Supplementary information

Vibronic quantum beating between electronic excited states in a heterodimer

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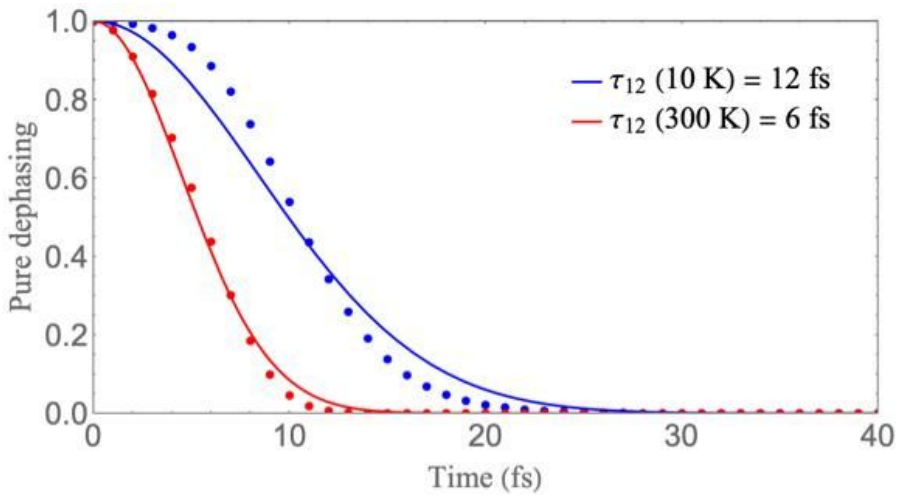

Figure S1. Pure dephasing function $D_{12}(t)$ for the AB heterodimer evaluated from the EHR-NEXMD simulations.

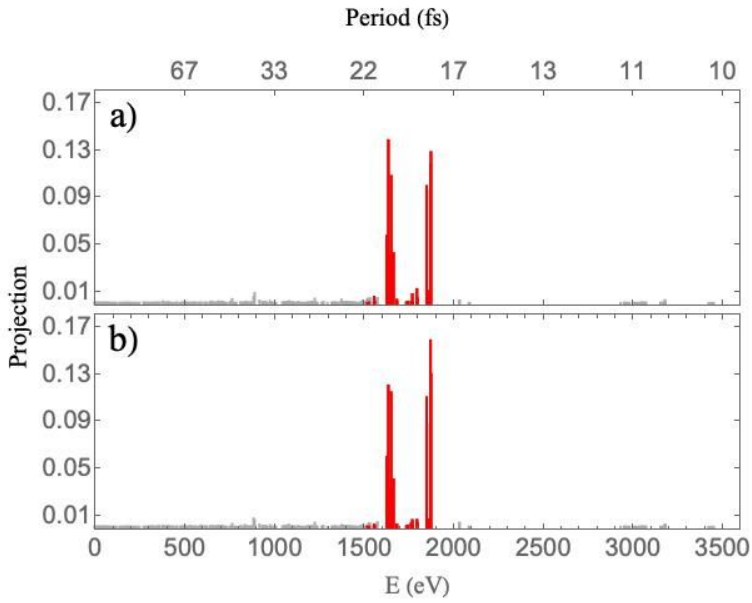

Figure S2. Distribution of values of the projection of the SVD_1 vector on the basis of equilibrium normal modes. SVD_1 vector was calculated using $NACR_{12}$ vectors at *t*=20fs (maximum of $NACT_{12}$ shown in **Figure 3(b)**) during EHR-NEXMD simulations at a) 10K and b) 300K. Modes within the range [1620;1890] cm^{-1} are indicated in red.

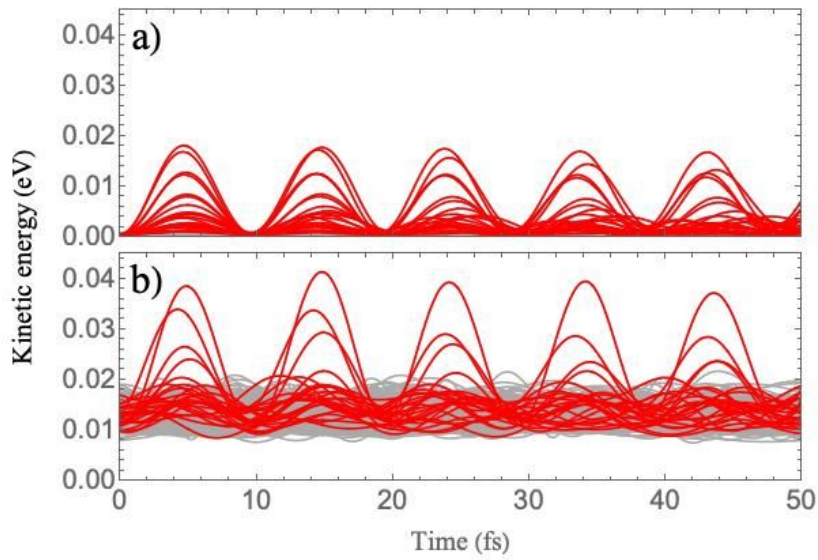

Figure S3. Time evolution of the average kinetic energy along equilibrium normal modes during EHR-NEXMD simulations at a) 10K and b) 300K. Modes within the range [1620;1890] cm^{-1} are indicated in red.

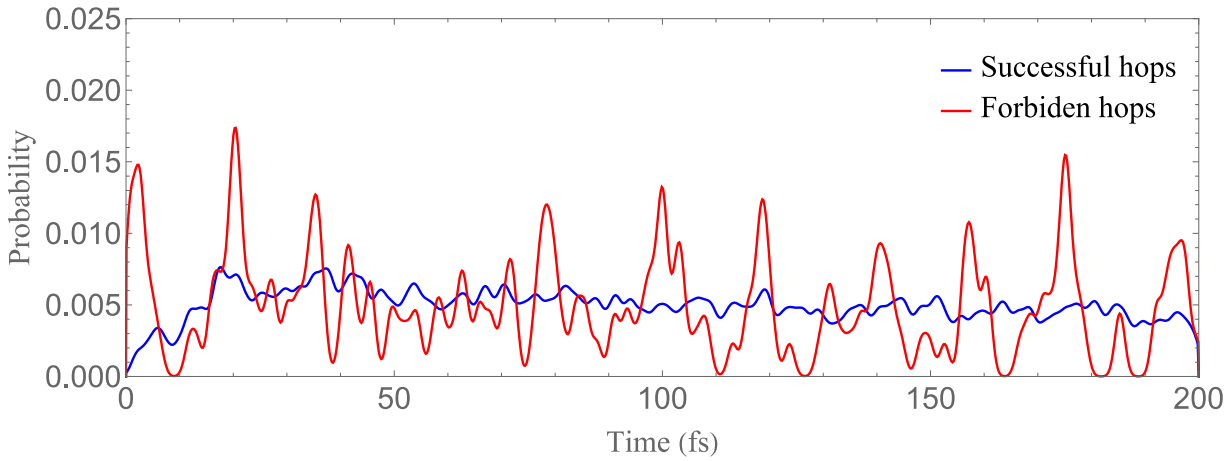

Figure S4. Probability density functions of successful and forbidden hops during SH-NEXMD simulations at 300 K.