The origin of chirality induced spin selectivity in photo-induced electron transfer

Thomas P. Fay\textsuperscript{1, a) and David T. Limmer\textsuperscript{1, 2, 3, 4}

\textsuperscript{1) Department of Chemistry, University of California, Berkeley, CA 94720, USA
\textsuperscript{2) Kavli Energy Nanoscience Institute at Berkeley, Berkeley, CA 94720, USA
\textsuperscript{3) Chemical Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA
\textsuperscript{4) Materials Science Division, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA

Here we propose a mechanism by which spin polarization can be generated dynamically in chiral molecular systems undergoing photo-induced electron transfer. The proposed mechanism explains how spin polarization emerges in systems where charge transport is dominated by incoherent hopping, mediated by spin orbit and electronic exchange couplings through an intermediate charge transfer state. We derive a simple expression for the spin polarization that predicts a non-monotonic temperature dependence consistent with recent experiments. We validate this theory using approximate quantum master equations and the numerically exact hierarchical equations of motion. The proposed mechanism of chirality induced spin selectivity should apply to many chiral systems, and the ideas presented here have implications for the study of spin transport at temperatures relevant to biology, and provide simple principles for the molecular control of spins in fluctuating environments.

Chirality induced spin selectivity (CISS), in which molecular chirality controls spin polarization of electrons, has been observed in a wide variety of systems,\textsuperscript{1–3} including in photo-induced electron transfer in artificial systems,\textsuperscript{4} such as quantum dots,\textsuperscript{5} and biological molecules, such as photosystem I\textsuperscript{6} and DNA.\textsuperscript{7, 8} Based on this, it has been suggested that CISS may serve some biological functions\textsuperscript{9} and that it could be exploited in nano- and molecular-scale spintronics technologies.\textsuperscript{1, 10}

Here we focus on the CISS effect in photo-induced molecular electron transfer.\textsuperscript{5} This effect is particularly puzzling, as it goes against the conventional notion that the initial singlet spin state of the system is preserved in this process.\textsuperscript{11}

Theoretical descriptions of CISS have primarily been confined to either the coherent regime,\textsuperscript{12–16} where electron transport is treated as a coherent tunneling process through a chiral molecular junction between leads, or static spin polarizations produced by spin-orbit coupling in the ground state of chiral molecules.\textsuperscript{17–19} However photo-induced electron transfer in molecules like photosystem I, where electrons incoherently hop between a discrete set of donor and acceptor sites, cannot be described by either of these theories.\textsuperscript{20} In such systems coupling of the electron transfers to molecular vibrations is strong,\textsuperscript{21} and electronic exchange interactions can also be significant.\textsuperscript{11} This necessitates the development of a theory of CISS that is appropriate for this incoherent regime of electron transport. Fortunately such techniques have been developed, primarily for understanding rates and dynamics of electron transfer reactions,\textsuperscript{22, 23} and through the tools of quantum master equations such theories can be adapted to describe spin transport.\textsuperscript{24, 25} These techniques have recently been used to show that spin coherence, but no spin polarization, arises in a single electron transfer step in a chiral environment mediated by spin-orbit coupling.\textsuperscript{25} Here we expand on this theory, and show how the interplay of chirality induced spin coherence, electron hopping, and electronic exchange coupling dynamically produce large spin polarizations in electron transfer reactions. The theory presented here will be shown to explain the observed temperature dependence of CISS in photosystem I, and it also provides a framework for engineering molecules to maximize the CISS effect.

Let us start by reviewing how photo-initiated charge transfer, between a donor D and acceptor A, in chiral molecules generates spin coherence in charge transfer states, as described in Ref. 25. This process generally proceeds via an electron transfer reaction from a bright locally excited singlet state, $S_1 = D^* - A$, to a charge transfer state, $CT = D^+ - A^-$, which can exist in either a singlet or triplet spin state,

$$S_1 \longrightarrow CT.$$ \hspace{1cm} (1)

As discussed in Ref. 25 direct diabatic coupling generates the CT state in a singlet $|S\rangle = (\langle \downarrow_D \uparrow_A \rangle - \langle \downarrow_D \uparrow_A \rangle) / \sqrt{2}$ spin state, whereas spin-orbit coupling (SOC) generates the CT state in the $i |T_0\rangle = i(|\uparrow_D \downarrow_A \rangle + |\downarrow_D \uparrow_A \rangle) / \sqrt{2}$ (taking the z axis to be defined by the spin-orbit coupling vector).\textsuperscript{26} So overall this electron transfer, mediated by spin-orbit coupling in a chiral molecule, generates the CT state in a coherent superposition of singlet and $|T_0\rangle$ triplet spin states, and its initial spin density operator, $\hat{\sigma}_{CT}(t)$, is given by

$$\hat{\sigma}_{CT}(0) = |\psi_0\rangle \langle \psi_0|,$$ \hspace{1cm} (1)

where $|\psi_0\rangle = \cos \theta |S\rangle + i \sin \theta |T_0\rangle$. The mixing angle $\theta$, is determined by the relative strength of the spin-preserving diabatic coupling $V_{DA}$ and the spin-orbit coupling $\Lambda_{DA}$, as $\theta = \arctan(\Lambda_{DA} / (2V_{DA}))$, and because the sign of $\Lambda_{DA}$ depends on the chirality of the molecule, the sign of $\theta$ also depends on chirality. The spin polarization of the CT state is defined as the difference in the z component of the spins between D and A. This is given by the expectation value of $\Delta S_z = \hat{\sigma}_{CT} - \hat{\sigma}_{\Lambda z} = |S\rangle \langle T_0| + |T_0\rangle \langle S|$, so the spin polarization is proportional to the real part of the singlet-triplet coherence, $\langle S|\hat{\sigma}_{CT}|T_0\rangle$. However the CT state is generated with purely imaginary singlet-triplet coherence, so no spin polarization is formed directly by the electron transfer.\textsuperscript{25}

Now let us consider how the spin state $\hat{\sigma}_{CT}$ evolves when there exists an exchange coupling between the donor and acceptor electron spins in the CT state. In this case the spin Hamiltonian for the CT state can be taken to be $\hat{H}_{CT} = -2J \hat{P}_T \cdot (\hat{P}_T$ is a triplet spin projection operator),\textsuperscript{27} and the time-evolution
The presence of exchange coupling effects a chirality-dependent transient oscillating spin polarization in the CT state. However this spin polarization clearly averages over time to zero. This naturally raises the question of how a static spin polarization can be generated in a photo-induced charge transfer reaction. The answer lies in the fact that many photo-generated CT states are not formed by a simple direct electron transfer, but rather the final CT state is often formed via a sequence of downhill electron transfers via intermediate CT states. The final CT state is often a well-separated radical ion pair state. In this state the exchange coupling between donor and acceptor spins is very weak, but the intermediate CT states often have a significantly larger exchange coupling, due to the closer proximity of the unpaired electrons. In this way, imaginary-valued singlet-triplet coherence created through spin-orbit coupled charge transfer can be transiently converted into a net spin polarization between the donor and acceptor electrons in an intermediate CT state with a large exchange coupling. This spin polarization can be transferred to the final CT state via a subsequent incoherent spin state preserving electron transfer. The spin polarization transferred to the final CT no longer oscillates due to the weak exchange coupling in this state, thus a net static spin polarization is generated. This is the basic mechanism by which static spin polarization can be generated in multi-step electron transfer reactions in chiral molecules.

We will now explore this further, by considering the simplest multi-state model including only one intermediate CT state in the chiral system (i.e. a three state model),

\[
S_1 \xrightarrow{k_{ET1}} CT_1 \xrightarrow{k_{ET2}} CT_2.
\]

We take the precursor state to be an excited donor state, \(S_1 = D^*-A_1-A_2\), the intermediate charge transfer state corresponds to an electron transfer from D to a primary acceptor \(A_1\), so \(CT_1 = D^*-A^*_1-A_2\), and the final charge transfer state \(CT_2\) is taken as the state formed by electron transfer from the primary acceptor \(A_1\) to the secondary acceptor \(A_2\), so \(CT_2 = D^*-A_1-A^*_2\). The CT states can exist in either singlet or triplet spin states but the \(S_1\) state only exists in the singlet spin state. A schematic of this system is shown in Fig. 1. To start with, for simplicity we will assume these downhill electron transfers occur irreversibly, and we will also assume that only the first electron transfer is spin-dependent, and occurs via chiral spin-orbit coupled charge transfer.

In this model, the spin density operators for each state obey the following set of equations,\(^{24,25}\)

\[
\frac{d}{dt} \hat{\sigma}_{S_1}(t) = -k_{ET1} \hat{\sigma}_{S_1}(t) \quad (4a)
\]

\[
\frac{d}{dt} \hat{\sigma}_{CT_1}(t) = -i \frac{\hat{H}_{CT_1}}{\hbar} + i \frac{\hat{H}_{CT_2}}{\hbar} \quad (4b)
\]

\[
\frac{d}{dt} \hat{\sigma}_{CT_2}(t) = -i \frac{\hat{H}_{CT_2}}{\hbar} \hat{\sigma}_{CT_1}(t) + k_{ET2} \hat{\sigma}_{CT_1}(t) \quad (4c)
\]

Here \(\hat{H}_{CT1}\) and \(\hat{H}_{CT2}\) are the spin Hamiltonians for the \(CT_1\) and \(CT_2\) states, describing all the spin interactions in these states. Here the spin Hamiltonians are simplified to just include the exchange couplings, so \(\hat{H}_{CT1} = -2J \hat{P}_x\) and \(\hat{H}_{CT2} = 0\) (the energy differences between different CT states enter into the master equations via the rate constants). This set of coupled equations can be obtained straightforwardly using perturbative Nakajima-Zwanzig theory,\(^{26,29}\) as has been described previously (a summary of the approximations in Refs. 24 and 25 will be discussed shortly). The shift term \(\delta \epsilon\) naturally emerges from the master equation theory, and its value will depend on the details of the electron transfer process. For a large downhill driving force, \(\Delta G_{CT1}\), it can be estimated as \(\delta \epsilon \approx -(\epsilon^{DA_1}_D + (\epsilon^{DA_2}_A/2)^2)/(\epsilon^{ET1} - \Delta G_{ET1})\), where \(\epsilon^{ET1}\) is the reorganization energy for the first electron transfer. We can also understand the \(\delta \epsilon\) term as a net chiral superexchange spin-orbit coupling term, which couples S and \(T_0\) states via the \(S_1\) state.

One can then solve these Eq. (4) analytically for an initial state where only \(S_1\) is populated, with \(\hat{\sigma}_{S_1}(0) = |S\rangle\langle S|\), from which the final spin polarization in \(CT_2\), given by \(\langle \Delta P_z \rangle = \lim_{t \to \infty} \text{tr}[\hat{\sigma}_{CT2}(t)]\), is found to be

\[
\langle \Delta P_z \rangle = -\frac{k_{ET2}(2J/\hbar) \sin(2\theta)}{k_{ET2}^2 + \Omega^2}.
\]
the potentials are harmonic. Given in the SI, Eq. (S.1)). Using the Hierarchical Equations of Motion (HEOM), we can compute the exact dynamics when the potentials are harmonic. 

For comparison, we also perform simulations of this model with the full perturbative QMEs, Eq. (4), modified to include back reaction terms. To briefly summarise the approximations used in Refs. 24 and 25 to obtain these, in these QMEs we assume the coherences between different electron transfer states, e.g. $|S_1\rangle\langle CT_1, S_1\rangle$, are short-lived and small (due to the large differences between potential energy surfaces), so these coherences are projected out using Nakajima-Zwanzig theory (but spin coherences are retained). The Nakajima-Zwanzig kernel is then expanded at lowest order in the diabatic couplings, with spin Hamiltonian terms in the kernel ignored (due to the large separation in energy scale between the nuclear motion and spin dynamics), and the population transfer dynamics are treated as Markovian. For the harmonic bath model given above, the second order QME parameters (rate constants and $\delta \epsilon$) can be computed exactly from the spectral density; details of which are given in the SI. In the high temperature limit, these rates can be well approximated with Marcus theory, $k_{ET} = (1/\hbar)\Gamma_{DA}^2 (\pi/\lambda_{ET} k_B T)^{1/2} e^{-2\lambda_{ET}/\hbar k_B T}$, where $\Gamma_{DA} = (V_{DA}^2 + \Lambda_{DA}^2 / 4)^{1/2}$ is the combined diabatic/SOC coupling for the electron transfer. Although we only consider harmonic potential energy surfaces here, the QMEs apply to general potential energy surfaces for the electron transfer states.

We set the free energy changes of the electron transfers to be $\Delta G_{ET1} = -0.1$ eV and $\Delta G_{ET2} = -0.25$ eV, with reorganisation energies of $\lambda_{ET1} = 0.1$ eV and $\lambda_{ET2} = 0.2$ eV. Diabatic state couplings are taken as $\Gamma_{DA} = (V_{DA}^2 + \Lambda_{DA}^2 / 4)^{1/2} = 0.5$ meV ($S_1$-CT1 coupling) and $\Gamma_{DA} = V_{DA}^2 + \Lambda_{DA}^2 / 4 = 0.25$ meV (CT1-CT2 coupling), and $\theta = \pi/16$, which corresponds to ~4% of CT1 molecules being formed in the triplet state. In these models we treat the intramolecular vibrational modes and solvent bath as a single harmonic bath with a Debye spectral density. For comparison, we also perform simulations of this model with the full perturbative QMEs, Eq. (4), modified to include back reaction terms. To briefly summarise the approximations used in Refs. 24 and 25 to obtain these, in these QMEs we assume the coherences between different electron transfer states, e.g. $|S_1\rangle\langle CT_1, S_1\rangle$, are short-lived and small (due to the large differences between potential energy surfaces), so these coherences are projected out using Nakajima-Zwanzig theory (but spin coherences are retained). The Nakajima-Zwanzig kernel is then expanded at lowest order in the diabatic couplings, with spin Hamiltonian terms in the kernel ignored (due to the large separation in energy scale between the nuclear motion and spin dynamics), and the population transfer dynamics are treated as Markovian. For the harmonic bath model given above, the second order QME parameters (rate constants and $\delta \epsilon$) can be computed exactly from the spectral density; details of which are given in the SI. In the high temperature limit, these rates can be well approximated with Marcus theory, $k_{ET} = (1/\hbar)\Gamma_{DA}^2 (\pi/\lambda_{ET} k_B T)^{1/2} e^{-2\lambda_{ET}/\hbar k_B T}$, where $\Gamma_{DA} = (V_{DA}^2 + \Lambda_{DA}^2 / 4)^{1/2}$ is the combined diabatic/SOC coupling for the electron transfer. Although we only consider harmonic potential energy surfaces here, the QMEs apply to general potential energy surfaces for the electron transfer states.

We set the free energy changes of the electron transfers to be $\Delta G_{ET1} = -0.1$ eV and $\Delta G_{ET2} = -0.25$ eV, with reorganisation energies of $\lambda_{ET1} = 0.1$ eV and $\lambda_{ET2} = 0.2$ eV. Diabatic state couplings are taken as $\Gamma_{DA} = (V_{DA}^2 + \Lambda_{DA}^2 / 4)^{1/2} = 0.5$ meV ($S_1$-CT1 coupling) and $\Gamma_{DA} = V_{DA}^2 + \Lambda_{DA}^2 / 4 = 0.25$ meV (CT1-CT2 coupling), and $\theta = \pi/16$, which corresponds to ~4% of CT1 molecules being formed in the triplet state. In these models we treat the intramolecular vibrational modes and solvent bath as a single harmonic bath with a Debye spectral density. For comparison, we also perform simulations of this model with the full perturbative QMEs, Eq. (4), modified to include back reaction terms. To briefly summarise the approximations used in Refs. 24 and 25 to obtain these, in these QMEs we assume the coherences between different electron transfer states, e.g. $|S_1\rangle\langle CT_1, S_1\rangle$, are short-lived and small (due to the large differences between potential energy surfaces), so these coherences are projected out using Nakajima-Zwanzig theory (but spin coherences are retained). The Nakajima-Zwanzig kernel is then expanded at lowest order in the diabatic couplings, with spin Hamiltonian terms in the kernel ignored (due to the large separation in energy scale between the nuclear motion and spin dynamics), and the population transfer dynamics are treated as Markovian. For the harmonic bath model given above, the second order QME parameters (rate constants and $\delta \epsilon$) can be computed exactly from the spectral density; details of which are given in the SI. In the high temperature limit, these rates can be well approximated with Marcus theory, $k_{ET} = (1/\hbar)\Gamma_{DA}^2 (\pi/\lambda_{ET} k_B T)^{1/2} e^{-2\lambda_{ET}/\hbar k_B T}$, where $\Gamma_{DA} = (V_{DA}^2 + \Lambda_{DA}^2 / 4)^{1/2}$ is the combined diabatic/SOC coupling for the electron transfer. Although we only consider harmonic potential energy surfaces here, the QMEs apply to general potential energy surfaces for the electron transfer states.

We set the free energy changes of the electron transfers to be $\Delta G_{ET1} = -0.1$ eV and $\Delta G_{ET2} = -0.25$ eV, with reorganisation energies of $\lambda_{ET1} = 0.1$ eV and $\lambda_{ET2} = 0.2$ eV. Diabatic state couplings are taken as $\Gamma_{DA} = (V_{DA}^2 + \Lambda_{DA}^2 / 4)^{1/2} = 0.5$ meV ($S_1$-CT1 coupling) and $\Gamma_{DA} = V_{DA}^2 + \Lambda_{DA}^2 / 4 = 0.25$ meV (CT1-CT2 coupling), and $\theta = \pi/16$, which corresponds to ~4% of CT1 molecules being formed in the triplet state. In these models we treat the intramolecular vibrational modes and solvent bath as a single harmonic bath with a Debye spectral density. For comparison, we also perform simulations of this model with the full perturbative QMEs, Eq. (4), modified to include back reaction terms. To briefly summarise the approximations used in Refs. 24 and 25 to obtain these, in these QMEs we assume the coherences between different electron transfer states, e.g. $|S_1\rangle\langle CT_1, S_1\rangle$, are short-lived and small (due to the large differences between potential energy surfaces), so these coherences are projected out using Nakajima-Zwanzig theory (but spin coherences are retained). The Nakajima-Zwanzig kernel is then expanded at lowest order in the diabatic couplings, with spin Hamiltonian terms in the kernel ignored (due to the large separation in energy scale between the nuclear motion and spin dynamics), and the population transfer dynamics are treated as Markovian. For the harmonic bath model given above, the second order QME parameters (rate constants and $\delta \epsilon$) can be computed exactly from the spectral density; details of which are given in the SI. In the high temperature limit, these rates can be well approximated with Marcus theory, $k_{ET} = (1/\hbar)\Gamma_{DA}^2 (\pi/\lambda_{ET} k_B T)^{1/2} e^{-2\lambda_{ET}/\hbar k_B T}$, where $\Gamma_{DA} = (V_{DA}^2 + \Lambda_{DA}^2 / 4)^{1/2}$ is the combined diabatic/SOC coupling for the electron transfer. Although we only consider harmonic potential energy surfaces here, the QMEs apply to general potential energy surfaces for the electron transfer states.

We set the free energy changes of the electron transfers to be $\Delta G_{ET1} = -0.1$ eV and $\Delta G_{ET2} = -0.25$ eV, with reorganisation energies of $\lambda_{ET1} = 0.1$ eV and $\lambda_{ET2} = 0.2$ eV. Diabatic state couplings are taken as $\Gamma_{DA} = (V_{DA}^2 + \Lambda_{DA}^2 / 4)^{1/2} = 0.5$ meV ($S_1$-CT1 coupling) and $\Gamma_{DA} = V_{DA}^2 + \Lambda_{DA}^2 / 4 = 0.25$ meV (CT1-CT2 coupling), and $\theta = \pi/16$, which corresponds to ~4% of CT1 molecules being formed in the triplet state. In these models we treat the intramolecular vibrational modes and solvent bath as a single harmonic bath with a Debye spectral density. For comparison, we also perform simulations of this model with the full perturbative QMEs, Eq. (4), modified to include back reaction terms. To briefly summarise the approximations used in Refs. 24 and 25 to obtain these, in these QMEs we assume the coherences between different electron transfer states, e.g. $|S_1\rangle\langle CT_1, S_1\rangle$, are short-lived and small (due to the large differences between potential energy surfaces), so these coherences are projected out using Nakajima-Zwanzig theory (but spin coherences are retained). The Nakajima-Zwanzig kernel is then expanded at lowest order in the diabatic couplings, with spin Hamiltonian terms in the kernel ignored (due to the large separation in energy scale between the nuclear motion and spin dynamics), and the population transfer dynamics are treated as Markovian. For the harmonic bath model given above, the second order QME parameters (rate constants and $\delta \epsilon$) can be computed exactly from the spectral density; details of which are given in the SI. In the high temperature limit, these rates can be well approximated with Marcus theory, $k_{ET} = (1/\hbar)\Gamma_{DA}^2 (\pi/\lambda_{ET} k_B T)^{1/2} e^{-2\lambda_{ET}/\hbar k_B T}$, where $\Gamma_{DA} = (V_{DA}^2 + \Lambda_{DA}^2 / 4)^{1/2}$ is the combined diabatic/SOC coupling for the electron transfer. Although we only consider harmonic potential energy surfaces here, the QMEs apply to general potential energy surfaces for the electron transfer states.
FIG. 2. Population and spin polarization dynamics for a three CT state model of electron transfer calculated with HEOM (solid lines) and the second order QME (dashed lines). Left column: total populations of $S_1$ (grey), CT$_1$ (orange) and CT$_2$ (purple) as a function of time. Right column: spin polarization in CT$_1$ (orange) and CT$_2$ (purple) as a function of time, with the value predicted by Eq. (5) indicated by the black dashed line. From top to bottom the value of the exchange coupling in the CT$_1$ state is varied with $J = 100$ mT (top), 10 mT (middle) and 1 mT (bottom), where $\mu_B$ is the Bohr magneton and $g_e$ is the $g$ factor for the free electron spin.

where second order perturbation theory is valid for the rate constants and $\delta \epsilon$. The general form of the master equation presented above is only slightly altered on including higher order effects in the electronic coupling; specifically we should add a decoherence term of the form $-(k_D/2)\langle [\psi_\theta | [\psi_\theta , \sigma_{\text{CT}_1}(t)] \rangle$ to the equation for $\sigma_{\text{CT}_i}(t)$. This causes the spin polarization in the intermediate state to decay, but for sufficiently large $2J$ significant spin polarization can still emerge and subsequently be transferred to the final CT state. This is demonstrated in Fig. 3 where we show the population dynamics (top panel), spin polarization (bottom panel, solid lines), and zero quantum coherence (bottom panel, dashed lines) for the three state model with $\Gamma_{DA_1} = 10$ meV, $V_{A_1A_2} = 5$ meV and $J/g_e\mu_B = 2$ T. In this limit the second order rate constant for the first electron transfers are approximately a factor of 5 too large compared to those obtained by fitting the population dynamics, so this example is clearly outside of the limits of second order perturbation theory. However, we still clearly see the emergence of a large static spin polarization ($\sim 30\%$) in the CT$_2$ state, as well as significant zero quantum coherence. This demonstrates that this mechanism can produce significant spin polarizations even outside the second order limit.

Having validated the general theory on a model condensed phase electron transfer, let us consider how this hopping mechanism predicts a temperature dependent spin polarization in chiral systems. Returning to Eq. (5) for $\langle \Delta P_z \rangle$, we can see how this temperature dependence emerges. Typically the exchange coupling, and energy shift terms are, to a good approximation, independent of temperature, whereas if the electron transfer is activated, $k_{\text{ET2}}$ will have an exponential dependence on inverse temperature. Therefore increasing $T$ will generally increase the ratio $k_{\text{ET2}}/\Omega$, so the spin polarization will
The fitted parameters are $a = 8.346 \times 10^6$ K$^{1/2}$ and $E_a = 0.32$ eV.

ACKNOWLEDGEMENTS

We would like to thank Anthony Poggio for useful comments on this manuscript. We are also thankful to Peter Hore for pointing out the connection between this work and the CIDEP effect in the EPR literature. TPF and DTL were supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, CPIMS Program Early Career Research Program under Award No. DE-FOA0002019.

SUPPORTING INFORMATION

Further details of the HEOM and QME calculations, a brief analysis of the effects of competing back reactions and singlet-triplet dephasing on spin polarization, and a discussion of the connection between SOC mediated CISS and chemically induced dynamic electron polarization (CIDEP).

REFERENCES

1. R. Naaman and D. H. Waldeck, “Spintronics and Chirality: Spin Selectivity in Electron Transport Through Chiral Molecules,” Annu. Rev. Phys. Chem. 66, 263–281 (2015).
2. R. Naaman, Y. Paltiel, and D. H. Waldeck, “Chiral Molecules and the Spin Selectivity Effect,” J. Phys. Chem. Lett. 11, 3660–3666 (2020).
3. D. H. Waldeck, R. Naaman, and Y. Paltiel, “The spin selectivity effect in chiral materials,” APL Mater. 9, 040902 (2021).
4. J. M. Abendroth, D. M. Sterner, B. P. Bloom, P. Roy, R. Naaman, D. H. Waldeck, P. S. Weiss, and P. C. Mondal, “Spin Selectivity in Photoinduced Charge-Transfer Mediated by Chiral Molecules,” ACSNano 13, 4928–4946 (2019).
5. B. P. Bloom, B. M. Graff, S. Ghosh, D. N. Beratan, and D. H. Waldeck, “Chirality Control of Electron Transfer in Quantum Dot Assemblies,” J. Am. Chem. Soc. 139, 9038–9043 (2017).
6. I. Carmeli, K. S. Kumar, O. Heifter, C. Carmeli, and R. Naaman, “Spin selectivity in electron transfer in photosystem i,” Angew. Chemie - Int. Ed. 53, 8953–8958 (2014).
7. K. Michaeli, N. Kantor-Uriel, R. Naaman, and D. H. Waldeck, “The electron’s spin and molecular chirality – how are they related and how do they affect life processes?” Chem. Soc. Rev. 45, 6478–6487 (2016).
J. R. Brandt, F. Salerno, and M. J. Fuchter, “The added value of small-molecule chirality in technological applications,” Nat. Rev. Chem. 1, 0045 (2017).
M. R. Wasielewski, “Energy, Charge, and Spin Transport in Molecules and Self-Assembled Nanostructures Inspired by Photosynthesis,” J. Org. Chem. 71, 5051–5066 (2006).
S. Dalm and P. Hedegård, “Theory of Chiral Induced Spin Selectivity,” Nano Lett. 19, 5253–5259 (2019).
P.-J. Hu, S.-X. Wang, X.-H. Gao, Y.-Y. Zhang, T.-F. Fang, A.-M. Guo, and Q.-F. Sun, “Spin-dependent electron transport along hairpinlike DNA molecules,” Phys. Rev. B 102, 195406 (2020).
M. Geyer, R. Gutierrez, and G. Cuniberti, “Effective Hamiltonian model for helically constrained quantum systems within adiabatic perturbation theory: Application to the chirality-induced spin selectivity (CISS) effect,” J. Chem. Phys. 152, 214105 (2020).
R. Gutierrez, E. Díaz, R. Naaman, and G. Cuniberti, “Spin-selective transport through helical molecular systems,” Phys. Rev. B 85, 081404 (2012).
K. Michaël and R. Naaman, “Origin of Spin-Dependent Tunneling Through Chiral Molecules,” J. Phys. Chem. C 123, 17043–17048 (2019).
A. Dianat, R. Gutiérrez, and G. Cuniberti, “Effective Hamiltonian model for helically constrained quantum systems within adiabatic perturbation theory: Application to the chirality-induced spin selectivity (CISS) effect,” J. Chem. Phys. 152, 214105 (2020).
R. Gutierrez, E. Díaz, R. Naaman, and G. Cuniberti, “Spin-selective transport through helical molecular systems,” Phys. Rev. B 85, 081404 (2012).
K. Michaël and R. Naaman, “Origin of Spin-Dependent Tunneling Through Chiral Molecules,” J. Phys. Chem. C 123, 17043–17048 (2019).
A. Dianat, R. Gutiérrez, H. Alpern, V. Mujica, A. Ziv, S. Yochemis, O. Millo, Y. Paltiel, and G. Cuniberti, “Role of Exchange Interactions in the Magnetic Response and Intermolecular Recognition of Chiral Molecules,” Nano Lett. 20, 7077–7086 (2020).
J. Fransson, “Vibrational origin of exchange splitting and “chiral-induced spin selectivity,” Phys. Rev. B 102, 235416 (2020).
J. Fransson, “Charge Redistribution and Spin Polarization Driven by Correlation Induced Electron Exchange in Chiral Molecules,” Nano Lett. 21, 3026–3032 (2021).
M. G. Muller, C. Slavov, R. Luthra, K. E. Redding, and A. R. Holzwarth, “Independent initiation of primary electron transfer in the two branches of the photosystem I reaction center,” Proc. Natl. Acad. Sci. 107, 4123–4128 (2010).
J. Blumberger, “Recent Advances in the Theory and Molecular Simulation of Biological Electron Transfer Reactions,” Chem. Rev. 115, 11191–11238 (2015).
V. May and O. Kühn, Charge and Energy Transfer Dynamics in Molecular Systems (Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim, 2000).
A. Nitzan, Chemical Dynamics in Condensed Phases (Oxford University Press, 2006).
T. P. Fay, L. P. Lindoy, and D. E. Manolopoulos, “Spin-selective electron transfer reactions of radical pairs: Beyond the Haberkorn master equation,” J. Chem. Phys. 149, 064107 (2018).
T. P. Fay, “Chirality-Induced Spin Coherence in Electron Transfer Reactions,” J. Phys. Chem. Lett. 12, 1407–1412 (2021).