Supplementary Information for

Nonadiabatic quantum dynamics explores non-monotonic photodissociation branching of N_2 into the $N(^4S)+N(^2D)$ and $N(^4S)+N(^2P)$ product channels

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Figures S1 to S7 provide details of key potential energy curves, their nonadiabatic couplings and their spin-orbit couplings.

	$^1\Sigma_u^+$	--	--	--	--	--	--	--	--	--	--	--	$^1\Sigma_u^-$ (m_S=0)
$^1\Sigma_u^+$ (m_S=0)	--	$^1\Sigma_u^-$	--	--	--	--	--	--	--	--	--	--	$^1\Delta_u$ (m_S=0)
$^1\Sigma_u^-$ (m_S=0)	--	--	$^1\Delta_u$	--	LSZ	LSX/Y	--	--	LSZ	LSX/Y	--	LSX/Y	$^3\Sigma_u^+$ (m_S=+/-1)
$^1\Delta_u$ (m_S=0)	--	--	--	$^3\Sigma_u^+$	--	LSX/Y	--	LSZ	--	LSX/Y	--	LSX/Y	$^3\Sigma_u^-$ (m_S=+/-1)
$^3\Sigma_u^+$ (m_S=0)	--	LSZ	--	--	$^3\Sigma_u^-$	--	LSX/Y	LSX/Y	LSX/Y	LSZ	LSX/Y	LSZ	$^3\Pi_u$ (m_S=0)
$^3\Sigma_u^-$ (m_S=0)	LSZ	--	--	--	--	$^3\Pi_u$	LSZ	--	--	LSX/Y	LSZ	LSX/Y	$^3\Delta_u$ (m_S=+/-1)
$^3\Pi_u$ (m_S=+/-1)	LSX/Y	LSX/Y	LSX/Y	LSX/Y	LSX/Y	LSZ	$^3\Delta_u$	--	LSZ	LSX/Y	--	--	$^5\Sigma_u^+$ (m_S=+/-1)
$^3\Delta_u$ (m_S=0)	--	--	LSZ	--	--	LSX/Y	--	$^5\Sigma_u^+$	--	LSX/Y	--	--	$^5\Sigma_u^-$ (m_S=+/-1)
$^5\Sigma_u^+$ (m_S=0,+/-2)	--	--	--	--	LSZ	LSX/Y	--	--	$^5\Sigma_u^-$	LSZ	LSX/Y	--	$^5\Pi_u$ (m_S=0,+/-2)
$^5\Sigma_u^-$ (m_S=0,+/-2)	--	--	--	LSZ	--	LSX/Y	--	LSZ	--	$^5\Pi_u$	LSZ	--	$^5\Delta_u$ (m_S=+/-1)
$^5\Pi_u$ (m_S=+/-1)	--	--	--	LSX/Y	LSX/Y	LSZ	LSX/Y	LSX/Y	LSX/Y	LSZ	$^5\Delta_u$	--	$^1\Pi_u$ (m_S=0)
$^5\Delta_u$ (m_S=0,+/-2)	--	--	--	--	--	LSX/Y	LSZ	--	--	LSX/Y	LSZ	$^1\Pi_u$	

Fig. S1.Schematical representation of spin-orbit couplings between the electronic accounting for their magnetic, m_S, quantum number (in parenthesis). LSX/Y and LSZ are the Cartesian components of the spin–orbit coupling in the molecular frame. Depending on the symmetry of the optically excited singlets, $^1\Sigma_u^+$ or $^1\Pi_u$, two sets of couplings are considered: for $^1\Sigma_u^+$ at the bottom left corner (in red) and for $^1\Pi_u$ at the top right corner (in blue).

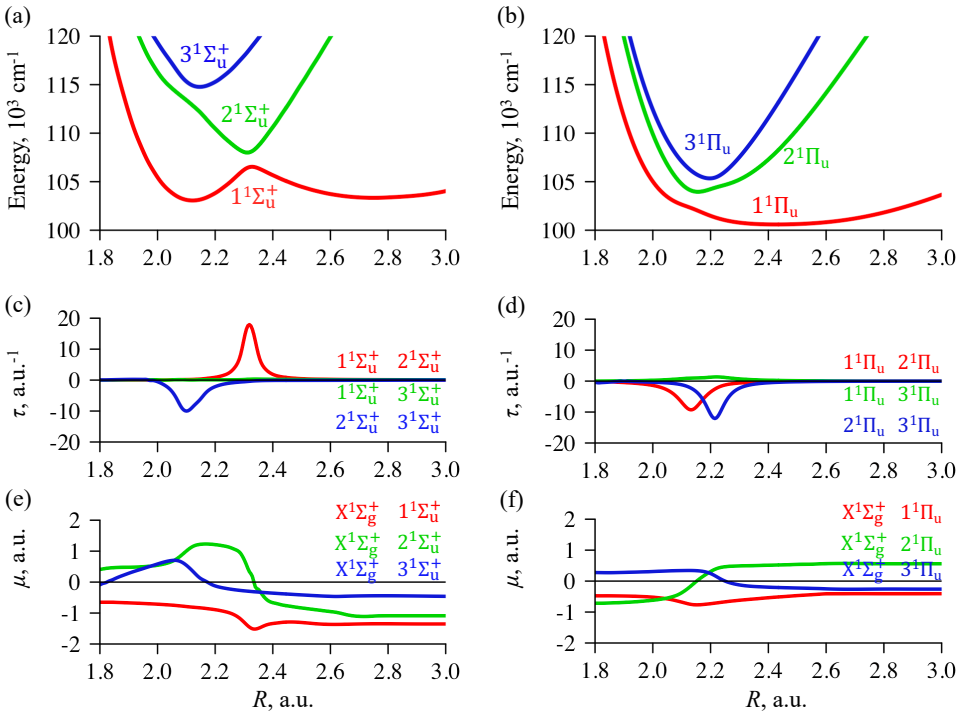

Fig. S2. Potential energy curves of the three lowest ${}^1\Sigma_u^+$ and ${}^1\Pi_u$ electronic states that are one-photon accessible from the ground state (a and b), respective $X^1\Sigma_g^+ - {}^1\Sigma_u^+$ and $X^1\Sigma_g^+ - {}^1\Pi_u$ electronic transition dipole moments (c and d) and their nonadiabatic couplings (e and f) as a function of the internuclear distance, *R*.

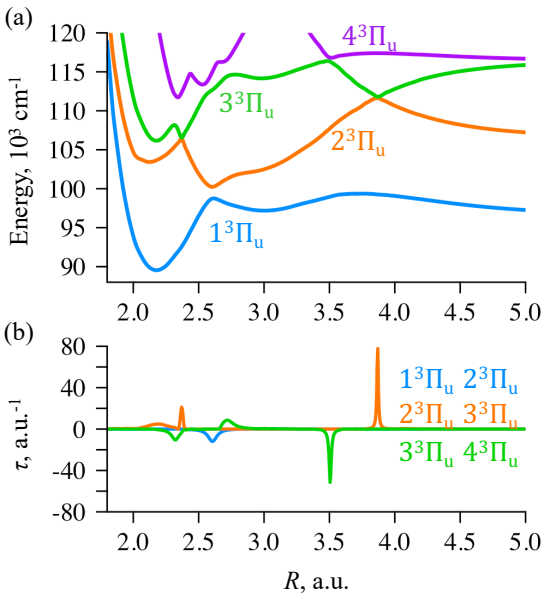

Fig. S3. Potential energy curves of the four lowest ${}^3\Pi_u$ electronic states (a) and their quite strong non-adiabatic couplings (b) as a function of the internuclear distance, *R*.

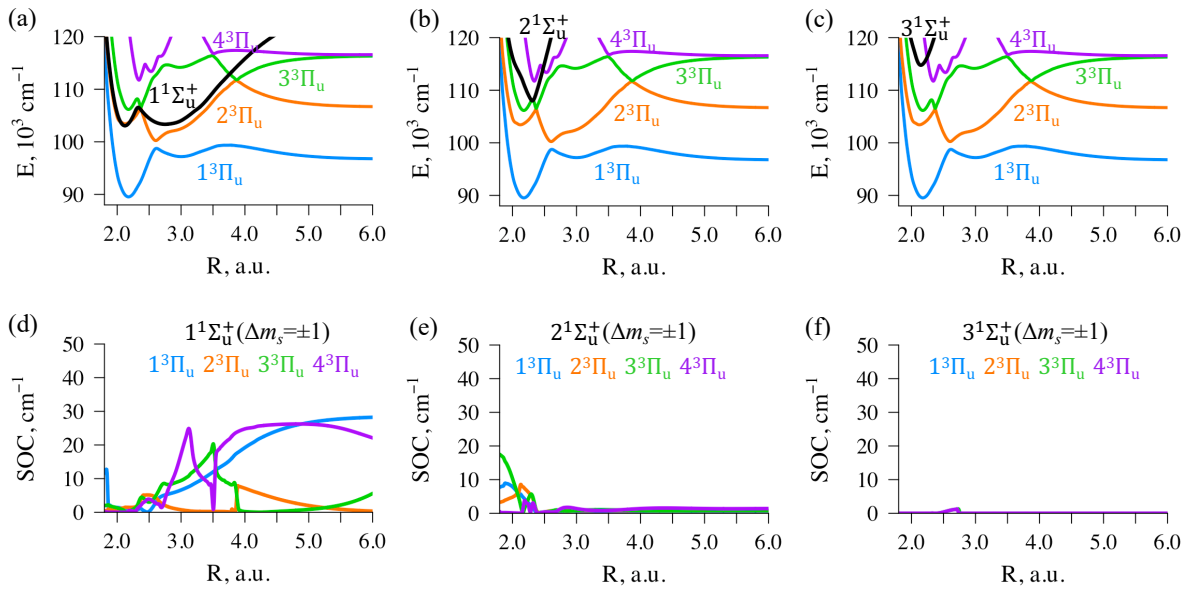

Fig. S4. Potential energy curves (a-c) and LSX/LSY spin-orbit coupling elements (d-f) between $1^1\Sigma_u^+$ (m_s=0) and $^3\Pi_u$ (m_s=1) (a, d), $2^1\Sigma_u^+$ (m_s=0) and $^3\Pi_u$ (m_s=1) (b, e), $3^1\Sigma_u^+$ (m_s=0) and $^3\Pi_u$ (m_s=1) (c, f) electronic states.

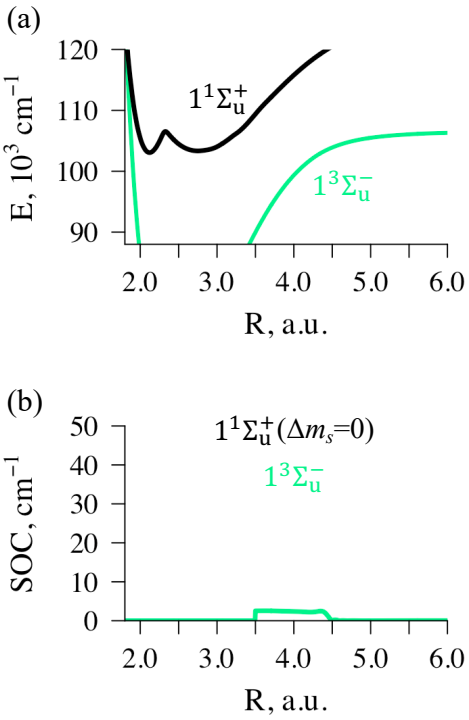

Fig. S5. Potential energy curves (a) and spin-orbit coupling elements (b) between electronic $1^1\Sigma_u^+$ (m_s=0) and $1^3\Sigma_u^-$ (m_s=0) (LSZ component).

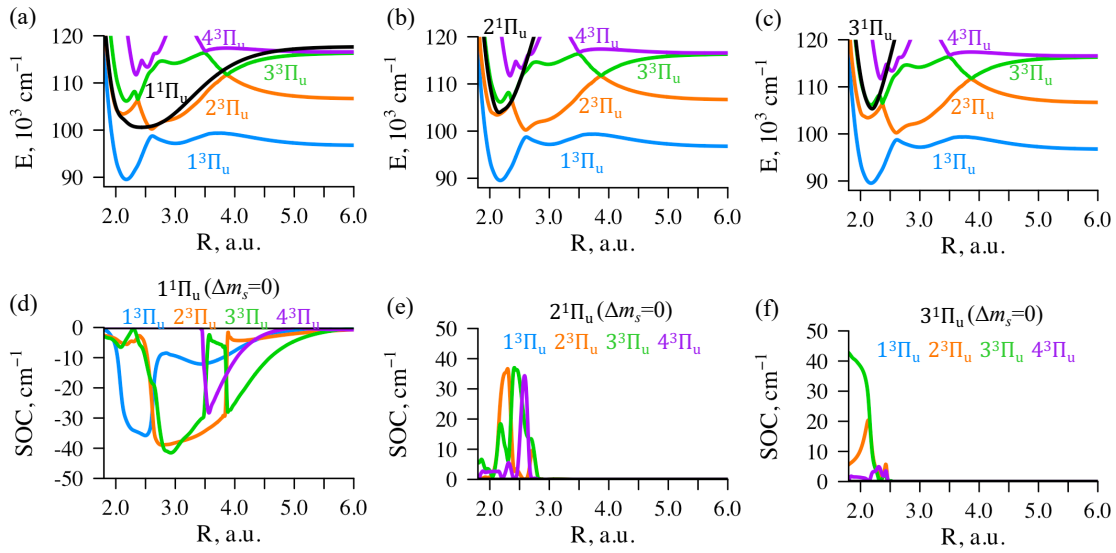

Fig. S6. Potential energy curves (a-c) and LSZ spin-orbit coupling elements (d-f) between 1 $^1\Pi_u$ (m_s=0) and $^3\Pi_u$ (m_s=0) (a, d), 2 $^1\Pi_u$ (m_s=0) and $^3\Pi_u$ (m_s=0) (b, e), 3 $^1\Pi_u$ (m_s=0) and $^3\Pi_u$ (m_s=0) (c, f) electronic states.

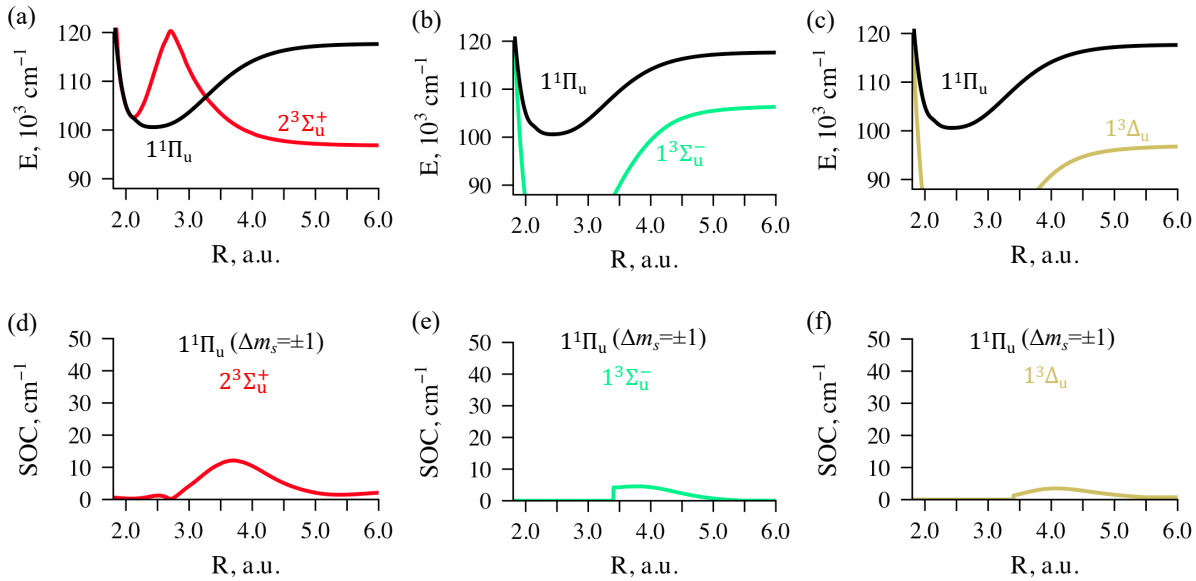

Fig. S7. Potential energy curves (a-c) and spin-orbit LSX/LSY coupling elements (d-f) between different electronic states: 1 $^1\Pi_u$ (m_s=0) and 2 $^3\Sigma_u^+$ (m_s=0), $1^3\Sigma_u^-$ (m_s=0), 1 $^3\Delta_u$ (m_s=0).