Chiral induced spin selectivity and time-reversal symmetry braking

Amnon Aharony

TEL AVIV UNIVERSITY אוניברסיטת תל-אביב

Ora Entin-Wohlman and Yasuhiro Utsumi (Mie)

Shlomi Mattiyahu (BGU), Guy Cohen (BGU), Yasuhiro Tokura (Tsukuba), Seigo Tarucha (U Tokyo) , Shingo Katsumoto (ISSP), Robert Shekhter & Mats Jonson (Göteborg), Wei-Min Zhang (Tainan), Carlos Balseiro (CNEA)

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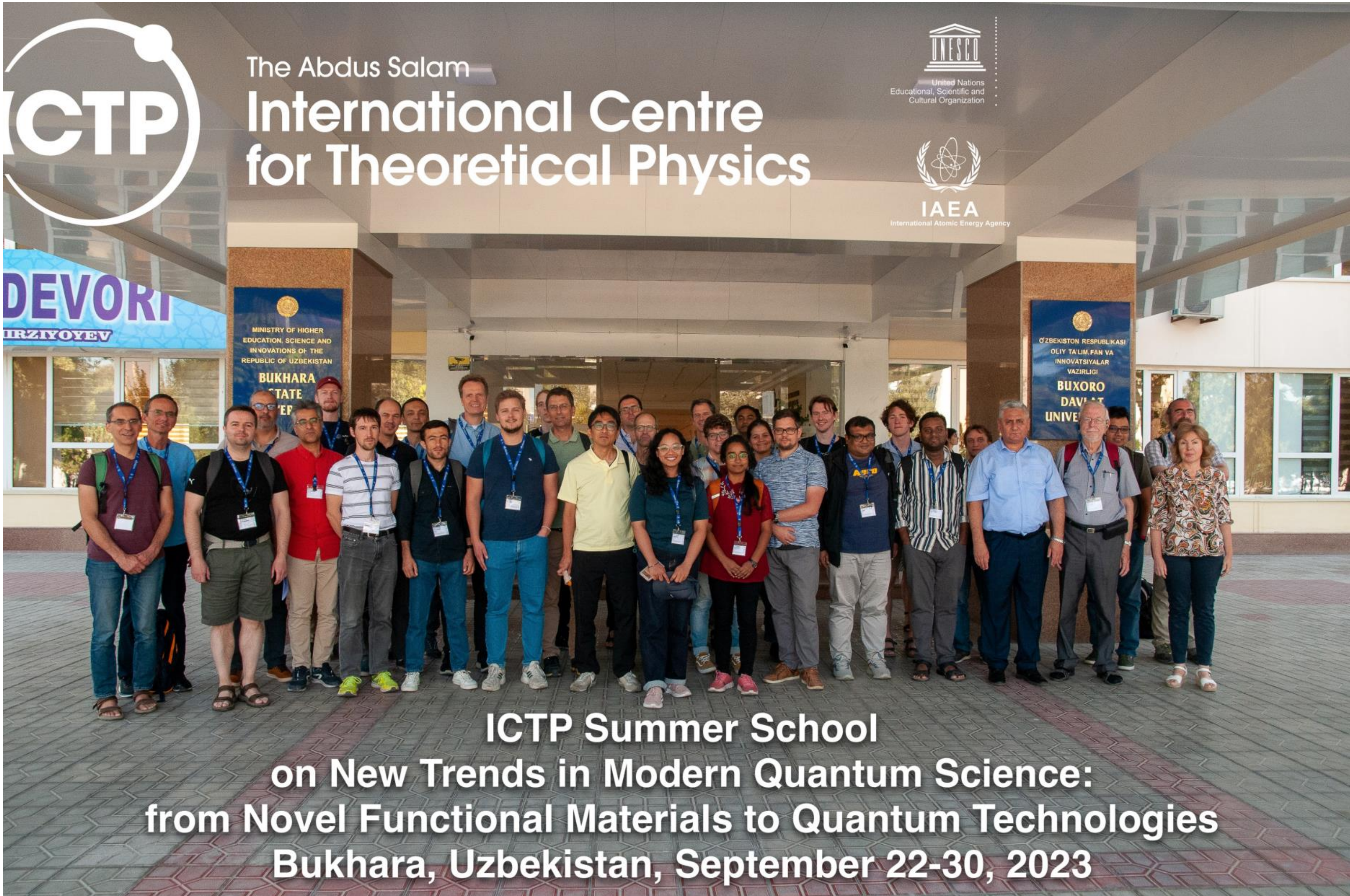
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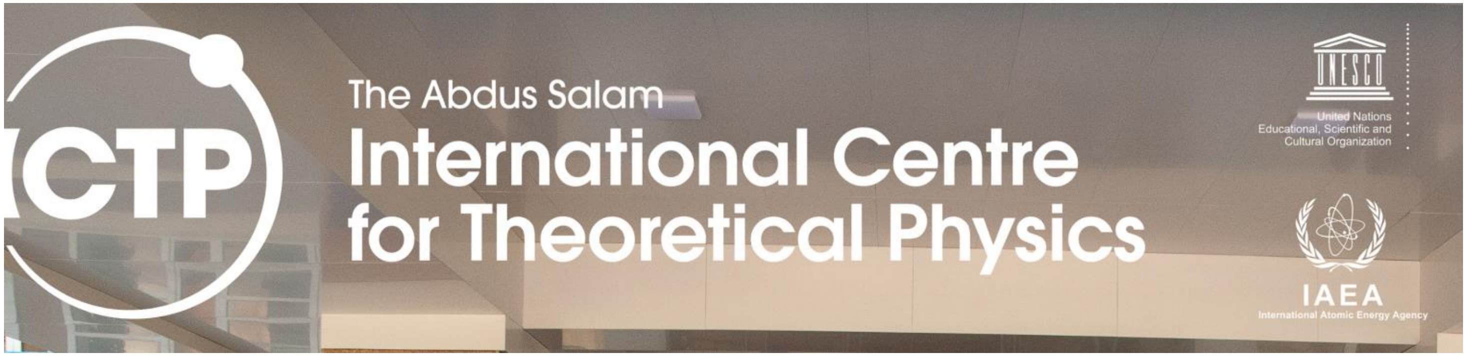

Abdus Salam

Yuval Ne’eman

Amnon Aharony

Yuval Gefen, Yigal Meir,…

CISS = chiral-induced spin selectivity

CISS

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The CISS Effect | - Weizmann Institute of Science

The chiral-induced spin selectivity (**CISS**) effect was recently established experimentally and theoretically. The ...

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About | The CISS Effect - Weizmann Institute of Science

The Chiral Induced Spin Selectivity (**CISS**) effect is a multidisciplinary phenomenon with implications in Chemistry, Physics and Biology. We constructed this ...


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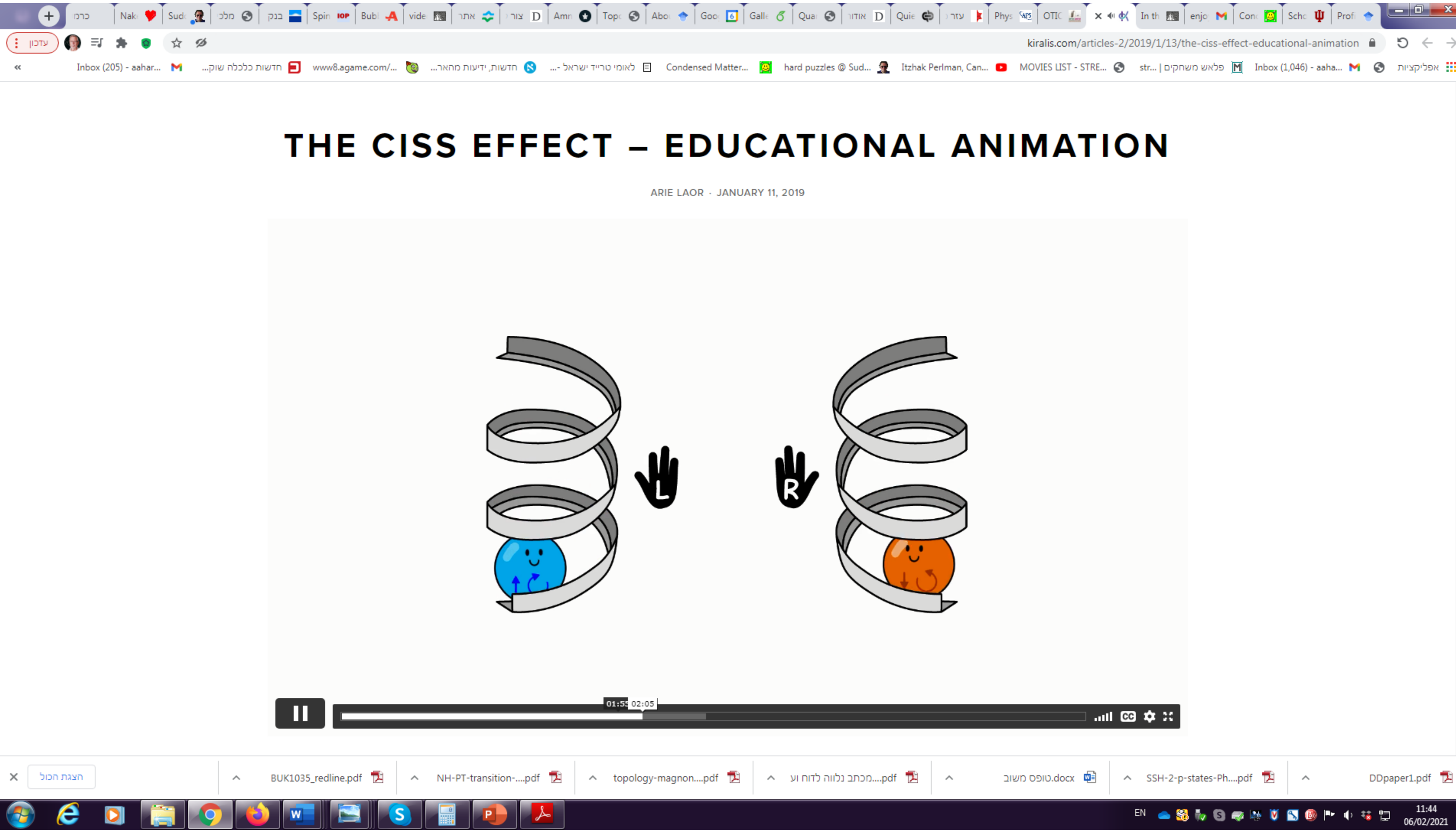
Ron Naaman


kiralis.com/articles-2/2019/1/13/the-ciss-effect-educational-animation
THE CISS EFFECT – EDUCATIONAL ANIMATION
ARIE LAOR · JANUARY 11, 2019
L
R

Chiral-induced spin selectivity (CISS)

The Journal of Physical Chemistry Letters

Letter

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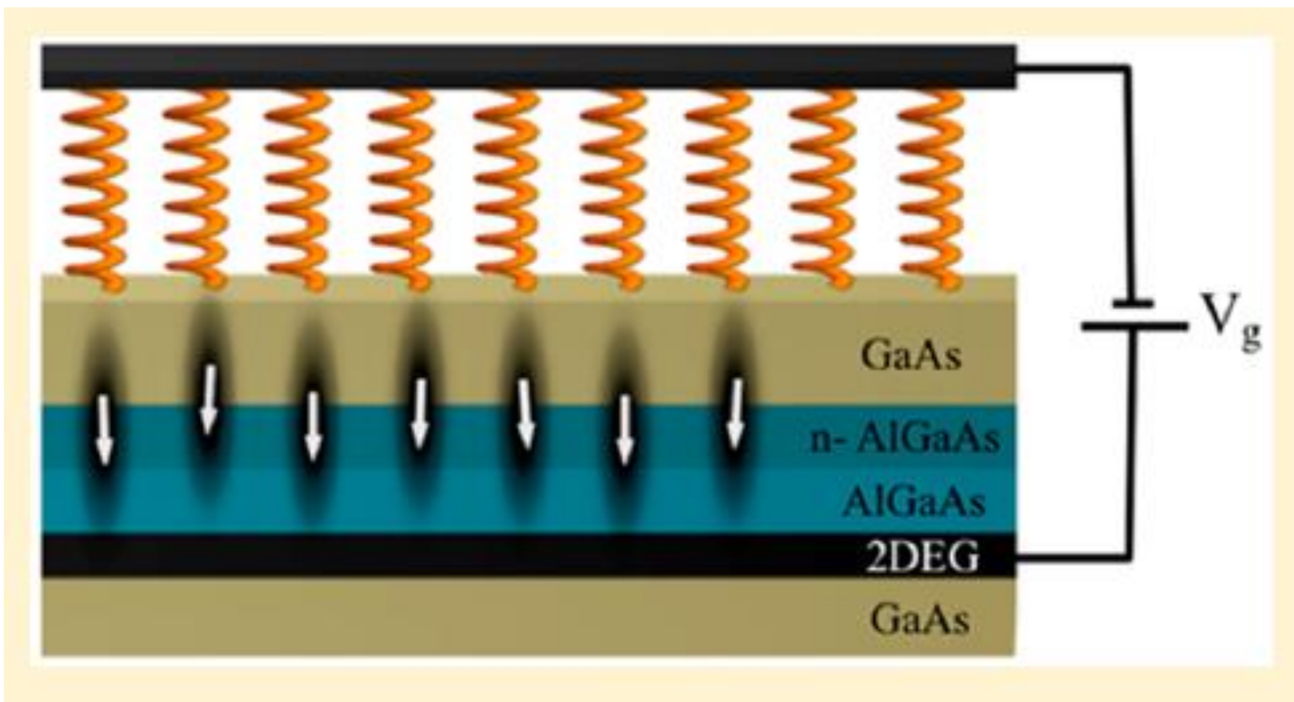
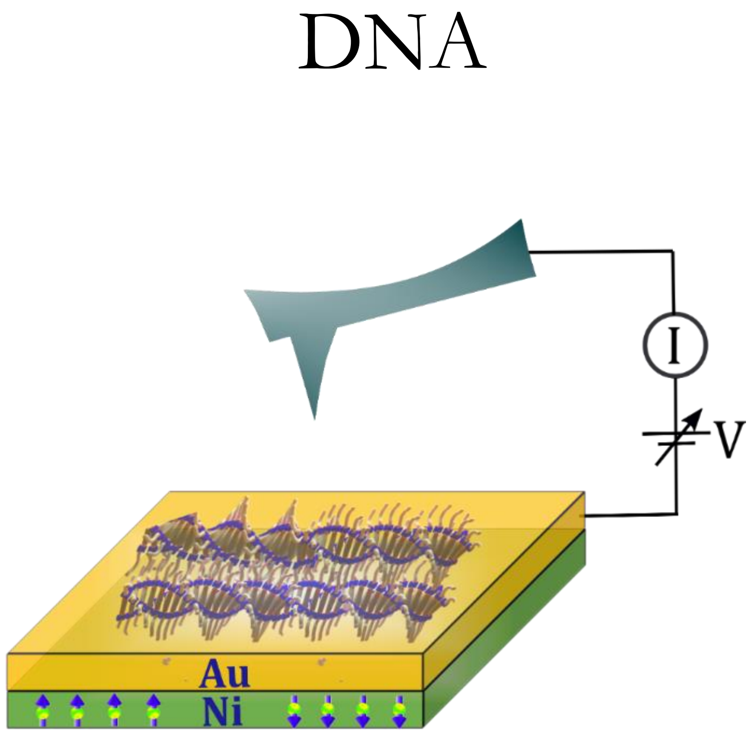
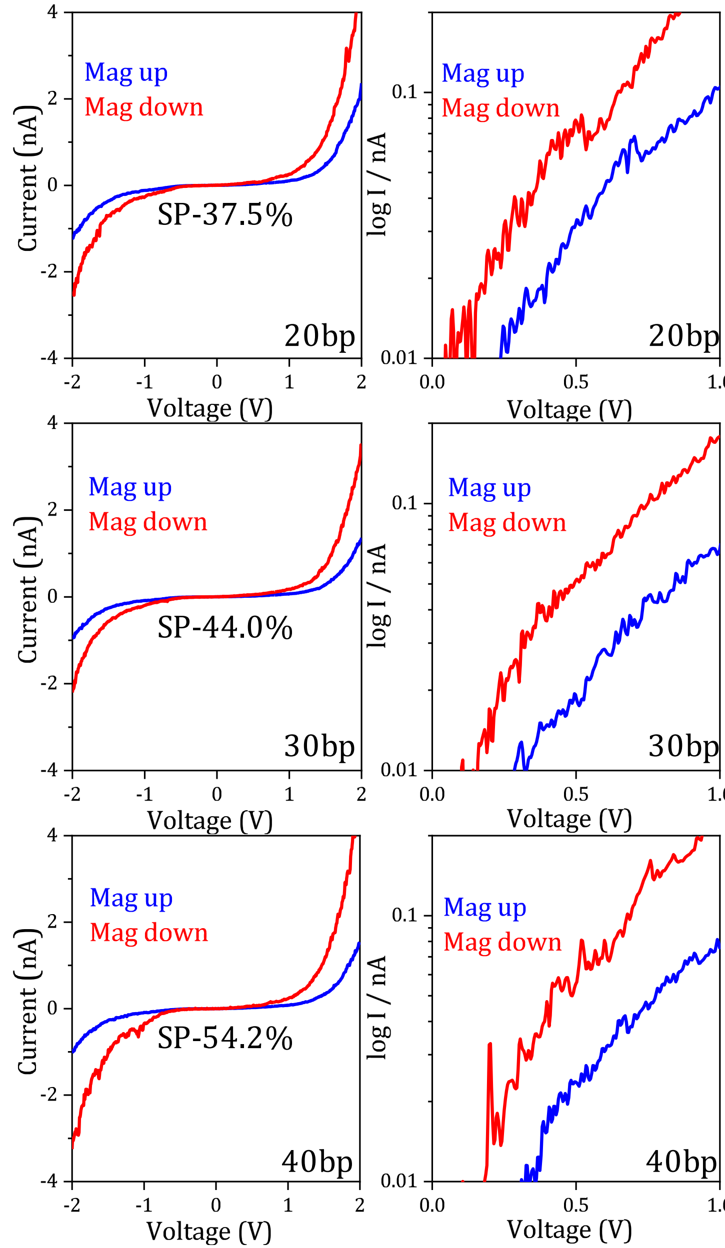
Electric Field-Controlled Magnetization in GaAs/AlGaAs Heterostructures–Chiral Organic Molecules Hybrids

Eilam Z. B. Smolinsky,[#,†] Avner Neubauer,[#,‡] Anup Kumar,[†] Shira Yochelis,[‡] Eyal Capua,[†] Raanan Carmieli,[§] Yossi Paltiel,[*,‡] Ron Naaman,[*,†] and Karen Michaeli[*,∥]



Spin Selective Conduction





S. Mishra, A. K. Mondal, S. Pal, T. K. Das, E.Z. B. Smolinsky, G. Siligardi, R. Naaman,
JPC C **124**, 10776-10782 (2020).

NANO LETTERS

LETTER

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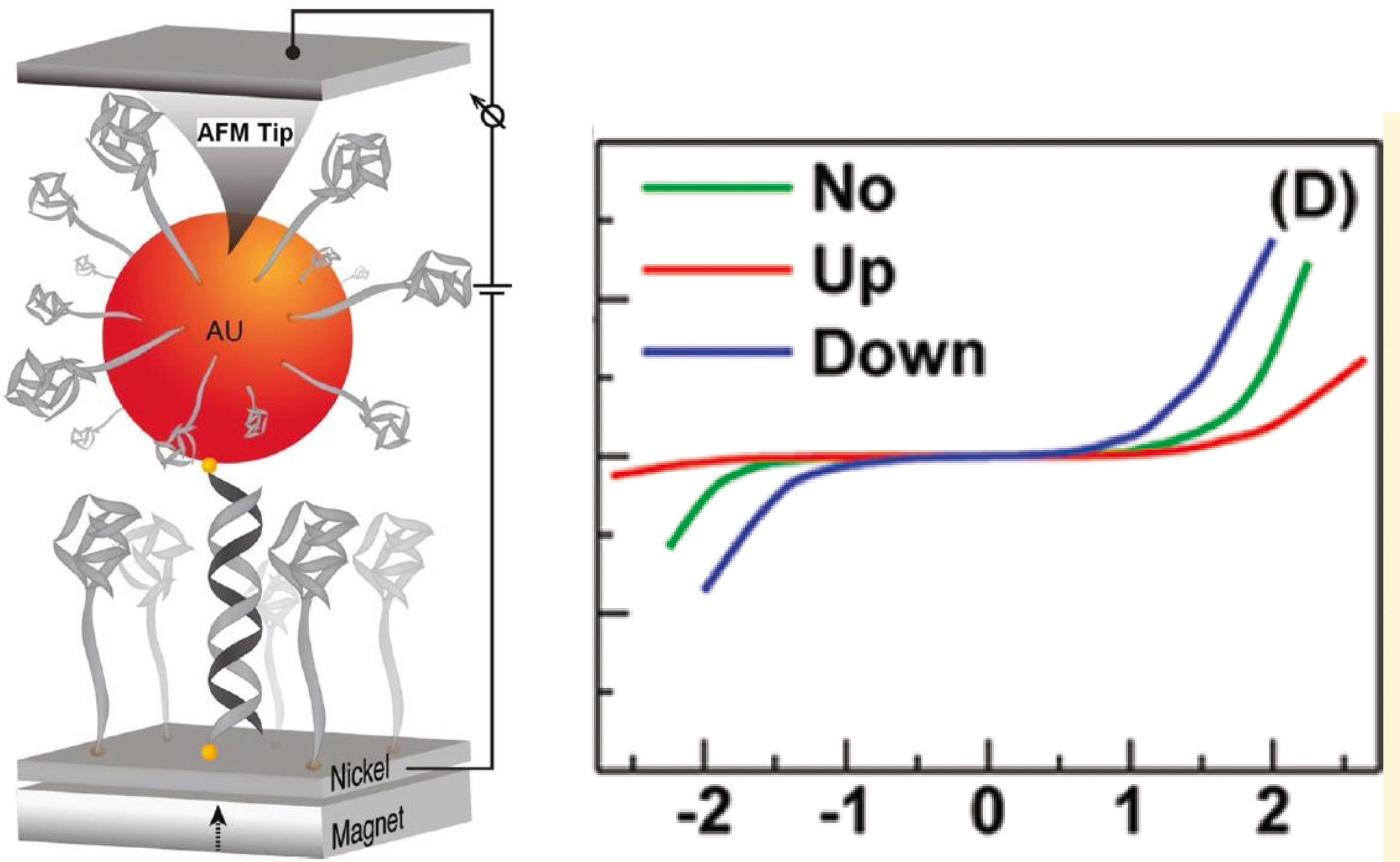
Spin Specific Electron Conduction through DNA Oligomers

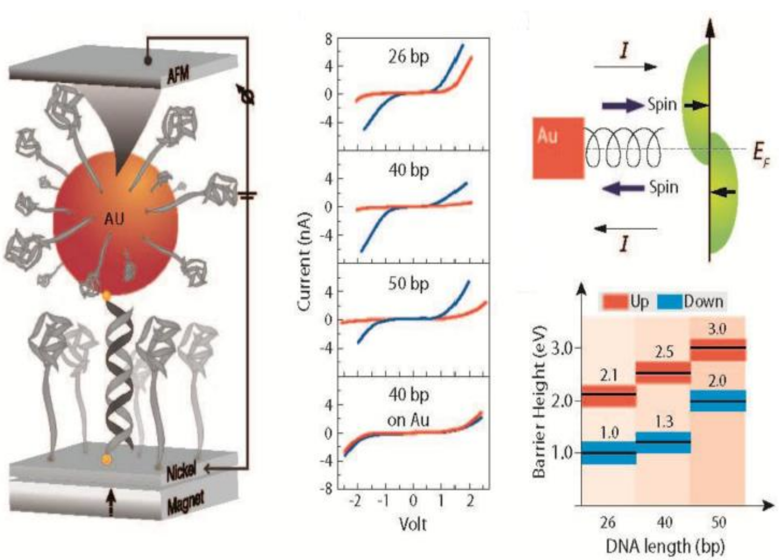
Zouti Xie,[†] Tal Z. Markus,[†] Sidney R. Cohen,[‡] Zeev Vager,[§] Rafael Gutierrez,[||] and Ron Naaman[*,†]

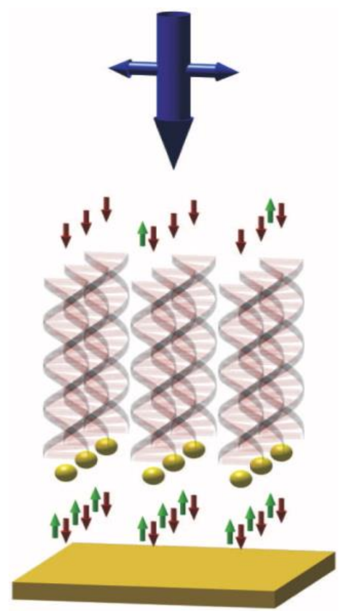


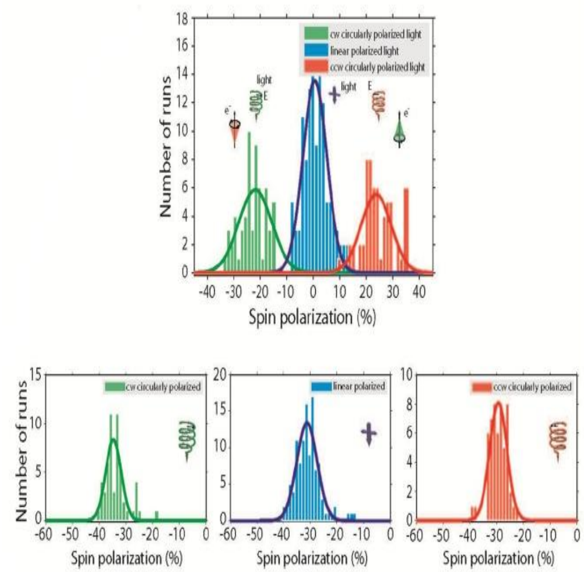
Chiral-induced spin selectivity (CISS)

Ron Naaman *et al*:

Chiral molecules can generate spin selectivity







REVIEW

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Theory of Chirality Induced Spin Selectivity: Progress and Challenges

Ferdinand Evers, Amnon Aharony, Nir Bar-Gill, Ora Entin-Wohlman, Per Hedegård, Oded Hod, Pavel Jelinek, Grzegorz Kamieniarz, Mikhail Lemeshko, Karen Michaeli, Vladimiro Mujica, Ron Naaman, Yossi Paltiel, Sivan Refaely-Abramson, Oren Tal, Jos Thijssen, Michael Thoss, Jan M. van Ruitenbeek, Latha Venkataraman, David H. Waldeck, Binghai Yan, and Leeor Kronik**

A critical overview of the theory of the chirality-induced spin selectivity (CISS) effect, that is, phenomena in which the chirality of molecular species imparts significant spin selectivity to various electron processes, is provided. Based on discussions in a recently held workshop, and further work published since, the status of CISS effects—in electron transmission, electron transport, and chemical reactions—is reviewed. For each, a detailed discussion of the state-of-the-art in theoretical understanding is provided and remaining challenges and research opportunities are identified.

1. Introduction

Chirality-induced spin selectivity (CISS), first discovered some two decades ago in the context of photoemission,[1] is now an umbrella term that defines a wide range of phenomena in which the chirality of molecular species imparts significant spin selectivity to various electron processes.[2–9] The interplay between

Adv. Mater. **2022**, *34*, 2106629

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Arxiv:2309.07588 **Condensed Matter > Mesoscale and Nanoscale Physics**

[Submitted on 14 Sep 2023]

Spin-Selective Electron Transport Through Single Chiral Molecules

Mohammad Reza Safari, Frank Matthes, Claus M. Schneider, Karl-Heinz Ernst, Daniel E. Bürgler

The interplay between chirality and magnetism has been a source of fascination among scientists for over a century. In recent years, chirality-induced spin selectivity (CISS) has attracted renewed interest. It has been observed that electron transport through layers of homochiral molecules leads to a significant spin polarization of several tens of percent. Despite the abundant experimental evidence gathered through mesoscopic transport measurements, the exact mechanism behind CISS remains elusive. In this study, we report spin-selective electron transport through single helical aromatic hydrocarbons that were sublimed in vacuo onto ferromagnetic cobalt surfaces and examined with spin-polarized scanning tunneling microscopy (SP-STM) at a temperature of 5 K. Direct comparison of two enantiomers under otherwise ide

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Outline

- Spin-orbit interaction and spin filters
- Time reversal symmetry – no polarization with 2 leads?
- Ways to overcome this limitation
- Explain experiments?

Spin-Orbit interaction

Expanding the **relativistic** Dirac Hamiltonian

$$\mathcal{H} \simeq \underbrace{\frac{\mathbf{p}^2}{2m} + V}_{\text{Schrodinger}} \underbrace{- \frac{\mathbf{p}^4}{8m^3c^2}}_{\text{correction of kinetic energy}} + \underbrace{\frac{1}{2m^2c^2}\mathbf{S}\cdot(\nabla V)\times\mathbf{p}}_{\text{spin-orbit coupling}} + \underbrace{\frac{\hbar^2}{8m^2c^2}(\nabla^2 V)}_{\text{Darwin term}}$$

spin-orbit Hamiltonian
-electrons in solid

$$\mathcal{H}_{\mathrm{so}} \propto \underbrace{\mathbf{S}}_{\frac{\hbar}{2}\boldsymbol{\sigma}} \cdot \underbrace{(\nabla V)}_{-\mathbf{E}} \times \mathbf{p}$$

electron spin operator: $\frac{\hbar}{2}\boldsymbol{\sigma}$

$-\mathbf{E}$ Electric field

$\updownarrow$

for a rotationally symmetric potential

$\leftrightarrow$ $\mathbf{S}\cdot\mathbf{L}$

spin

angular momentum

brief modern history
spin-orbit coupling

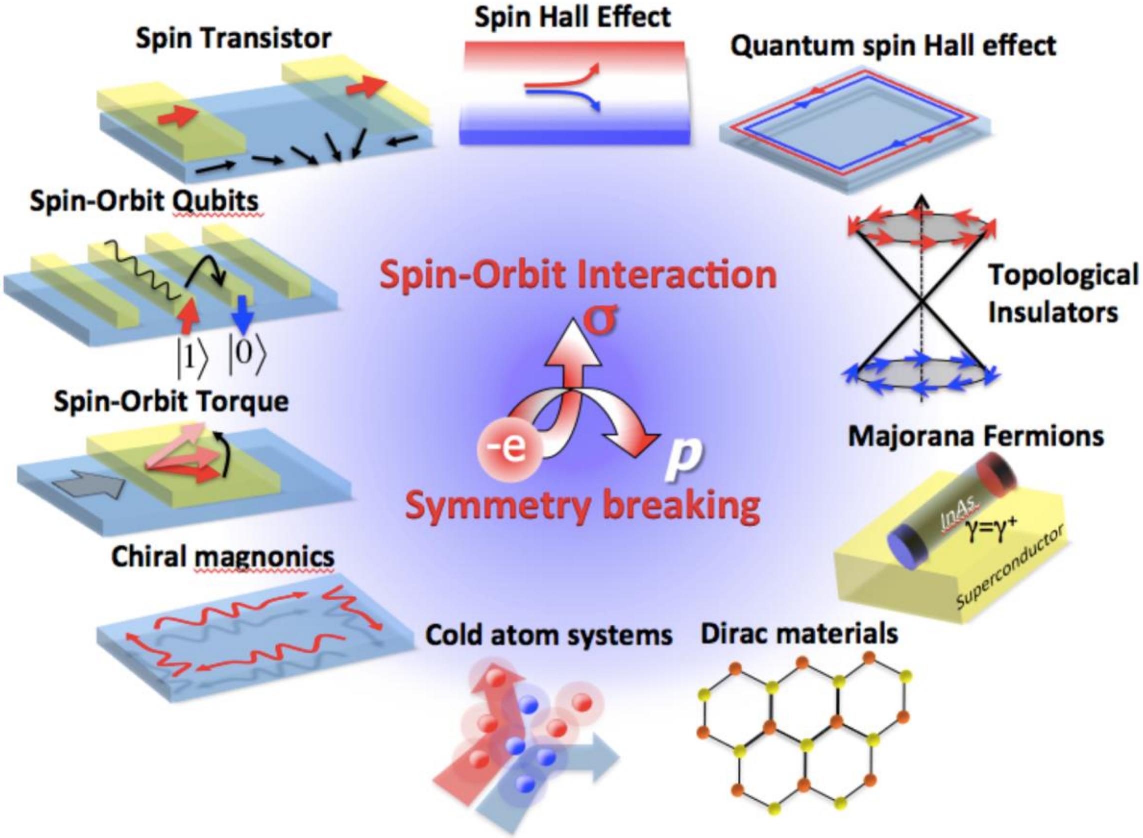
1984 Bychkov & Rashba Hamiltonian—spin resonance of 2D semiconductors

1990 Datta & Das spin transistor

1

1997 Gate control of spin-orbit interaction

2005-now manipulating spin orientaton by moving electrons, controlling electron trajectories using spin as a steering wheel, topological classes of materials…….



→ Flying qubits

Two-dimensional (in the x-y plane) Rashba interaction

רבי שלמה בן אברהם

E Rashba

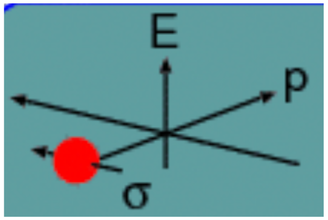
$$\hat{H}_{SO} = \frac{\hbar}{(2M_0c)^2} \nabla V(\mathbf{r})(\hat{\boldsymbol{\sigma}} \times \hat{\mathbf{p}}).$$

$$\mathcal{H}_R^{2d} = \alpha(p_x\sigma_y - p_y\sigma_x)$$

$$\alpha[\mathbf{p} \times \boldsymbol{\sigma}]_z$$

Strength of Rashba term can be tuned by gate voltage!

add kinetic energy $$\mathcal{H} = \frac{1}{2m^*}\Big(\mathbf{p} + \underbrace{k_{so}\boldsymbol{\sigma} \times \hat{\mathbf{z}}}_{\text{``vector potential''}}\Big)^2$$



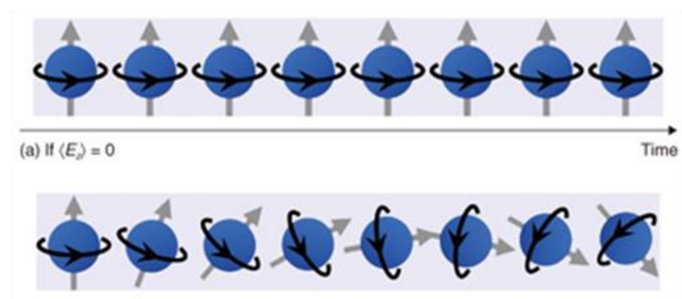
The Aharonov-Casher (**AC**) effect

Rashba spin-orbit interaction in a plane $\mathcal{H}_R = \dfrac{\hbar k_{\rm so}}{m^*}\hat{\mathbf{n}}\cdot[\boldsymbol{\sigma}\times\mathbf{p}]$

$$\mathbf{E} = -\boldsymbol{\nabla}V = E\hat{\mathbf{n}} \qquad \mathcal{H} = \frac{\mathbf{p}^2}{2m^*} + \mathcal{H}_R = \frac{\left(\mathbf{p} + \hbar k_{\rm so}[\hat{\mathbf{n}}\times\boldsymbol{\sigma}]\cdot\mathbf{p}\right)^2}{2m^*}$$

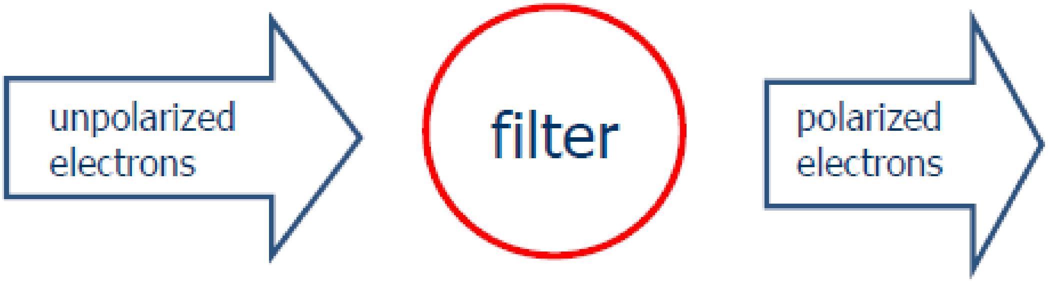
generates the AC phase,

$$e^{i\mathbf{k}\cdot\mathbf{R}}|\chi\rangle \Rightarrow e^{i[\mathbf{k}\cdot\mathbf{R}}e^{ik_{\rm so}[\hat{\mathbf{n}}\times\boldsymbol{\sigma}]\cdot\mathbf{R}}|\chi\rangle$$



Entin-Wohlman, Oreg, Meir, Gefen (1989, 1992)

Spin filters



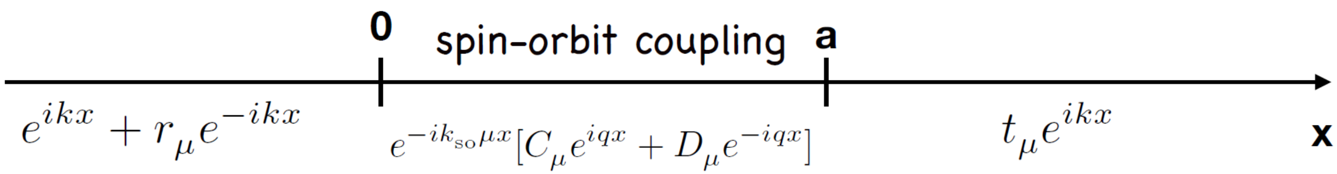
Can spin polarization be generated in a **2-terminal** setup with **spin-orbit interaction** (SOI)?

Outline

- Spin-orbit interaction and spin filters
- Time reversal symmetry – no polarization with 2 leads?
- Ways to overcome this limitation
- Explain experiments??

Bardarson's theorem: time-reversal symmetric Hamiltonian cannot generate a spin asymmetry for tunneling between two terminals

- Choose as a basis the eigenspinors of the spin-orbit coupling
- Solve the scattering for each of them



- reflection amp. independent of spin-orbit coupling
- transmission amp. acquires a phase $e^{-ia(k_{\mathrm{so}}\mu + k)}$
- transmission probability independent of spin-orbit coupling

J H Bardarson, J Phys. A: Math Theor. **41**, 405203 (2008)

Spin transmission between **2 terminals** with **time reversal symmetry?**

$$|\psi^L\rangle = c^{in,L}\,|n\rangle + c^{out,L}\,|Tn\rangle \qquad |\psi^R\rangle = c^{in,R}\,|m\rangle + c^{out,R}\,|Tm\rangle$$

$$\begin{pmatrix} c^{out,L} \\ c^{out,R} \end{pmatrix} = S \begin{pmatrix} c^{in,L} \\ c^{in,R} \end{pmatrix} = \begin{pmatrix} r & t' \\ t & r' \end{pmatrix} \begin{pmatrix} c^{in,L} \\ c^{out,L} \end{pmatrix}$$

Scattering matrix

$$T\,|\psi^L\rangle = (c^{in,L})^*\,|Tn\rangle - (c^{out,L})^*\,|n\rangle \qquad T\,|\psi^R\rangle = (c^{in,R})^*\,|Tm\rangle - (c^{out,R})^*\,|m\rangle$$

Time-reversal

$$\begin{pmatrix} (c^{in,L})^* \\ (c^{in,R})^* \end{pmatrix} = S \begin{pmatrix} -(c^{out,L})^* \\ -(c^{out,R})^* \end{pmatrix}$$

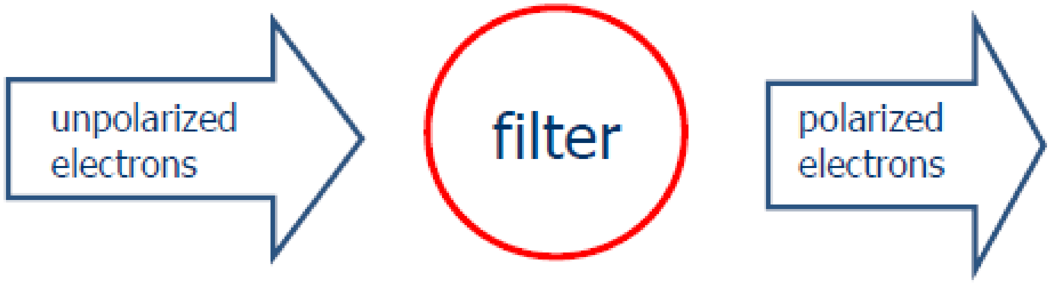
S is unitary

$$S^T \begin{pmatrix} c^{in,L} \\ c^{in,R} \end{pmatrix} = -\begin{pmatrix} c^{out,L} \\ c^{out,R} \end{pmatrix} \Rightarrow S^T = -S \Rightarrow r^T = -r \Rightarrow r = \begin{pmatrix} 0 & \lambda \\ -\lambda & 0 \end{pmatrix}$$

$$\boxed{r^\dagger r = |\lambda|^2 I} \qquad \boxed{t^\dagger t = 1 - r^\dagger r}$$

Same transmissions for both spin polarizations

J. H. Bardarson, J. Phys. A: Math. Theor. **41**, 405203 (2008)



Can spin polarization be generated in a **2-terminal** setup with **spin-orbit interaction** (SOI)?

Bardarson: NO, since SOI obeys **time reversal symmetry --- Kramer's degeneracy**

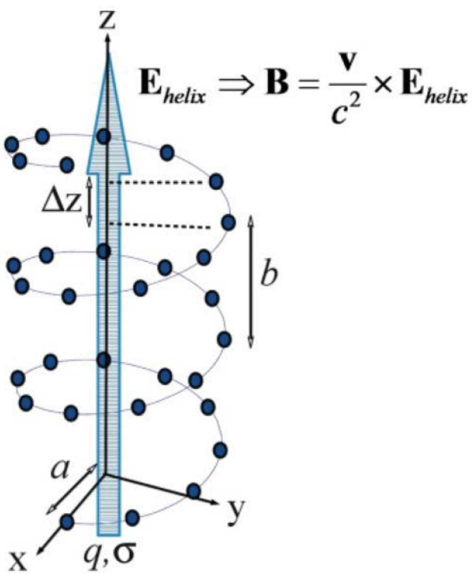
Bardarson's theorem: no spin splitting with 2 terminals and with time-reversal symmetry

However, several papers contradicted the theorem!

PHYSICAL REVIEW B **85**, 081404(R) (2012)

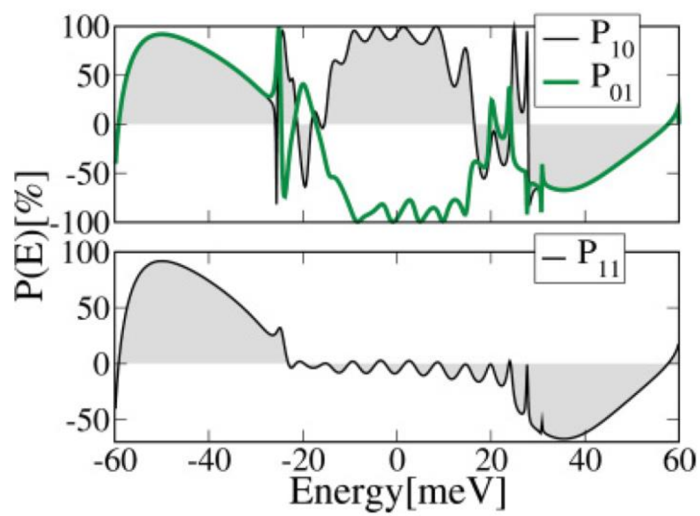
Spin-selective transport through helical molecular systems

R. Gutierrez,[1] E. Díaz,[1,2] R. Naaman,[3] and G. Cuniberti[1,4]

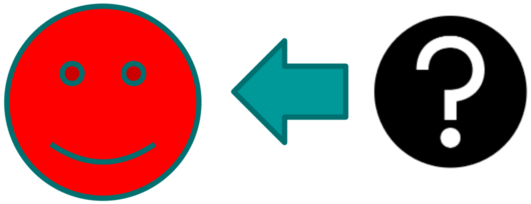


$$H = \sum_{\sigma=\uparrow,\downarrow} \sum_{n=1}^{N} U_n c^{\dagger}_{n,\sigma} c_{n,\sigma} + V \sum_{\sigma=\uparrow,\downarrow} \sum_{n=1}^{N-1} (c^{\dagger}_{n,\sigma} c_{n+1,\sigma} + \text{H.c.})$$

$$+ \sum_{n,m=1}^{N} (c^{\dagger}_{n,\uparrow} W_{n,m} c_{m,\downarrow} + c^{\dagger}_{m,\downarrow} W^{\times}_{m,n} c_{n,\uparrow}) + H_{\text{leads}}. \qquad (2)$$



Unpolarized Incoming electrons



Received: February 18, 2013
Revised: May 17, 2013
Published: May 21, 2013

dx.doi.org/10.1021/jp401705x | *J. Phys. Chem. C* 2013, 117, 22276−22284

THE JOURNAL OF PHYSICAL CHEMISTRY C

Article

pubs.acs.org/JPCC

Modeling Spin Transport in Helical Fields: Derivation of an Effective Low-Dimensional Hamiltonian

R. Gutierrez,[*,†] E. Díaz,[‡] C. Gaul,[‡,§] T. Brumme,[†] F. Domínguez-Adame,[‡] and G. Cuniberti[†,∥]

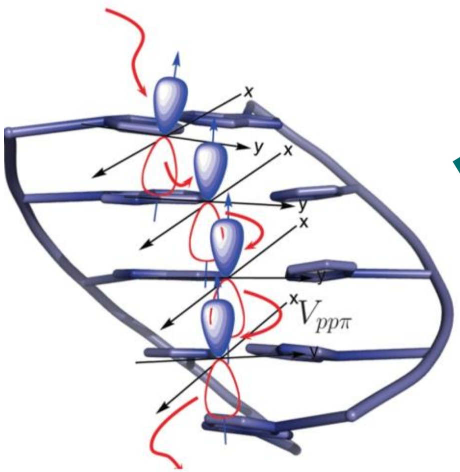
setup. Reference 18 addressed for the first time in the context of a *quantum transport model* the possibility that an electrostatic field with helical symmetry could induce a spin−orbit interaction. An effective one-dimensional (1D) Hamiltonian was formulated, assuming that only the *z*-component (along the helical axis) of the electron momentum was not vanishing. Although strong spin-dependent effects were found, it turns out that the model needs to break time-reversal symmetry to reveal the spin polarization. This is unsatisfactory from a formal point

PHYSICAL REVIEW B **101**, 241410(R) (2020)

Rapid Communications

Spin-orbit interaction and spin selectivity for tunneling electron transfer in DNA

Solmar Varela,[1,*] Iskra Zambrano,[2] Bertrand Berche,[3] Vladimiro Mujica,[4] and Ernesto Medina[2,5,†]

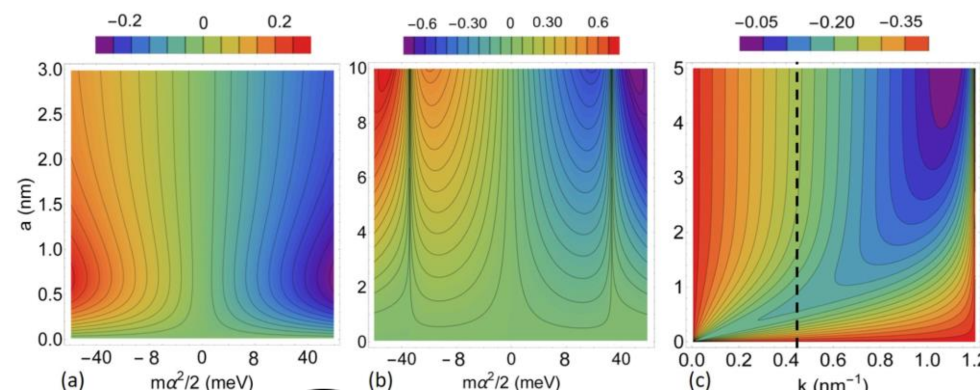


L SOI R

$$H = \begin{cases} \left(\frac{p_x^2}{2m} + V_o\right)\mathbf{1} + \alpha\sigma_y p_x, & 0 \leqslant x \leqslant a, \\ \text{donor/acceptor states}, & \text{outside}. \end{cases}$$

$$\psi_2 = \begin{pmatrix} C_\uparrow e^{iq_\uparrow x} \\ C_\downarrow e^{iq_\downarrow x} \end{pmatrix} + \begin{pmatrix} D_\uparrow e^{-iq_\uparrow x} \\ D_\downarrow e^{-iq_\downarrow x} \end{pmatrix}, \quad 0 \leqslant x \leqslant a$$

$$\boxed{q_s = \sqrt{k^2 - q_0^2 + \left(\frac{m\alpha}{\hbar}\right)^2} + s\left(\frac{m\alpha}{\hbar}\right),}$$



?

Step 1:

Comment on: "Spin-orbit interaction and spin selectivity for tunneling electron transfer in DNA"

Ora Entin-Wohlman,[1,*] Amnon Aharony,[1,†] and Yasuhiro Utsumi[2]

$$\mathcal{H} = \left[\frac{p_x^2}{2m} + V_0\right]\mathbf{1} + \alpha\sigma_y p_x \quad \text{for} \quad 0 < x < a$$

$$\psi_\mu(x) \propto e^{iQ_\mu x} \qquad \boxed{Q_\mu^\pm = -k_{\rm so}\mu \pm q\ , \quad \text{with} \quad q = \sqrt{k^2 + k_{\rm so}^2 - q_0^2}}$$

$$Q_\mu^\pm(\text{Varela}) = \pm(k_{\rm so}\mu + q)$$

$$\begin{aligned}
\psi_\mu &= \left[e^{ikx} + r_\mu e^{-ikx}\right]\ , \quad x < 0\ ,\\
\psi_\mu &= e^{-ik_{\rm so}\mu x}\left[C_\mu e^{iqx} + D_\mu e^{-iqx}\right]\ , \quad 0 < x < a\\
\psi_\mu &= t_\mu e^{ikx}\ , \quad a < x\ .
\end{aligned}$$

$$\boxed{T_\mu = |t_\mu|^2 = \frac{4k^2q^2}{4k^2q^2 + (k^2 - q^2)^2\sin^2(qa)}}$$

Independent of spin!

BC: $$\boxed{v_\mu^\pm = \hbar(Q_\mu^\pm + k_{\rm so}\mu)/m = \pm\hbar q/m}$$

$$\widetilde{\mathcal{H}} = U(x)^\dagger\mathcal{H}U(x)\ , \quad U(x) = e^{ik_{\rm so}x\sigma_y}$$

$$\widetilde{\mathcal{H}} = \frac{p_x^2 - (\hbar k_{\rm so})^2}{2m} + V_0\ .$$

Accepted!

Step 2:

Response to Comment on: Tunneling in DNA with Spin Orbit coupling

Solmar Varela,[1,2] Iskra Zambrano,[2] Bertrand Berche,[3] Vladimiro Mujica,[4] and Ernesto Medina[2,5]

Us

$$\Psi_s = \begin{pmatrix} is \\ 1 \end{pmatrix} e^{i\lambda|q|x} \qquad |\Psi_\mu(x)\rangle = e^{i\bar{Q}_\mu x}|\mu\rangle$$

$$q = sk_{so} + \lambda\sqrt{k^2 + k_{so}^2 - q_0^2}.$$

$$Q_\mu^\pm = -\mu k_{\mathrm{so}} \pm \sqrt{k^2 + k_{\mathrm{so}}^2 - q_0^2}$$

Abstract: "... we show that the allowed wavevectors are the ones
Assumed in the original paper and thus the original conclusions follow."

Accepted?

Comments in Physical Review B

The Comment

Comments are publications that criticize or correct specific papers of other authors previously published in Physical Review B. Each Comment should state clearly to which paper it refers. The normal publication schedule is followed. Authors of potential Comments are encouraged to try to resolve and clarify any disagreement with the authors of the original paper before submission of the Comment. The content in a Comment should be directed to the physics in the paper being criticized; statements on other matters, such as perceived citation omissions, are not generally suitable for publication as Comments, and can usually be addressed most effectively through direct contact with the authors of the original paper. Criticism should be free of polemics and personal or ad hominem remarks.

The Reply

When a Comment is deemed suitable for publication by the Editor, the criticized authors will be given the opportunity to write a Reply for possible simultaneous publication. The Reply will also be reviewed and to be suitable for publication should contain new physics material or discussion; it is not appropriate simply to repeat what has already appeared in the literature. If a Reply is not found suitable for publication it may be rejected even if the Comment is accepted. It is the responsibility of the corresponding author of the original work being criticized (to whom a copy of the Comment is sent as part of the review process) to ensure that all the original authors are aware of the criticism and to ensure that all appropriate individuals are listed as authors of the Reply.

The Review Process

The paper is first sent to the authors whose work is being criticized. These authors may (a) act as reviewers (usually nonanonymously) and recommend that the paper be accepted, be accepted after revision, or be rejected; (b) submit a Reply for simultaneous consideration, although it is often more productive to wait until the Comment is in a form that we intend to publish; (c) respond following review by an independent referee. If they choose to review the paper they may or may not want to publish a Reply to the Comment. Authors should indicate their intentions to the editors as soon as possible. 2. After the issues in question have been addressed by the authors of the Comment and the authors of the work being criticized, the Editor will usually consult an independent, anonymous referee. When the Editor is ready to accept a Comment, the authors being criticized will have an opportunity to submit a Reply (or to revise their Reply if one has already been submitted). 3. After the Comment and Reply have been accepted for publication, the author of the Comment is sent a copy of the Reply for information, but should not alter the text of the Comment in proof. The Comment and Reply are usually (but not always) published in the same issue.

Step 3:

Comment on "Response to Comment on: Tunneling in DNA with Spin-Orbit coupling"

Ora Entin-Wohlman,[1,*] Amnon Aharony,[1,†] and Yasuhiro Utsumi[2]

Reply:

$$q = sk_{so} + \lambda\sqrt{k^2 + k_{so}^2 - q_0^2}.$$

Original:

$$\boxed{Q_\mu^\pm(\mathrm{Varela}) = \pm(k_{\mathrm{so}}\mu + q)}$$

PRB: see the rules !

We: Talked to chief editor Molenkamp.

He knew the physics, but also sent to a member of the editorial board

PHYSICAL REVIEW B **103**, 077401 (2021)

Comment on "Spin-orbit interaction and spin selectivity for tunneling electron transfer in DNA"

Ora Entin-Wohlman,[1,*] Amnon Aharony,[1,†] and Yasuhiro Utsumi[2]
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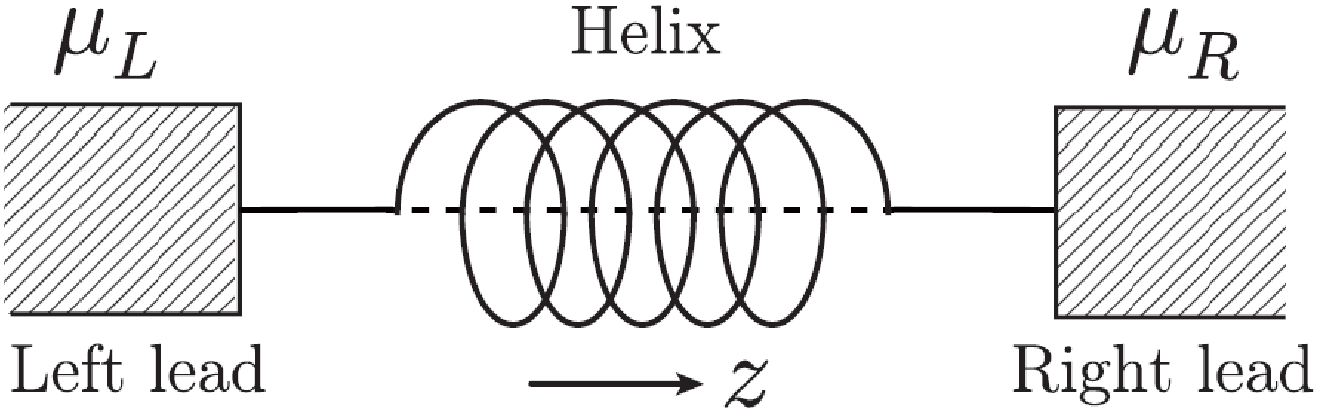
(Received 22 July 2020; revised 8 September 2020; accepted 25 January 2021; published 22 February 2021)

Response **canceled** acceptance

Outline

- Spin-orbit interaction and spin filters
- Time reversal symmetry – no polarization with 2 leads
- Ways to overcome this limitation
- Explain experiments?

Our explanations of CISS



Is helix equivalent to effective rnormalized single wire?

PHYSICAL REVIEW B **93**, 075407 (2016)

Spin-dependent transport through a chiral molecule in the presence of spin-orbit interaction and nonunitary effects

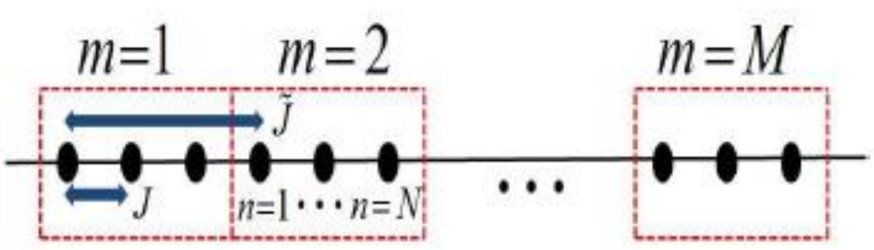
Shlomi Matityahu,[1,*] Yasuhiro Utsumi,[2] Amnon Aharony,[1,3,4] Ora Entin-Wohlman,[1,3,4] and Carlos A. Balseiro[5,6]

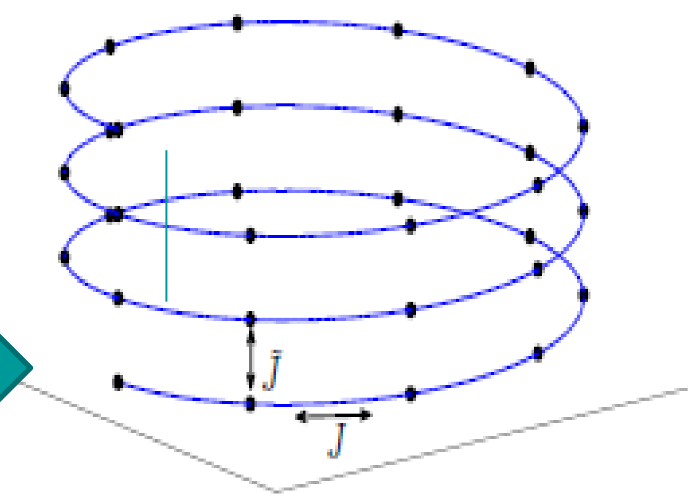
Our approach: scattering with helix between 2 leads

Tight binding hopping on helix

Interference: hopping between helix steps

Spin-orbit interaction





Tight binding model

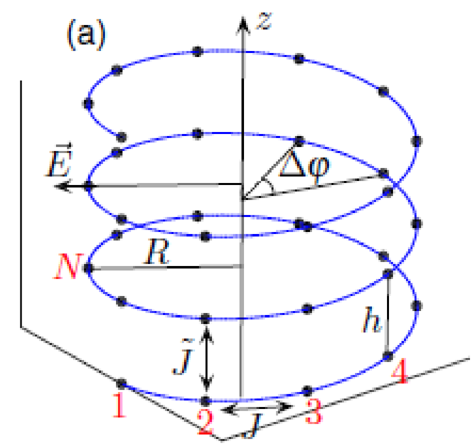
$$\mathcal{H}_{\text{mol}} = \varepsilon_0 \sum_{m=1}^{M} \sum_{n=1}^{N} c_{m,n}^{\dagger} c_{m,n}$$

$$- \sum_{m=1}^{M} \sum_{n=1}^{N} [J c_{m,n+1}^{\dagger} V_n c_{m,n} + \tilde{J} c_{m+1,n}^{\dagger} c_{m,n} + \text{H.c.}]$$

$$V_n = e^{i\mathbf{K}_n \cdot \boldsymbol{\sigma}} \qquad \mathbf{K}_n = \lambda\, \mathbf{d}_{n,n+1} \times \mathbf{E}_{n,n+1}$$

Scattering approach

$$|\psi_l\rangle = \begin{cases} |\chi_{in}\rangle\, e^{ik_0(l-1)} + r\,|\chi_r\rangle\, e^{-ik_0(l-1)}, & l \leqslant 1, \\ t\,|\chi_t\rangle\, e^{ik_0(l-NM)}, & l \geqslant NM \end{cases}$$



Spin polarization

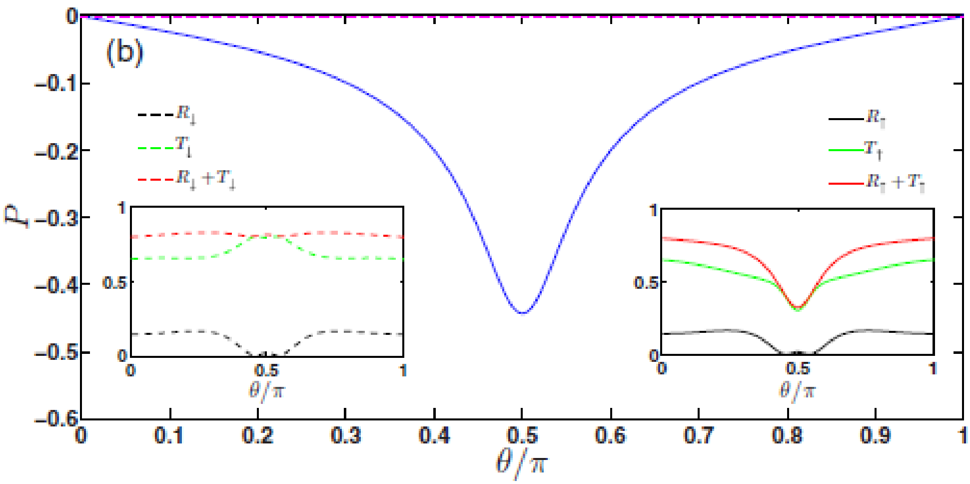
$$P_{\hat{\mathbf{n}}'} \equiv \frac{\text{Tr}[\mathcal{T}^{\dagger}(\hat{\mathbf{n}}' \cdot \boldsymbol{\sigma})\mathcal{T}]}{\text{Tr}[\mathcal{T}^{\dagger}\mathcal{T}]} = \frac{|t_{\uparrow\uparrow}|^2 - |t_{\downarrow\downarrow}|^2}{|t_{\uparrow\uparrow}|^2 + |t_{\downarrow\downarrow}|^2}.$$

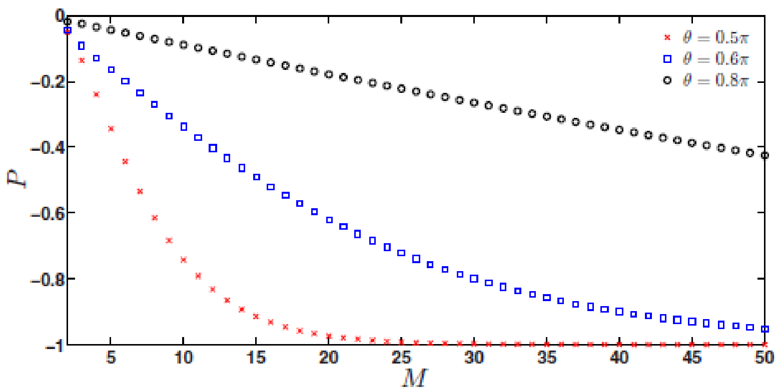
NO POLARIZATION WITH TIME REVERSAL SYMMETRY AND 2 TERMINALS!

Leakage of electrons or loss of coherence

--- Electrons can escape from every site on helix

$$\tilde{\varepsilon}_0 = \varepsilon_0 - \frac{|J_x|^2 e^{iq}}{J_0}$$





Length

Other alternatives:

- More terminals
- Magnetic fields or polarized electrons
- Time-dependence: AC electric and magnetic fields
- More orbital states

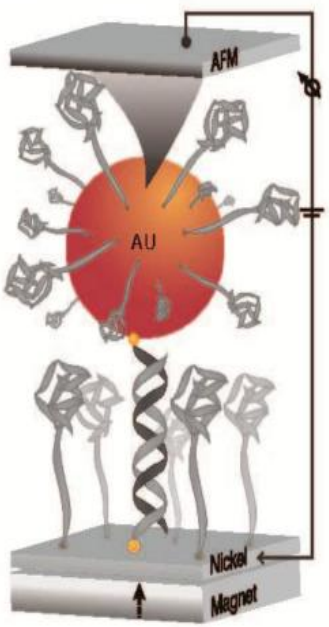
- Non-linear response – needs T(E) (Fransson, vWees)
- Orbital filtering (Binghai Yan)
- Molecule-molecule coupling? (Leakage, cooperative effect)
- Role of exchange with substrate (Paltiel)
- Molecule parallel to substrate (Ruitenbeek)?
- Double helix?
- More???

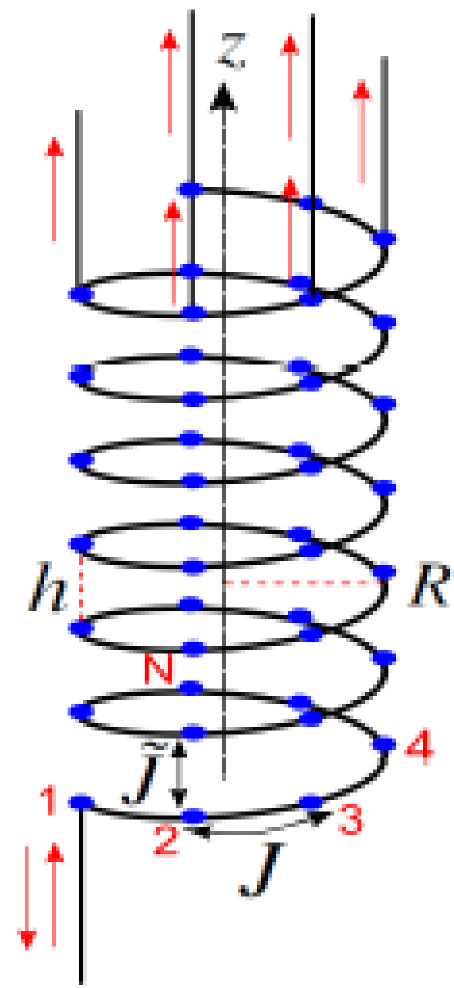
Alternative: **more terminals**;
collect electrons at the end from the **2** last sites on the helix

PHYSICAL REVIEW B **95**, 085411 (2017)

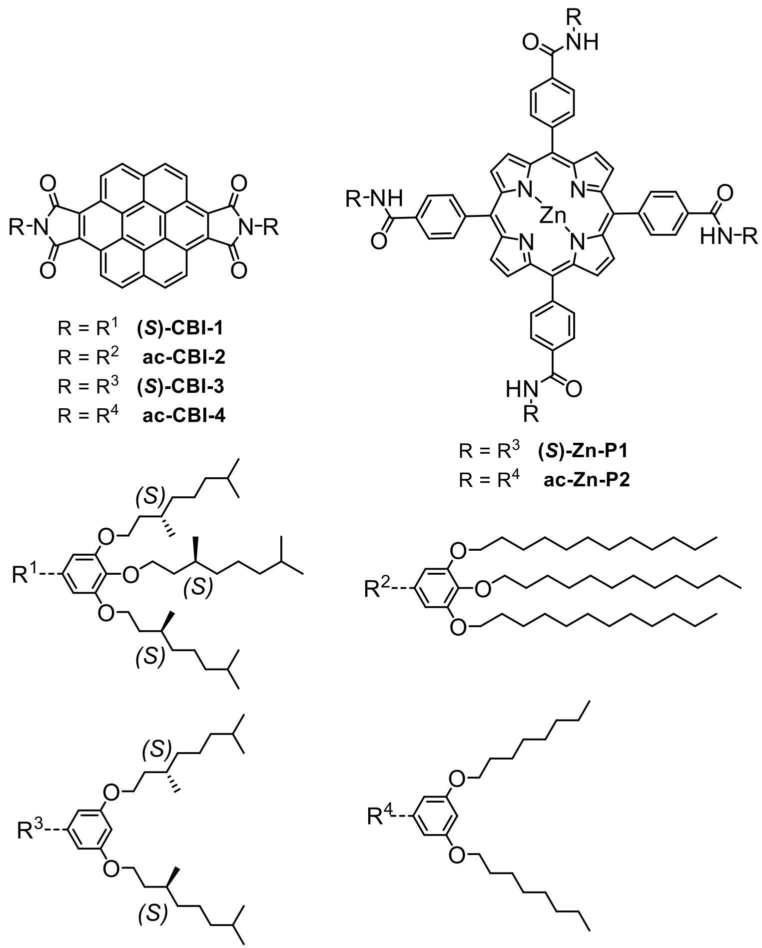
Spin filtering in all-electrical three-terminal interferometers

S. Matityahu,[1,2,*] A. Aharony,[1,3] O. Entin-Wohlman,[1,3] and C. A. Balseiro[4,5]

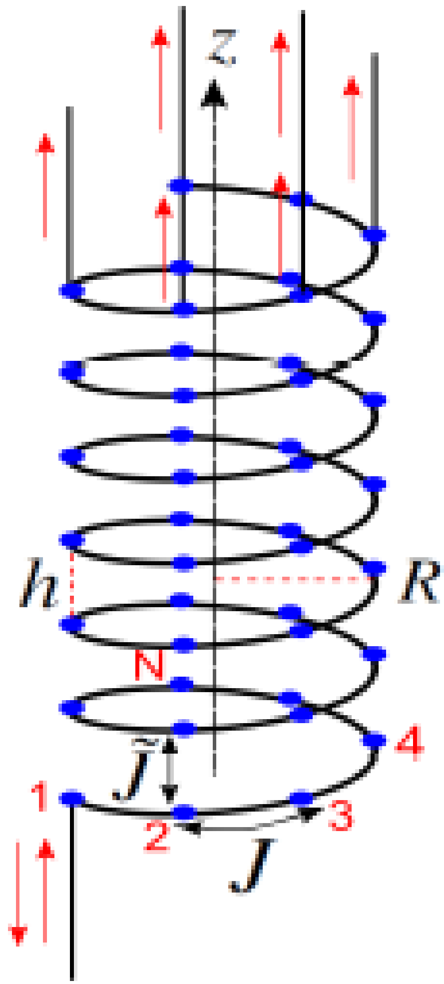




Alternative: **more terminals**;
collect electrons at the end from the **2** last sites on the helix



molecule
with several
arms
(Naaman)?

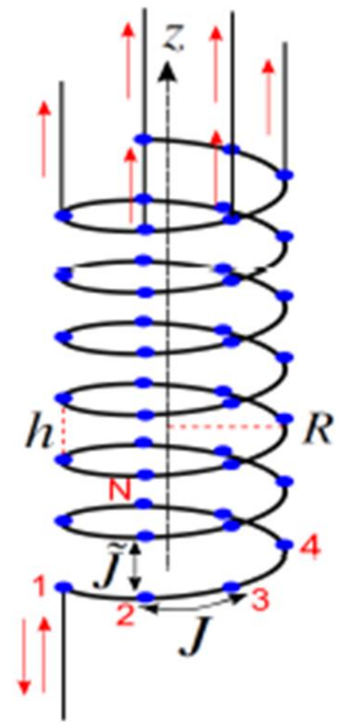


$$|\psi_n\rangle = \begin{cases} |\chi_{\text{in}}\rangle\, e^{ik_0(n-n_{\text{in}})} + r\,|\chi_r\rangle\, e^{-ik_0(n-n_{\text{in}})} & \text{input lead} \\ t^{(1)}\big|\chi_t^{(1)}\big\rangle e^{ik_0(n-n_{\text{out},1})} & \text{first output lead} \\ t^{(2)}\big|\chi_t^{(2)}\big\rangle e^{ik_0(n-n_{\text{out},2})} & \text{second output lead, etc.} \end{cases}$$

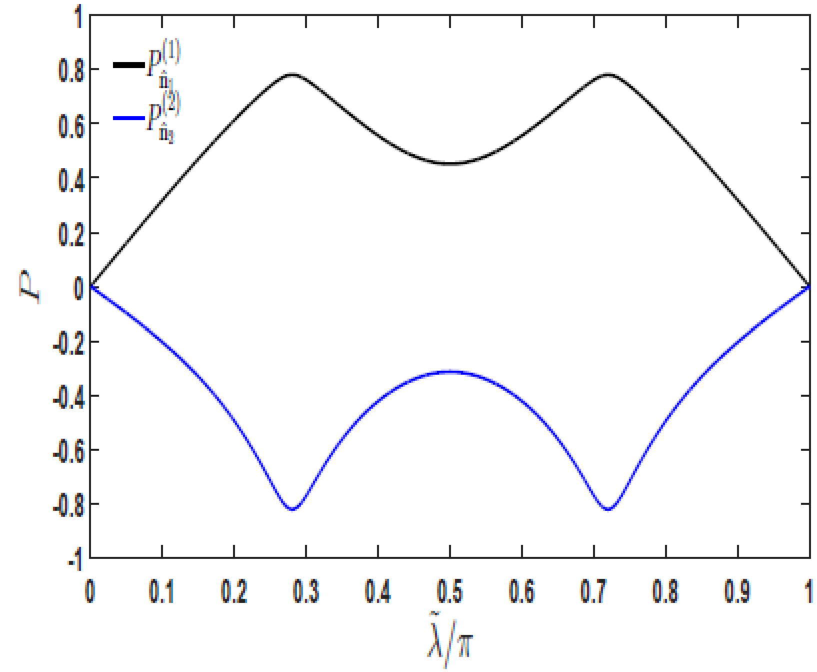
$$r|\chi_r\rangle = \mathcal{R}\,|\chi_{\text{in}}\rangle$$

$$t^{(n)}\big|\chi_t^{(n)}\big\rangle = \mathcal{T}_n\,|\chi_{\text{in}}\rangle$$

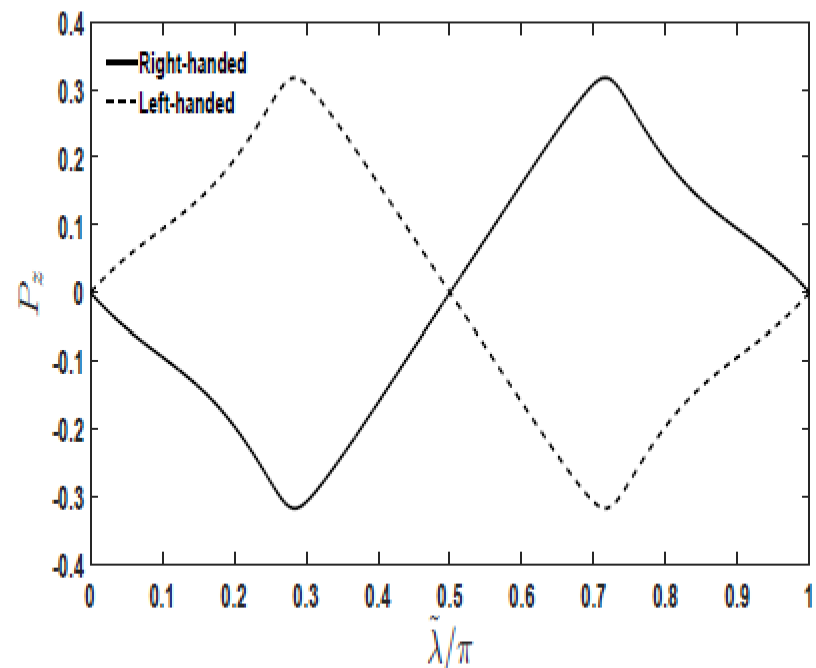
$$P_{\hat{\mathbf{n}}_n}^{(n)} \equiv \frac{\mathrm{Tr}[\mathcal{T}_n^\dagger(\hat{\mathbf{n}}_n\cdot\boldsymbol{\sigma})\mathcal{T}_n]}{\mathrm{Tr}[\mathcal{T}_n^\dagger\mathcal{T}_n]} = \frac{|t_+^{(n)}|^2 - |t_-^{(n)}|^2}{|t_+^{(n)}|^2 + |t_-^{(n)}|^2}.$$



Polarization along
Each quantization axis



Total polarization
Along helix axis

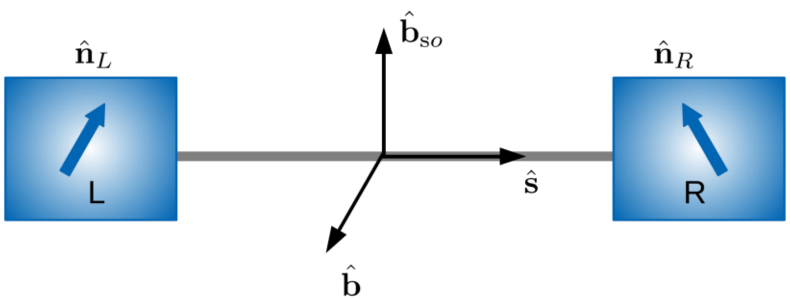


Magnetic Fields & polarized leads

PHYSICAL REVIEW B **102**, 115436 (2020)

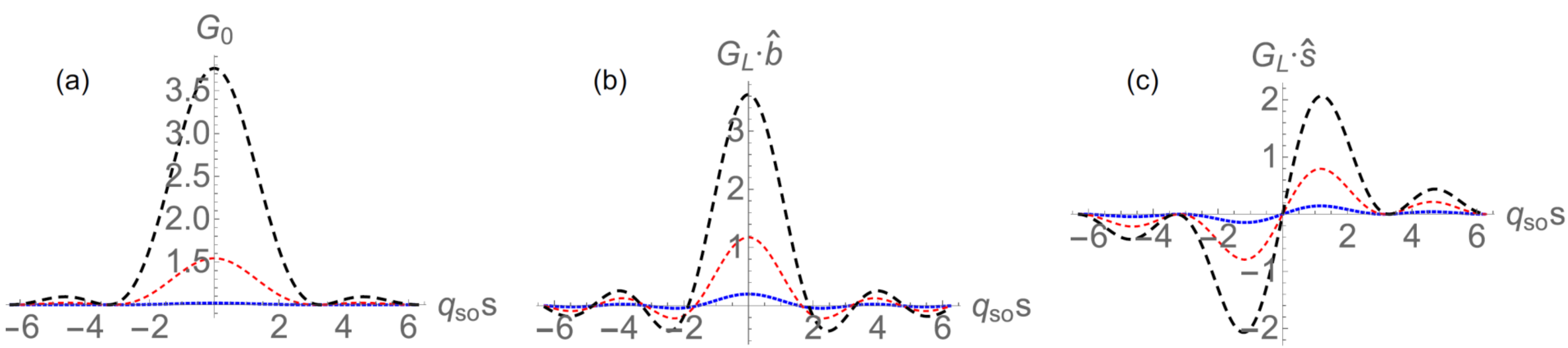
Effects of magnetic fields on the Datta-Das spin field-effect transistor

K. Sarkar,[1,2,*] A. Aharony,[2,†] O. Entin-Wohlman,[2] M. Jonson,[3] and R. I. Shekhter[3]



$$\widetilde{V}_{LR} = V_0\mathbf{1} + iV_{\rm so}(\hat{\mathbf{b}}_{\rm so}\cdot\boldsymbol{\sigma}) + V_b(\hat{\mathbf{b}}\cdot\boldsymbol{\sigma})$$

$$\dot{\mathbf{M}}^L = \mathbf{G}_L(\mu_R^0 - \mu_L^0) - G_0U_L\hat{\mathbf{n}}_L + \mathbf{G}_\times U_R.$$



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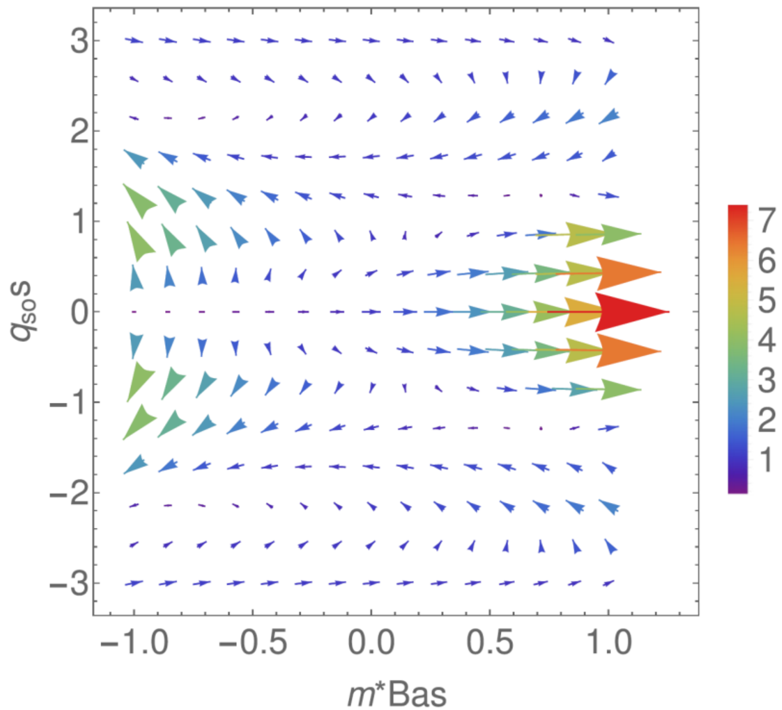
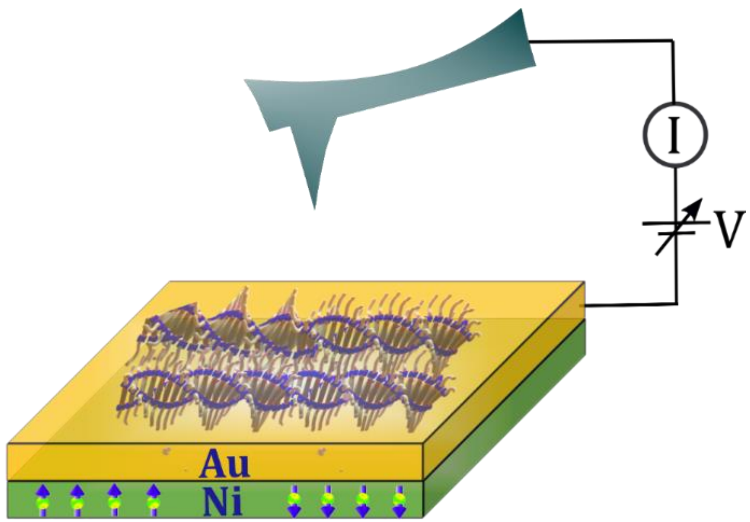
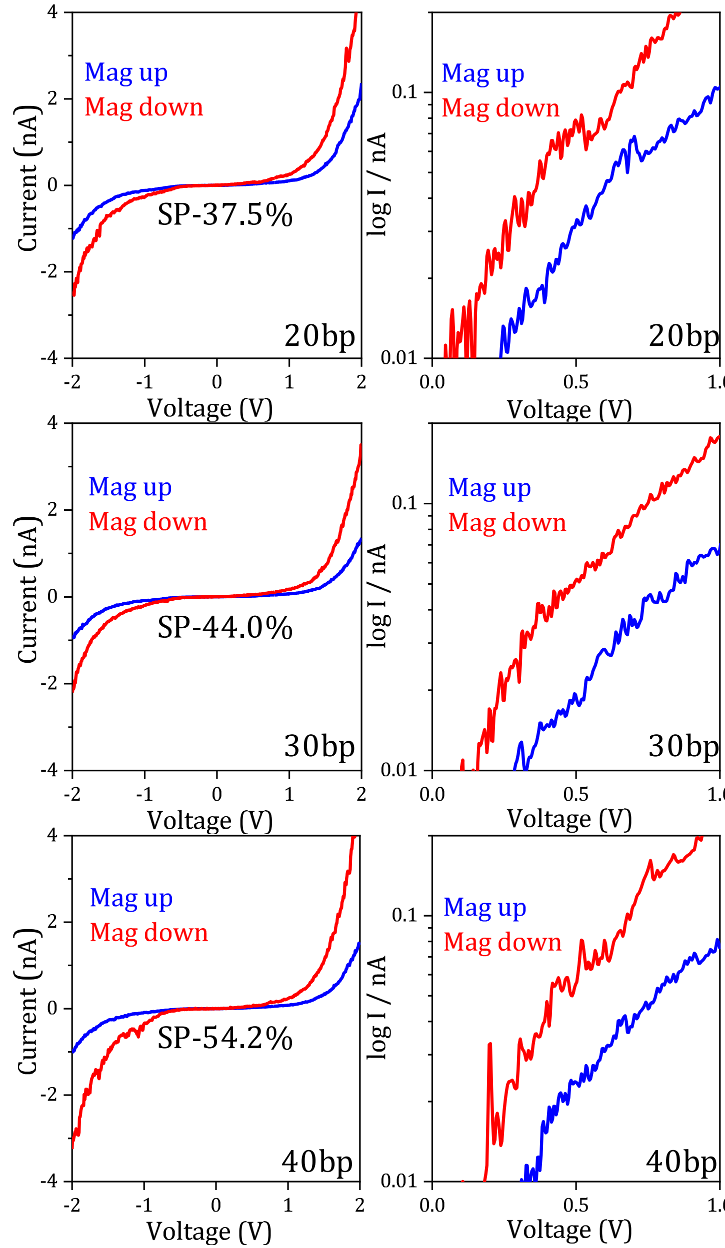


FIG. 3. The magnetization conductance $\mathbf{G}_L$ (in units of γ) injected into the left unpolarized lead ($p_L = 0$) due to a full polarization of the right lead ($p_R = 1$), for different values of the SOI and the Zeeman energy on the link, with $\hat{\mathbf{n}}_R = \hat{\mathbf{b}}$. The arrows are all in the $\hat{\mathbf{b}}$-$\hat{\mathbf{s}}$ plane.

Spin Selective Conduction

DNA





S. Mishra, A. K. Mondal, S. Pal, T. K. Das, E.Z. B. Smolinsky, G. Siligardi, R. Naaman,
JPC C **124**, 10776-10782 (2020).

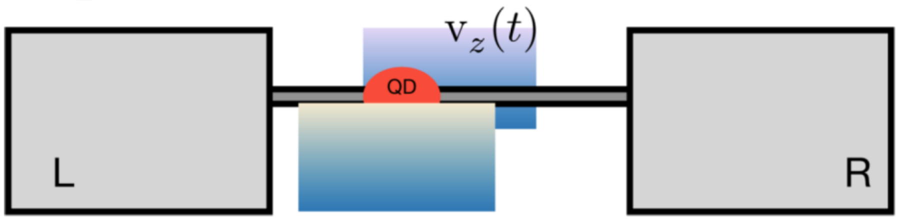
Time-dependence

PHYSICAL REVIEW B **101**, 121303(R) (2020)

Rapid Communications

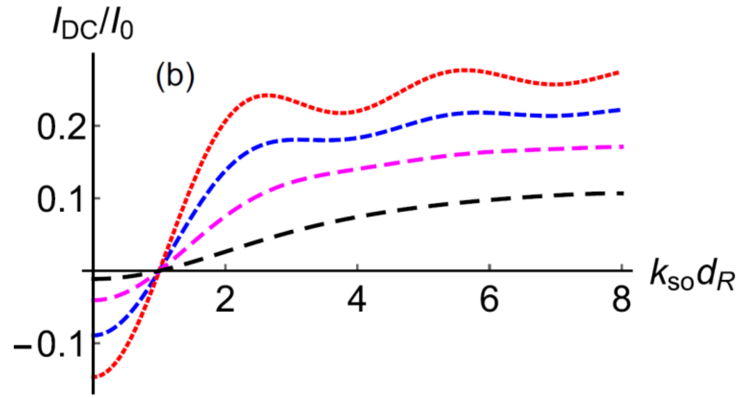
Photovoltaic effect generated by spin-orbit interactions

O. Entin-Wohlman,[1,*] R. I. Shekhter,[2] M. Jonson,[2] and A. Aharony[1]



Note oscillations

DC current generated by time-dependent SOI

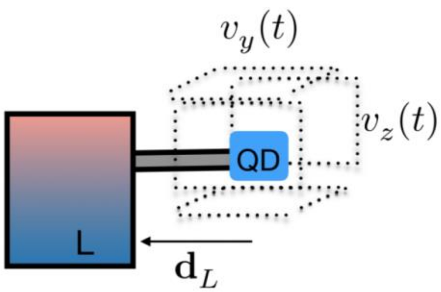


Time-dependence

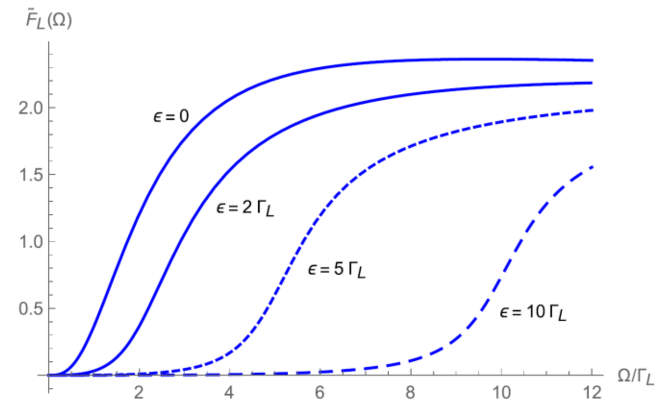
PHYSICAL REVIEW B **102**, 075419 (2020)

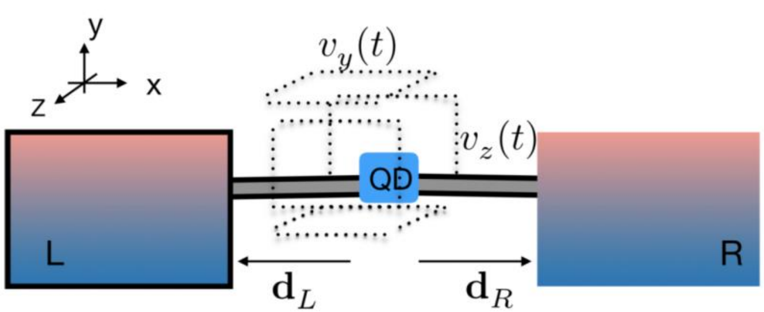
Magnetization generated by microwave-induced Rashba interaction

O. Entin-Wohlman,[1,*] R. I. Shekhter,[2] M. Jonson,[2] and A. Aharony[1]



$$\dot{\mathbf{M}}_L(t)|^{\rm dc} = 2\hat{\mathbf{x}}\gamma\alpha_L^2\Gamma_L\widetilde{F}_L(\Omega),$$





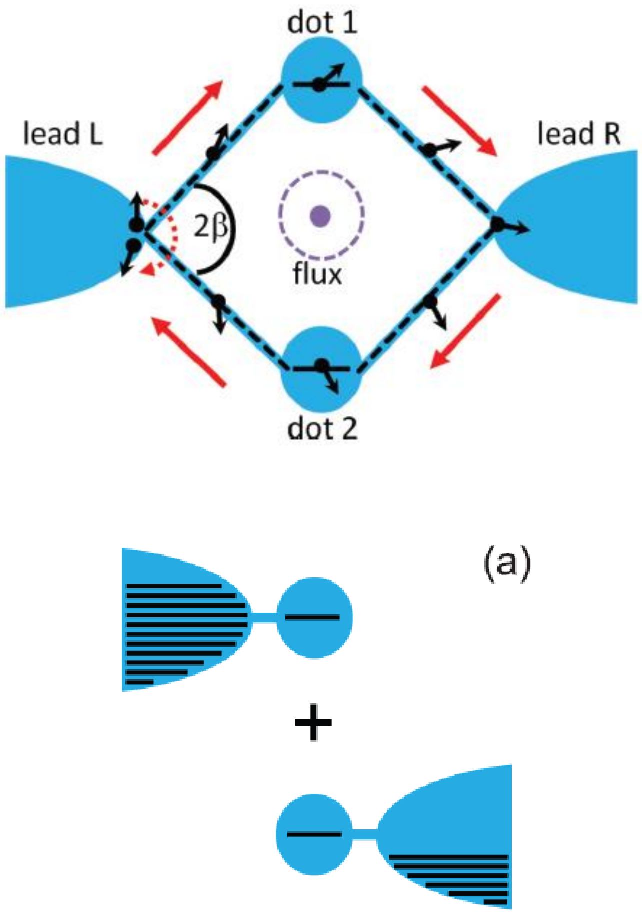
$$\dot{\mathbf{M}}_L^{\rm dc} = \hat{\mathbf{x}}\big(\gamma\alpha_L^2[2\Gamma\widetilde{F}_L(\Omega) - 4\Gamma_R F_L(\Omega)] + \gamma\alpha_R^2 4\Gamma_L F_R(\Omega) - \gamma\alpha_L F_{LR}(\Omega)\big),$$

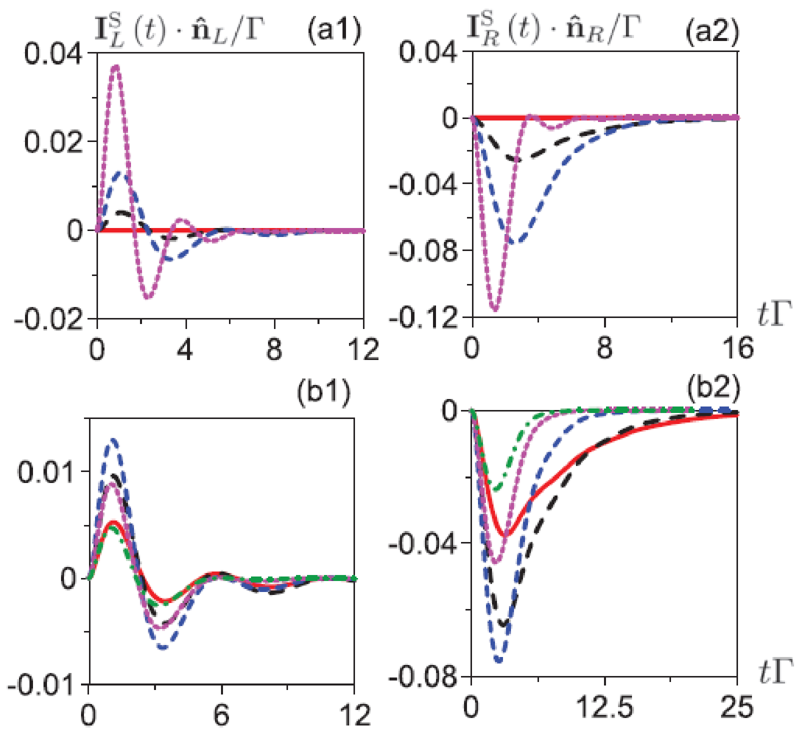
Another way: look at transient currents

PHYSICAL REVIEW B **90**, 165422 (2014)

Real-time dynamics of spin-dependent transport through a double-quantum-dot Aharonov-Bohm interferometer with spin-orbit interaction

Matisse Wei-Yuan Tu,[1] Amnon Aharony,[2,3,*] Wei-Min Zhang,[1,†] and Ora Entin-Wohlman[2,3]





The Journal of Physical Chemistry Letters

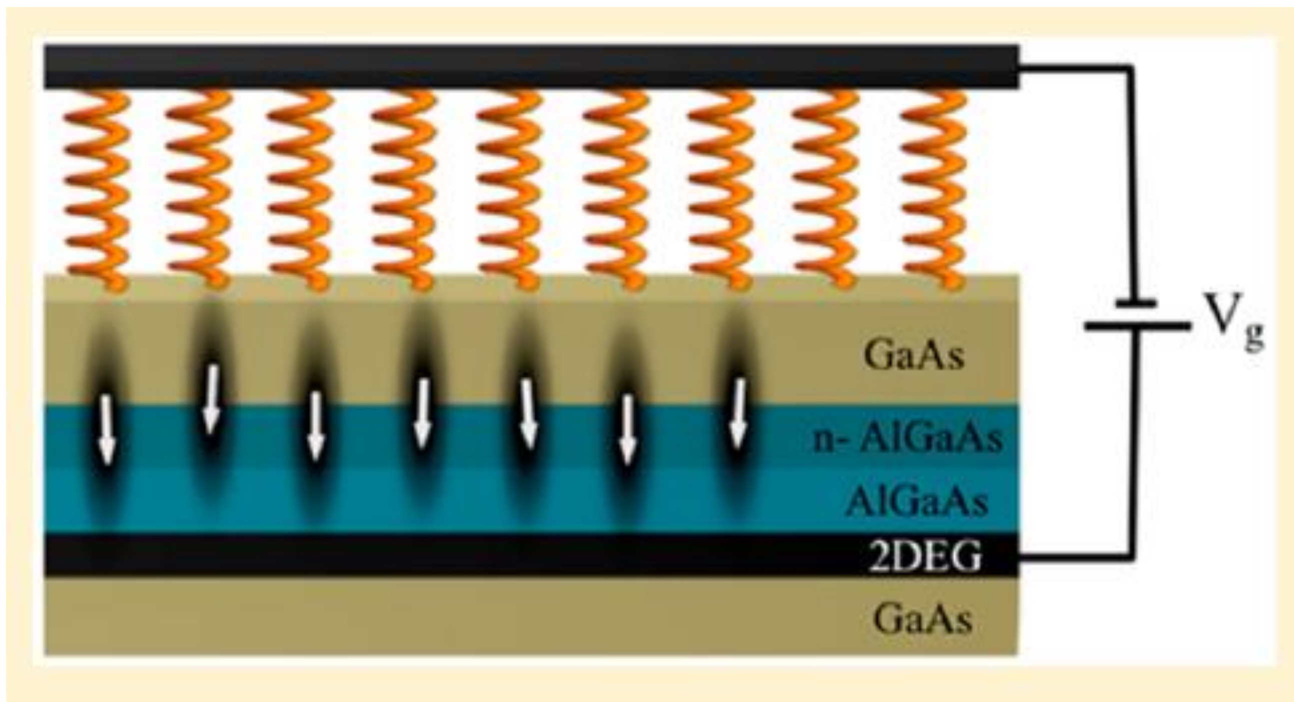
Letter

pubs.acs.org/JPCL

Electric Field-Controlled Magnetization in GaAs/AlGaAs Heterostructures–Chiral Organic Molecules Hybrids

Eilam Z. B. Smolinsky,[#,†] Avner Neubauer,[#,‡] Anup Kumar,[†] Shira Yochelis,[‡] Eyal Capua,[†] Raanan Carmieli,[§] Yossi Paltiel,[*,‡] Ron Naaman,[*,†] and Karen Michaeli[*,‖]

Explanation:
Transient following Exchange in substrate



Spin transmission between **2 terminals** with **time reversal symmetry?**

$$|\psi^L\rangle = c^{in,L}\,|n\rangle + c^{out,L}\,|Tn\rangle \qquad |\psi^R\rangle = c^{in,R}\,|m\rangle + c^{out,R}\,|Tm\rangle$$

$$\begin{pmatrix} c^{out,L} \\ c^{out,R} \end{pmatrix} = S \begin{pmatrix} c^{in,L} \\ c^{in,R} \end{pmatrix} = \begin{pmatrix} r & t' \\ t & r' \end{pmatrix} \begin{pmatrix} c^{in,L} \\ c^{out,L} \end{pmatrix}$$

$$T\,|\psi^L\rangle = (c^{in,L})^*\,|Tn\rangle - (c^{out,L})^*\,|n\rangle \qquad T\,|\psi^R\rangle = (c^{in,R})^*\,|Tm\rangle - (c^{out,R})^*\,|m\rangle$$

$$\begin{pmatrix} (c^{in,L})^* \\ (c^{in,R})^* \end{pmatrix} = S \begin{pmatrix} -(c^{out,L})^* \\ -(c^{out,R})^* \end{pmatrix}$$

S unitary

$$S^T \begin{pmatrix} c^{in,L} \\ c^{in,R} \end{pmatrix} = -\begin{pmatrix} c^{out,L} \\ c^{out,R} \end{pmatrix} \qquad S^T = -S \qquad r^T = -r \qquad r = \begin{pmatrix} 0 & \lambda \\ -\lambda & 0 \end{pmatrix}$$

$$\boxed{r^\dagger r = |\lambda|^2 I} \qquad \boxed{t^\dagger t = 1 - r^\dagger r}$$

Same transmissions for both spin polarizations

J. H. Bardarson, J. Phys. A: Math. Theor. **41**, 405203 (2008)

PHYSICAL REVIEW B **102**, 035445 (2020)

Editors' Suggestion

Spin selectivity through time-reversal symmetric helical junctions

Yasuhiro Utsumi,[1] Ora Entin-Wohlman,[2] and Amnon Aharony[2]

in time-reversal symmetric systems with half-integer spins, the transmission eigenvalues of the scattering matrix come in degenerate pairs. Assuming that this Kramers-type degeneracy involves spins with opposite eigenvalues, the theorem prohibits the two-terminal spin filtering because each pair of doubly degenerate transmission eigenvalues carries the same amount of up and down spins. However, the theorem does not specify which spin states are associated with the doubly degenerate transmission eigenvalues. Therefore, it is possible to consider, e.g., two pairs of doubly degenerate transmission eigenvalues in which one pair carries two up spins in one direction and the other pair carries two down spins in the opposite direction. Hence, the theorem does not rule out the "counterexamples" [36–39] of the no-go theorem of spin filtering by two-terminal setups.

Orbital states on sites, double helix DNA

PHYSICAL REVIEW B **102**, 035445 (2020)

Editors' Suggestion

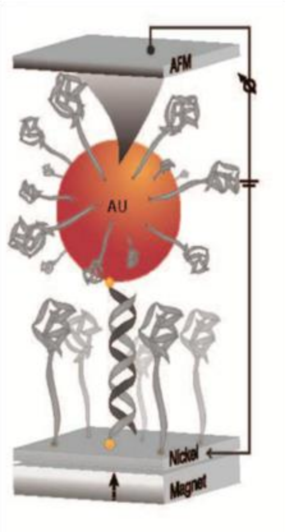
Spin selectivity through time-reversal symmetric helical junctions

Yasuhiro Utsumi,[1] Ora Entin-Wohlman,[2] and Amnon Aharony[2]

$$|\psi\rangle = \sum_{n=1}^{N_L} \left(c_n^{\mathrm{in,L}}|n\rangle + c_n^{\mathrm{out,L}}|Tn\rangle\right) \qquad T|\psi\rangle = \sum_{n=1}^{N_L} \left[(c_n^{\mathrm{in,L}})^*|Tn\rangle - (c_n^{\mathrm{out,L}})^*|n\rangle\right]$$

2 orbital states on each site (px & pz on Carbon)

Ot double helix DNA



Editors' Suggestion

Spin selectivity through time-reversal symmetric helical junctions

Yasuhiro Utsumi,[1] Ora Entin-Wohlman,[2] and Amnon Aharony[2]

$$\mathcal{H}_{\rm mol} = \sum_{n=1}^{N_{\rm mol}-1} (-J c_{n+1}^{\dagger} c_n + {\rm H.c.}) + \sum_{n=1}^{N_{\rm mol}} \epsilon_0 c_n^{\dagger} c_n$$
$$+ \Delta\epsilon c_n^{\dagger} \tau_z \otimes \sigma_0 c_n + \Delta_{\rm so} c_n^{\dagger} \tau_y \otimes \boldsymbol{t}(\phi_n) \cdot \boldsymbol{\sigma} c_n, \qquad (45)$$

where $N_{\rm mol}$ is the number of sites on the molecule. The creation operator on site n,

$$c_n^{\dagger} = [c_{n;x\uparrow}^{\dagger} \quad c_{n;x\downarrow}^{\dagger} \quad c_{n;z\uparrow}^{\dagger} \quad c_{n;z\downarrow}^{\dagger}], \qquad (46)$$

$$\mathbf{t}(\phi) = L\{-\tilde{\kappa}\ \sin(\phi), p\tilde{\kappa}\ \cos(\phi), |\tilde{\tau}|\}, \qquad (47)$$

where $L = \sqrt{R^2 + [\Delta h/(2\pi)]^2}$, and p specifies the chirality of helix: $p = 1$ (-1) for a right-handed (left-handed) helix [12]. The radius and the pitch determine the curvature $\tilde{\kappa}$ and torsion $\tilde{\tau}$ of the helix:

$$\tilde{\kappa} = R/L^2, \quad \tilde{\tau} = p\Delta h/(2\pi)/L^2. \qquad (48)$$

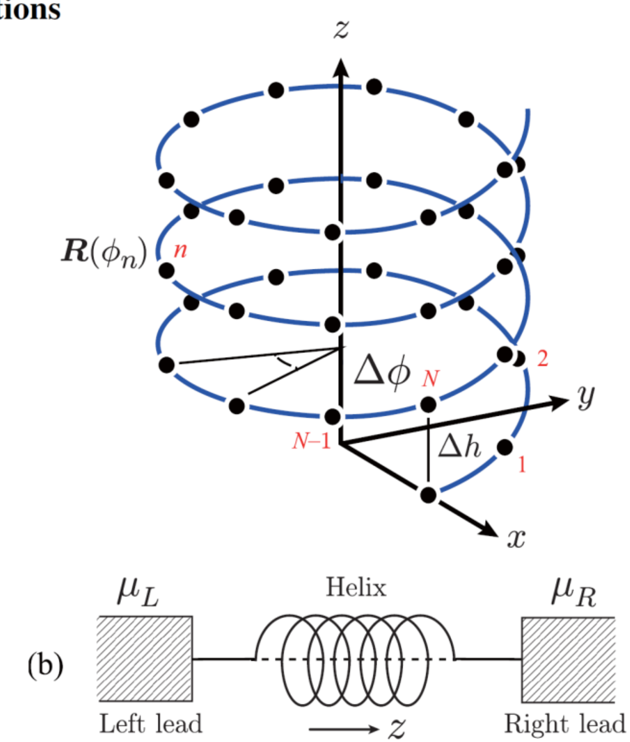


FIG. 2. (a) Schematic picture of a single strand of a double-stranded DNA. $\boldsymbol{R}(\phi_n)$ is the radius vector of site n within the Frenet-Serret scheme [Eq. (B1)], Δh is the pitch, $\Delta\phi = 2\pi/N$, and $\phi_n = n\Delta\phi$. The original tight-binding Hamiltonian (B4) is expressed in the coordinate system x, y, and z, shown in the figure. (b) A molecular junction. The left and right leads are attached to two edges of the single strand of the DNA molecule. A difference in the chemical potentials of the left and right leads, μ_L and μ_R, induces a flow of electrons.

PHYSICAL REVIEW B **102**, 035445 (2020)

Editors' Suggestion

Spin selectivity through time-reversal symmetric helical junctions

Yasuhiro Utsumi,[1] Ora Entin-Wohlman,[2] and Amnon Aharony[2]

Example—two orbitals

$$r = \begin{bmatrix} r_{1\uparrow,1\uparrow} & 0 & 0 & r_{1\uparrow,2\downarrow} \\ 0 & r_{1\downarrow,1\downarrow} & r_{1\downarrow,2\uparrow} & 0 \\ 0 & r_{2\uparrow,1\downarrow} & r_{2\uparrow,2\uparrow} & 0 \\ r_{2\downarrow,1\uparrow} & 0 & 0 & r_{2\downarrow,2\downarrow} \end{bmatrix} = \begin{bmatrix} r_{1\uparrow,1\uparrow} & 0 & 0 & r_{1\uparrow,2\downarrow} \\ 0 & r_{1\uparrow,1\uparrow} & -r_{2\downarrow,1\uparrow} & 0 \\ 0 & -r_{1\uparrow,2\downarrow} & r_{2\downarrow,2\downarrow} & 0 \\ r_{2\downarrow,1\uparrow} & 0 & 0 & r_{2\downarrow,2\downarrow} \end{bmatrix}$$

$$\Big\downarrow$$

time-reversal symmetric $\quad r_+ = \begin{bmatrix} r_{1\uparrow,1\uparrow} & r_{1\uparrow,2\downarrow} \\ r_{2\downarrow,1\uparrow} & r_{2\downarrow,2\downarrow} \end{bmatrix}, \; r_- = \begin{bmatrix} r_{2\downarrow,2\downarrow} & -r_{1\uparrow,2\downarrow} \\ -r_{2\downarrow,1\uparrow} & r_{1\uparrow,1\uparrow} \end{bmatrix}$

$$\Big\downarrow$$

Spin-polarization $\quad P \propto |r_{2\downarrow,1\uparrow}|^2 - |r_{1\uparrow,2\downarrow}|^2$

$\boxed{N_S = 1}$

$$r = \begin{array}{cc} \uparrow & \downarrow \\ \left[\begin{array}{cc} r_0 & 0 \\ 0 & r_0 \end{array}\right] \end{array} \begin{array}{c} \uparrow \\ \downarrow \end{array}$$

2 transmission eigenvalues $\{\Lambda, \Lambda\}$ $\Lambda = 1 - |r_0|^2$

$\Rightarrow$ $P_{z;L} = 0$

$\boxed{N_S = 2}$

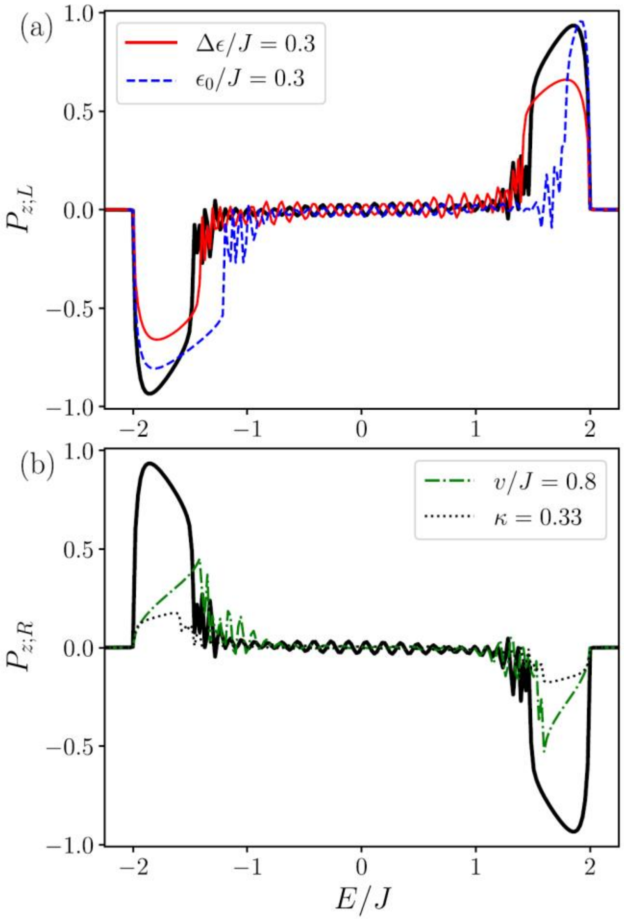
$$r = \begin{array}{cccc} 1\uparrow & 1\downarrow & 2\uparrow & 2\downarrow \\ \left[\begin{array}{cc|cc} r_{1\uparrow,1\uparrow} & 0 & 0 & r_{1\uparrow,2\downarrow} \\ 0 & r_{1\uparrow,1\uparrow} & -r_{2\downarrow,1\uparrow} & 0 \\ \hline 0 & -r_{1\uparrow,2\downarrow} & r_{2\downarrow,2\downarrow} & 0 \\ r_{2\downarrow,1\uparrow} & 0 & 0 & r_{2\downarrow,2\downarrow} \end{array}\right] \end{array} \begin{array}{c} 1\uparrow \\ 1\downarrow \\ 2\uparrow \\ 2\downarrow \end{array}$$

4 transmission eigenvalues $\{\Lambda_+, \Lambda_+, \Lambda_-, \Lambda_-\}$ $\Lambda_\pm = 1 - X \pm \sqrt{X^2 - |Y|^2}$

$$X = \frac{|r_{1\uparrow,1\uparrow}|^2 + |r_{1\uparrow,2\downarrow}|^2 + |r_{2\downarrow,1\uparrow}|^2 + |r_{2\downarrow,2\downarrow}|^2}{2} \qquad Y = r_{1\uparrow,1\uparrow} r_{2\downarrow,2\downarrow} - r_{1\uparrow,2\downarrow} r_{2\downarrow,1\uparrow}$$

$$\Rightarrow \quad P_{z;L} = \frac{|r_{2\downarrow,1\uparrow}|^2 - |r_{1\uparrow,2\downarrow}|^2}{\Lambda_+ + \Lambda_-} \quad \neq 0$$

Finite spin-polarization factor



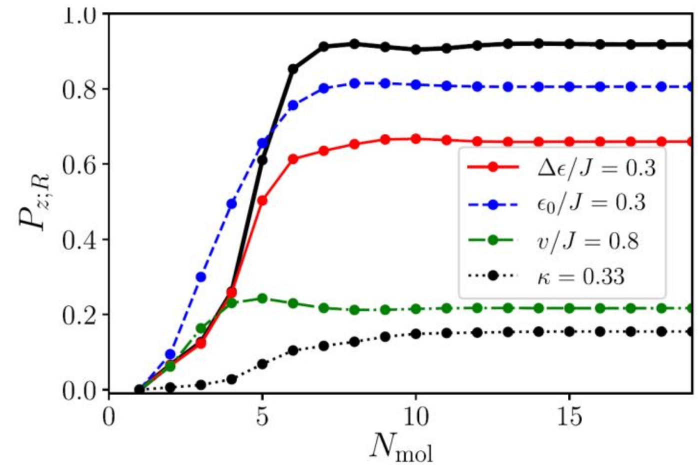


FIG. 4. The length dependence of z component of the spin-polarization factor in the right lead. The energy is fixed at $E/J = -1.8$. Other parameters are as in Fig. 3.

From the experimental point of view, perhaps the main feature that we find is the strong dependence of the spin-filtering effect on the energy of the charge carriers, in addition to its dependence on the chirality parameter of the helix-shaped molecule. The latter results in an experimentally accessible property: the directions of the spin polarizations in the left and the right leads are opposite.

Research Article

Israel Journal of Chemistry
www.ijc.wiley-vch.de

doi.org/10.1002/ijch.202200107

Spin-Filtering in a *p*-Orbital Helical Atomic Chain

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Abstract: We theoretically analyze spin filtering in two-terminal systems, induced by the spin-orbit interaction (SOI), as a possible origin of the "chirality-induced spin selectivity" (CISS) effect observed experimentally in chiral molecules, such as DNA. Due to Bardarson's theorem, spin filtering cannot be realized in a molecule containing one orbital-channel. However, when two orbitals are involved, SOI can induce spin filtering in a molecule coupled to two terminals without braking time-reversal symmetry. In particular, we provide an example of a 4×4 reflection matrix for a spinful electron passing through a molecule containing two orbital-channels, which complies with Bardarson's theorem and produces a finite spin conductance. As a microscopic toy model realizing a single strand of DNA, we consider a *p*-orbital helical atomic chain with intra-atomic SOI's and a strong crystalline field along the helix. This model exhibits two-orbital spin filtering: For various parameters preserving the helical symmetry, the model hosts spin asymmetric states carrying pairs of up and down spins propagating in opposite directions. The typical energy scale of the helical states is the product of the intra-atomic SOI and the curvature. The spin filtering mechanism is associated with the intra-atomic SOI, which would be larger than the inter-atomic SOI. In this respect, the present model may be a more likely candidate for the CISS in organic material than other models associated with the inter-atomic SOI.

Keywords: Chirality induced spin selectivity effect · Spin orbit interaction · Helical symmetry · Time reversal symmetry

Electronic States at Edges of Finite p-orbital Helical Atomic Chain

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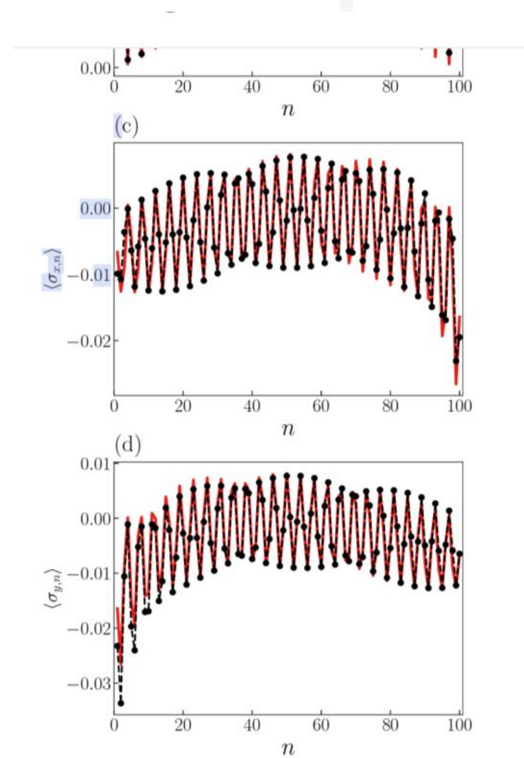
(Dated: 31 May 2023)

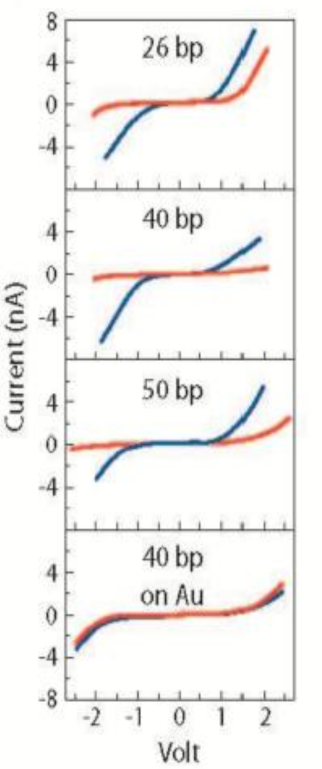
In connection to the chirality induced spin-selectivity (CISS) effect, we theoretically analyze the electron state of edges of a finite p-orbital helical atomic chain with the intra-atomic spin orbit interaction (SOI). This model can host the spin-filtering state in which two up spins propagate in one direction and two down spins propagate in the opposite direction without breaking the time-reversal symmetry. We found that this model can exhibit the enhancement of charge density concentrated at the edges due to the evanescent states induced by the spin and orbital flip by the SOI. Although the spin density is absent because of the time reversal symmetry of the SOI, the charge concentration at the edges may play a role in the enantioselective adsorption of CISS molecules on the ferromagnetic surface.

I. INTRODUCTION



Other alternatives:

- More terminals
- Magnetic fields or polarized electrons
- Time-dependence: AC electric and magnetic fields
- More orbital states
- Non-linear response – needs T(E) (Fransson, vWees)
- Orbital filtering (Binghai Yan)
- Molecule-molecule coupling? (Leakage, cooperative effect)
- Role of exchange with substrate (Paltiel)
- Molecule parallel to substrate (Ruitenbeek)?
- Double helix -- Utsumi?
- More???



Conclusions:

No spin splitting for 2 terminals plus spin orbit.

Many theoretical ways to overcome this limitation, **BUT**

Which model applies to each experiment??

Leakage,

Magnetic fields,

Time dependence (transients),

Double helix and more ionic levels,

Non-linearity?? ……..

감사합니다

gamsahamnida

Thank you

Instituto Balseiro