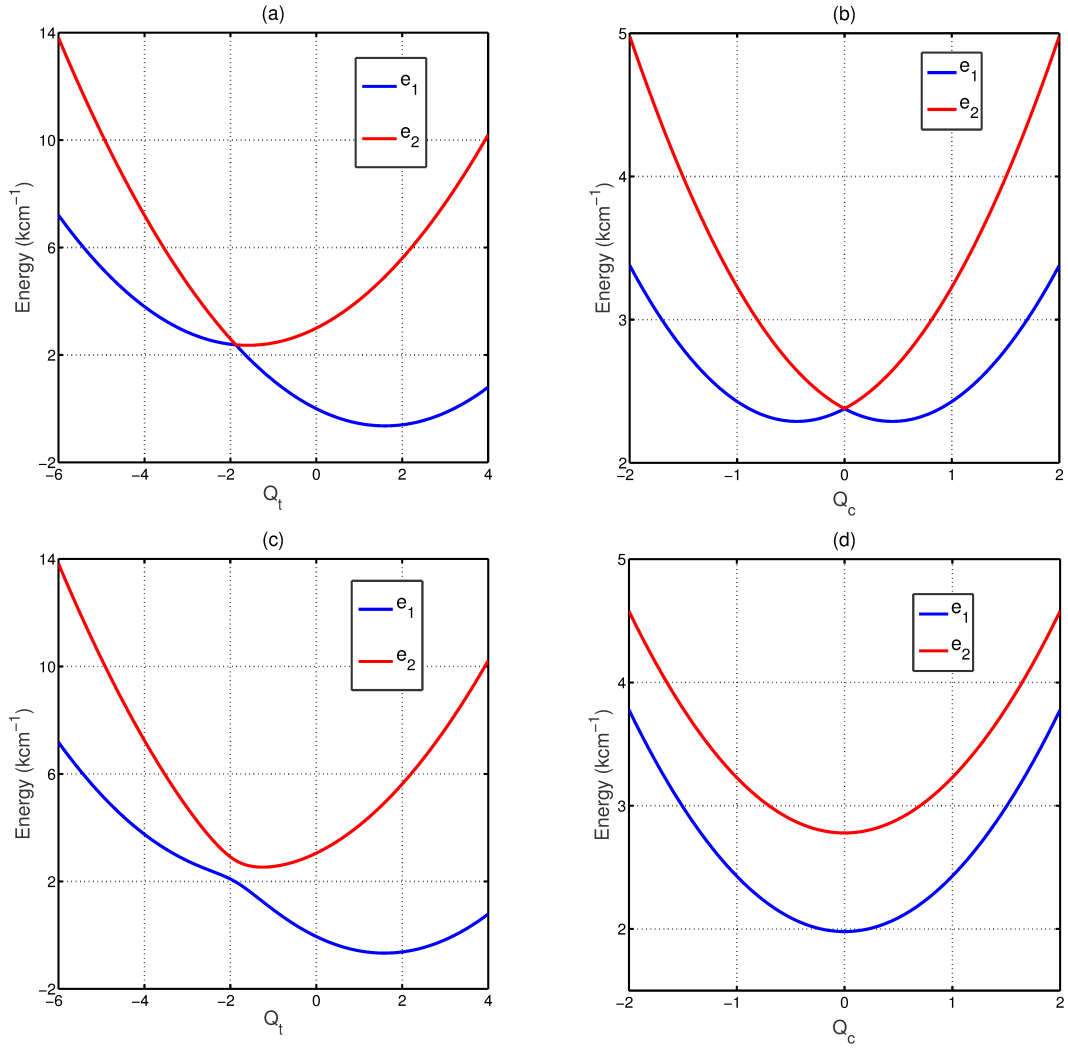
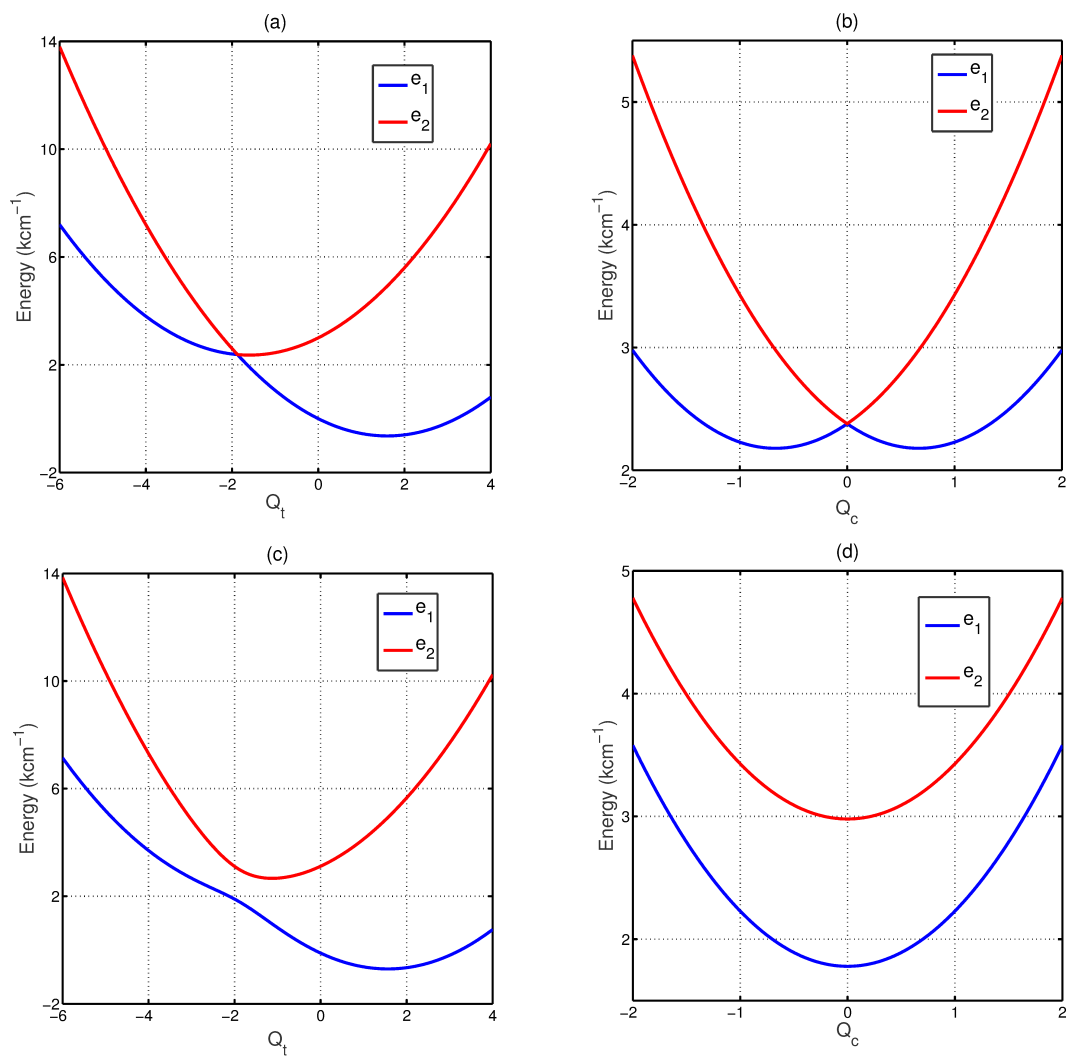


FIG. S1. PESs of the CI (a, b) and the AC (c, d) configuration along the tuning (Q_t) and the coupling (Q_c) modes for the intersurface coupling $\Lambda = 400 \text{ cm}^{-1}$.

FIG. S2. Same as Fig. S1, but for $\Lambda = 600 \text{ cm}^{-1}$.

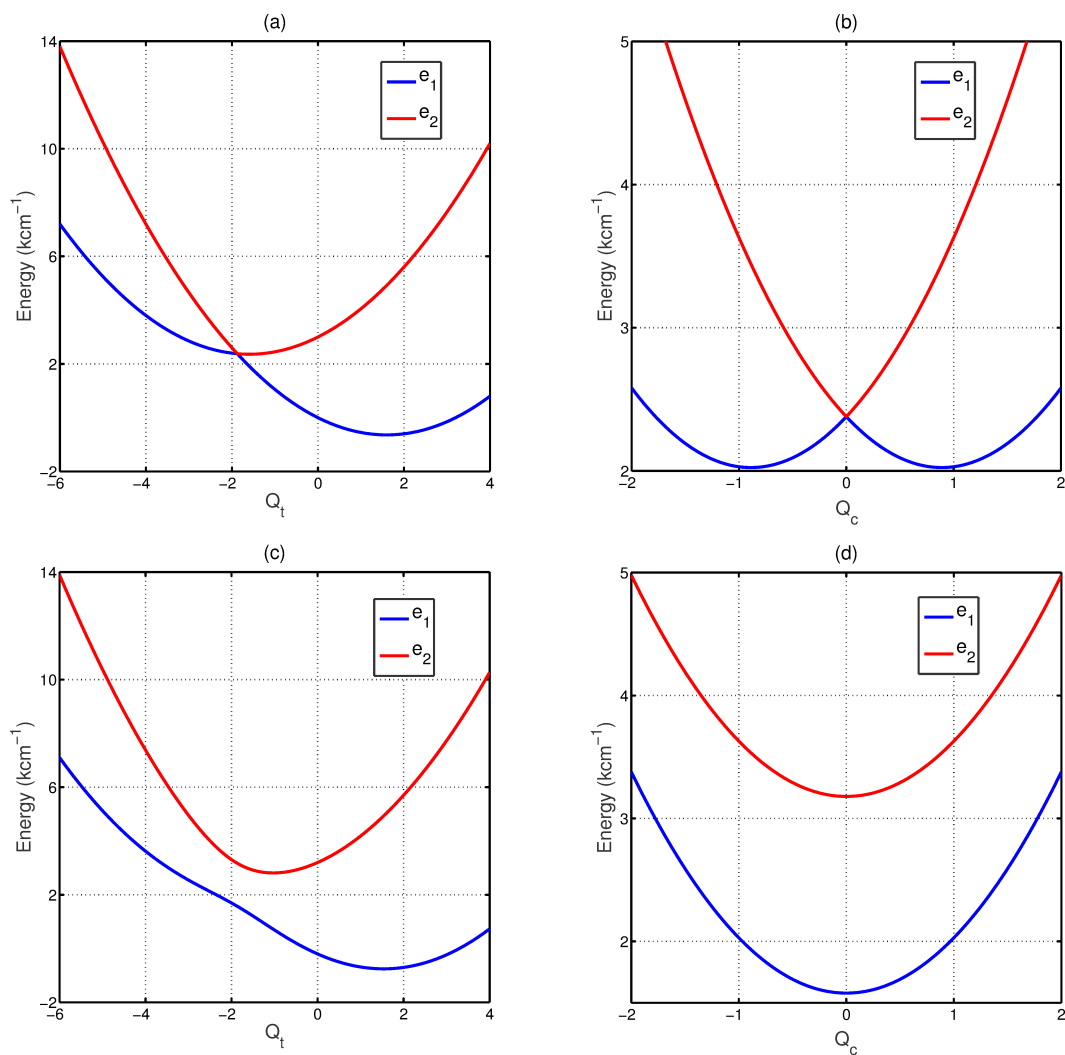


FIG. S3. Same as Fig. S1, but for $\Lambda = 800 \text{ cm}^{-1}$.

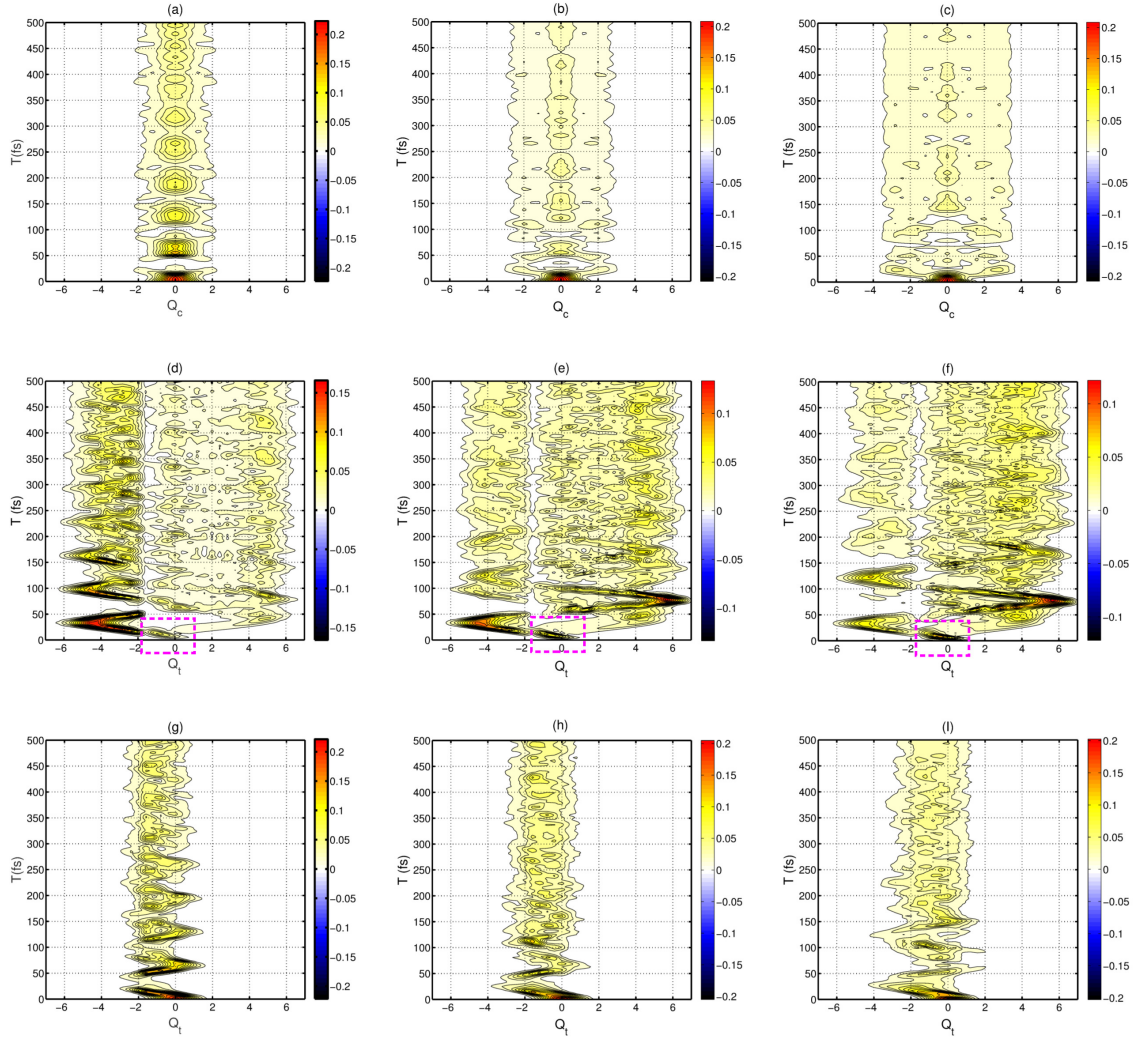


FIG. S4. The wave-packet dynamics of the CI configuration for $\Lambda = 400$ (a, d, g), 600 (b,e,h) and 800 (c, f, I) cm^{-1} . In (a), (b) and (c), the kinetics of the wave packet on the upper electronic PES $|\tilde{e}_2\rangle$ is plotted along coupling mode Q_c . In (d), (e) and (f), we show the time evolution of the wave packet on the lower excited PES $|\tilde{e}_1\rangle$ along the tuning mode Q_t . The wave-packet dynamics on the upper electronic PES $|\tilde{e}_2\rangle$ is plotted along the tuning mode Q_t , respectively.

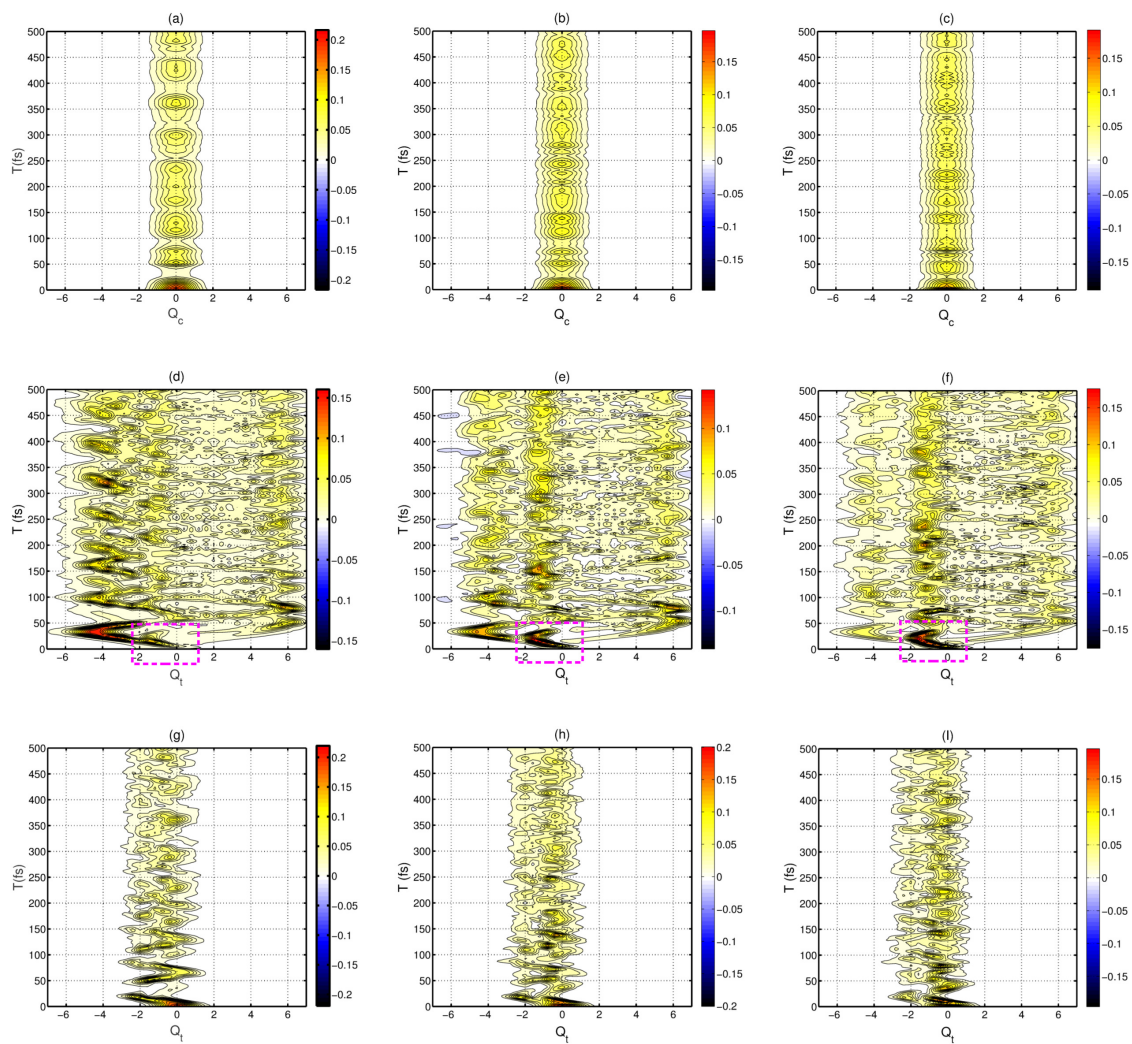


FIG. S5. Same as Fig. S4, but for the AC configuration.