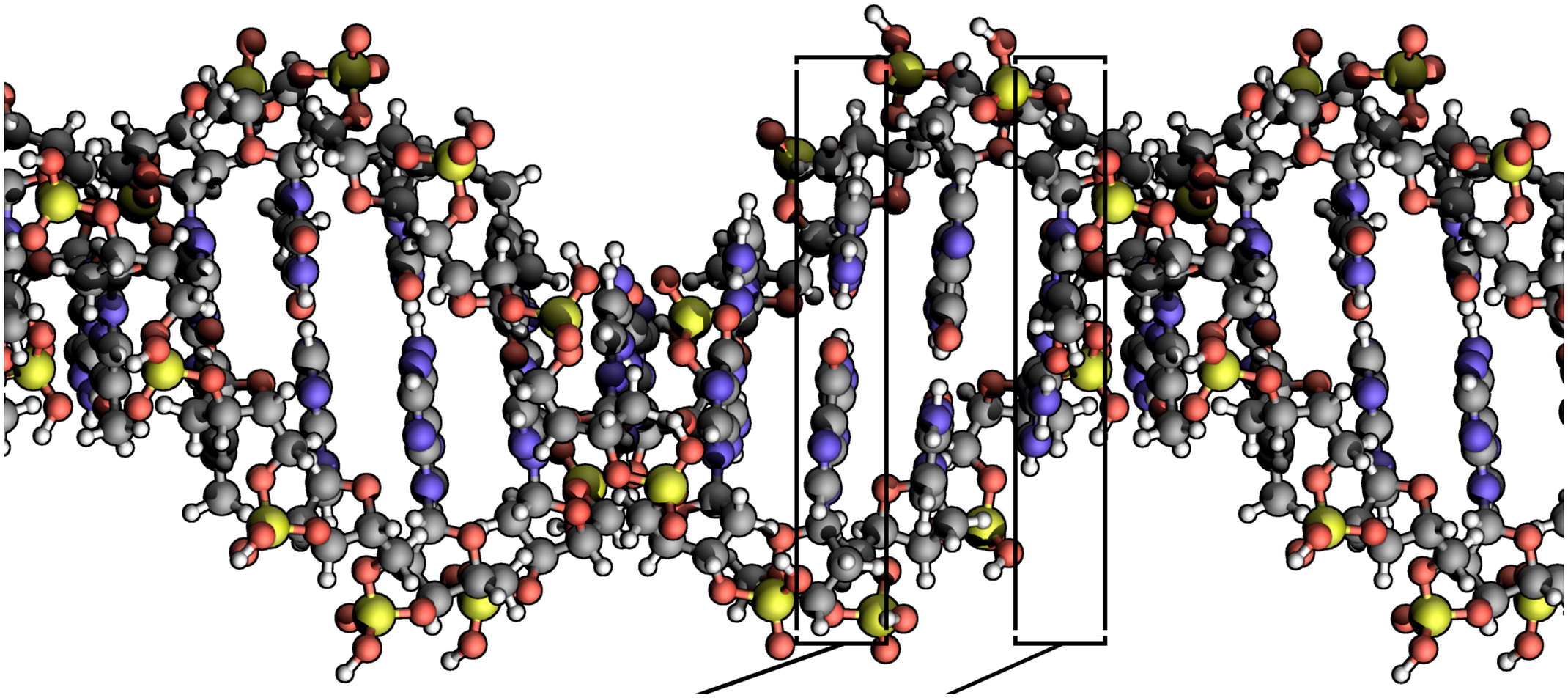

Electron and Spin–Phonon Interaction in DNA

Mayra Peralta, YachayTech University, Ecuador

Technical University of Dresden, Germany March 25th 2022

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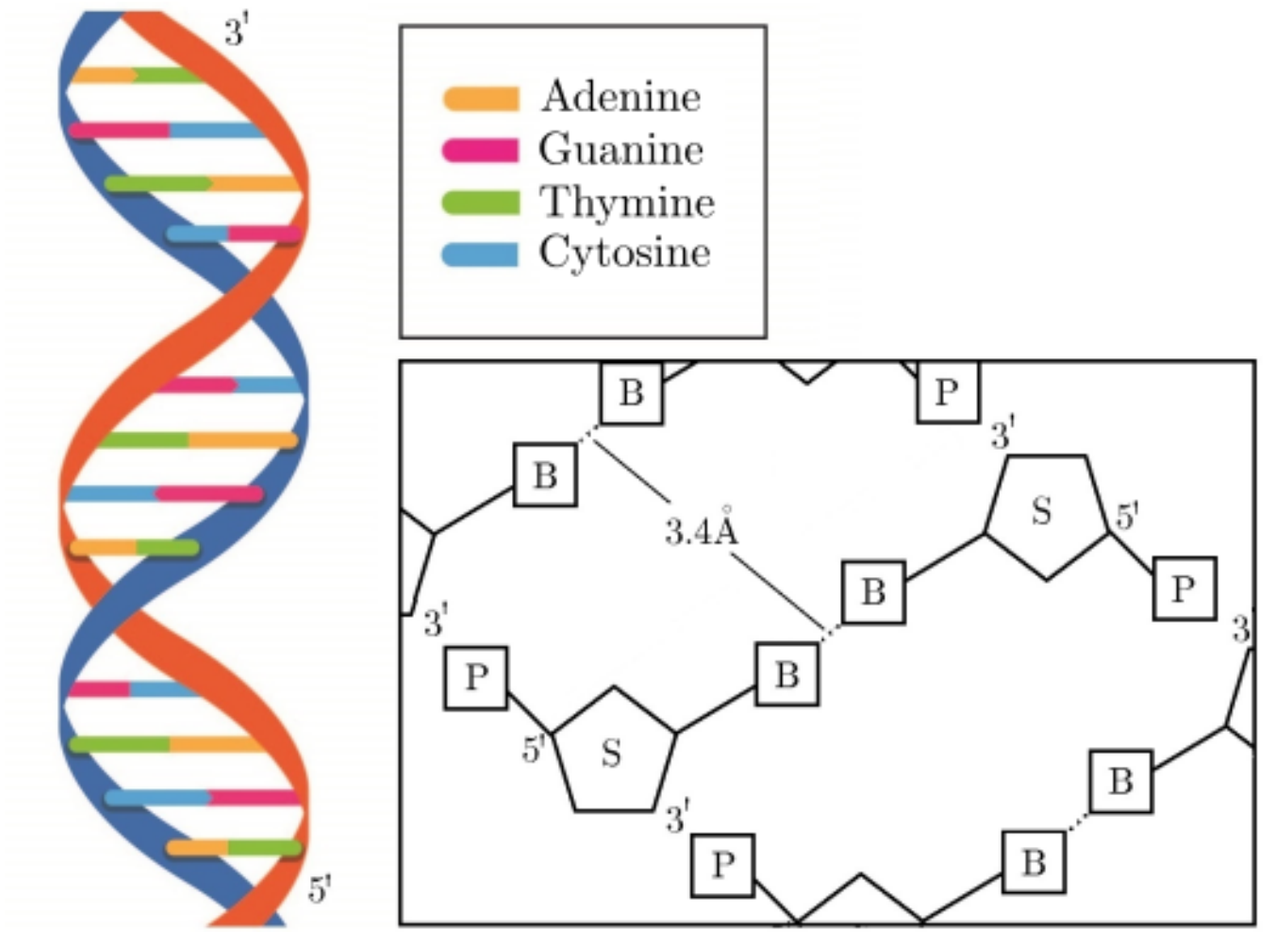
Introduction: Structure of DNA



- B form is the most common form.
- Double right handed helix polymer.
- Nucleotides are the building blocks, which are formed by a base, a sugar and a phosphate group.
- Bases can be Purines (A, G) or Pyrimidines (T, C).
- The sugar is a deoxyribose sugar.
- The phosphate group act as structural support

[1] Anirban Ghosh and Manju Bansal. A glossary of dna structures from a to z. Acta Crystallographica Section D: Biological Crystallography, 59(4):620–626, 2003.

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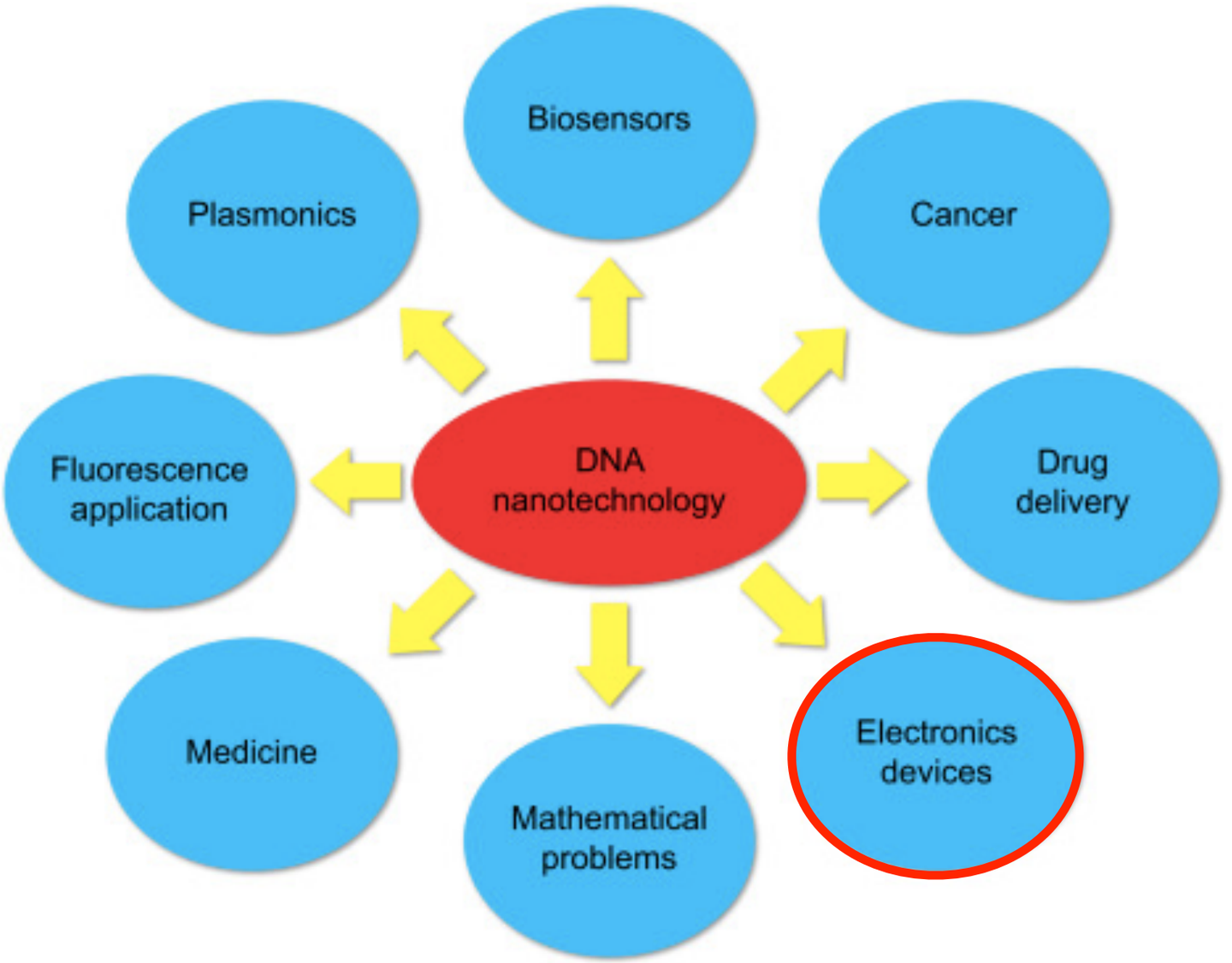
Introduction: Structure of DNA



- Self assembly and self recognition
- High transfer rates of charge
- Spin selectivity (CISS Effect)

[2] Nadrian C Seeman and Hanadi F Sleiman. Dna nanotechnology. Nature Reviews Materials, 3(1):1–23, 2017

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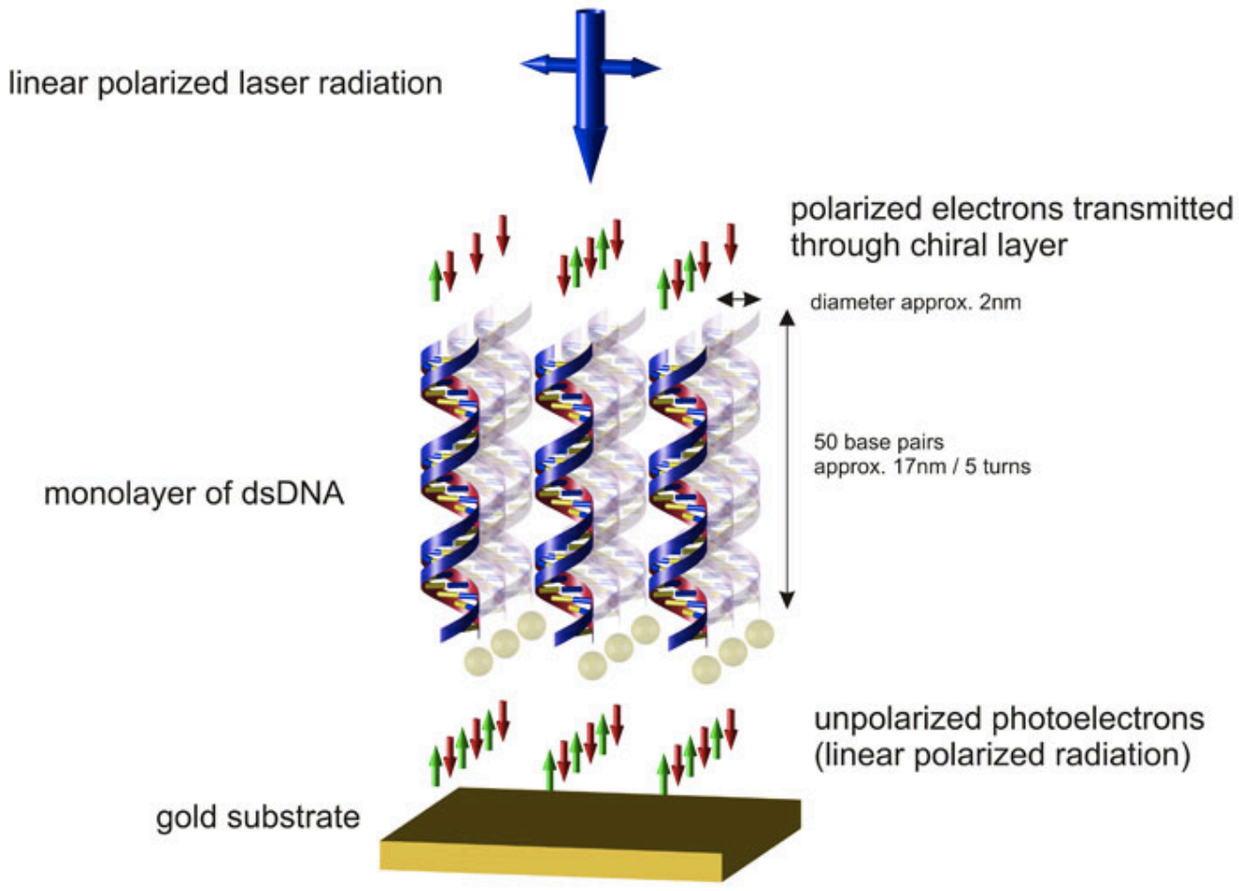
Introduction: DNA in the context of molecular spintronics



- Spintronics study: Inject, manipulate and detect spin polarization and spin polarized currents.
- Individual molecules.
- DNA properties: spin polarization, spin dependent transport, long distance electron transfer, chiral induced spin selectivity.

Chiral Induced Spin Selectivity! (CISS Effect)

[3] B Göhler, V Hamelbeck, TZ Markus, M Kettner, GF Hanne, Z Vager, R Naaman, and H Zacharias. Spin selectivity in electron transmission through self-assembled monolayers of double-stranded dna. Science, 331(6019):894–897, 2011.

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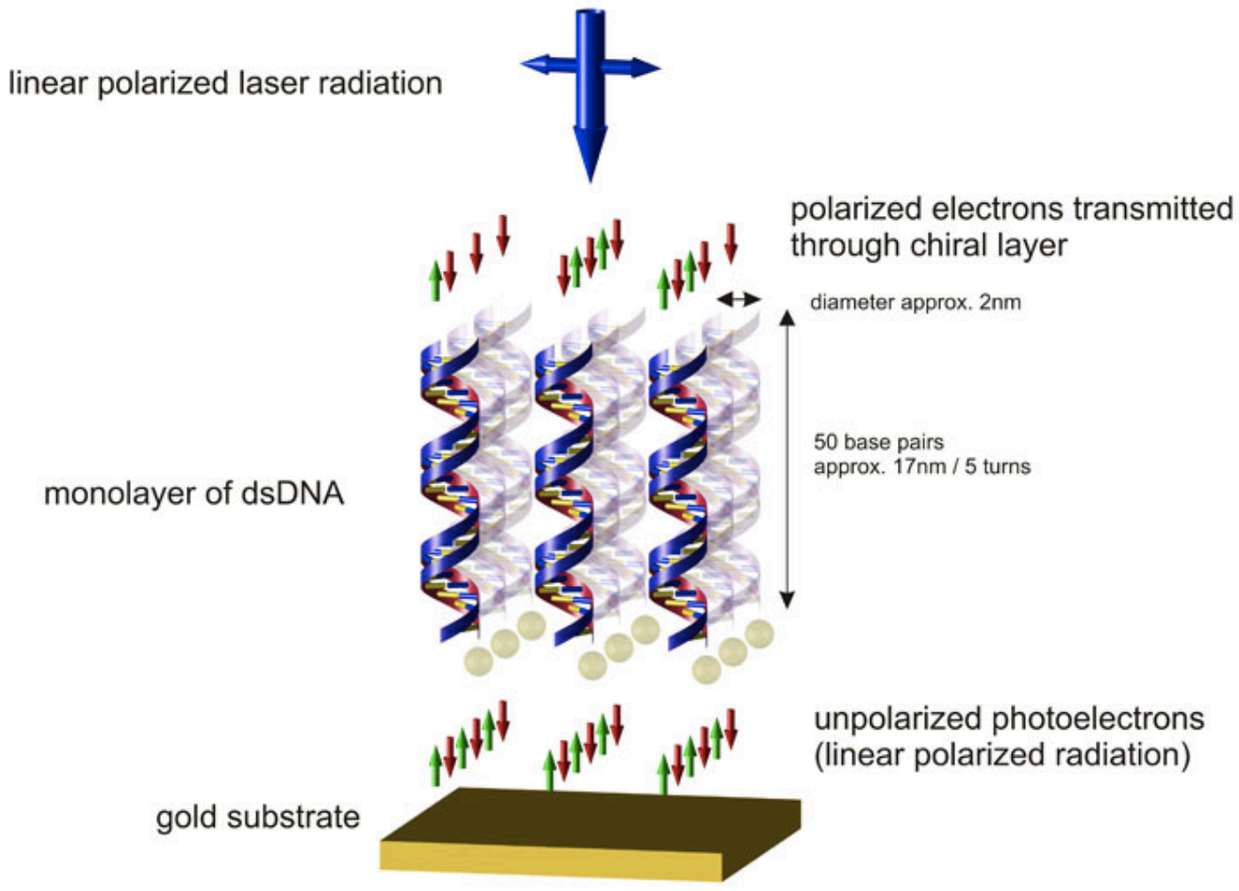

Other amazing applications!

- Quantum information science, quantum computers
- Sensors
- Spin injection through molecules in spintronic devices
- Spin selective chemistry

Chiral Induced Spin Selectivity! (CISS Effect)

[3] B Göhler, V Hamelbeck, TZ Markus, M Kettner, GF Hanne, Z Vager, R Naaman, and H Zacharias. Spin selectivity in electron transmission through self-assembled monolayers of double-stranded dna. Science, 331(6019):894–897, 2011.

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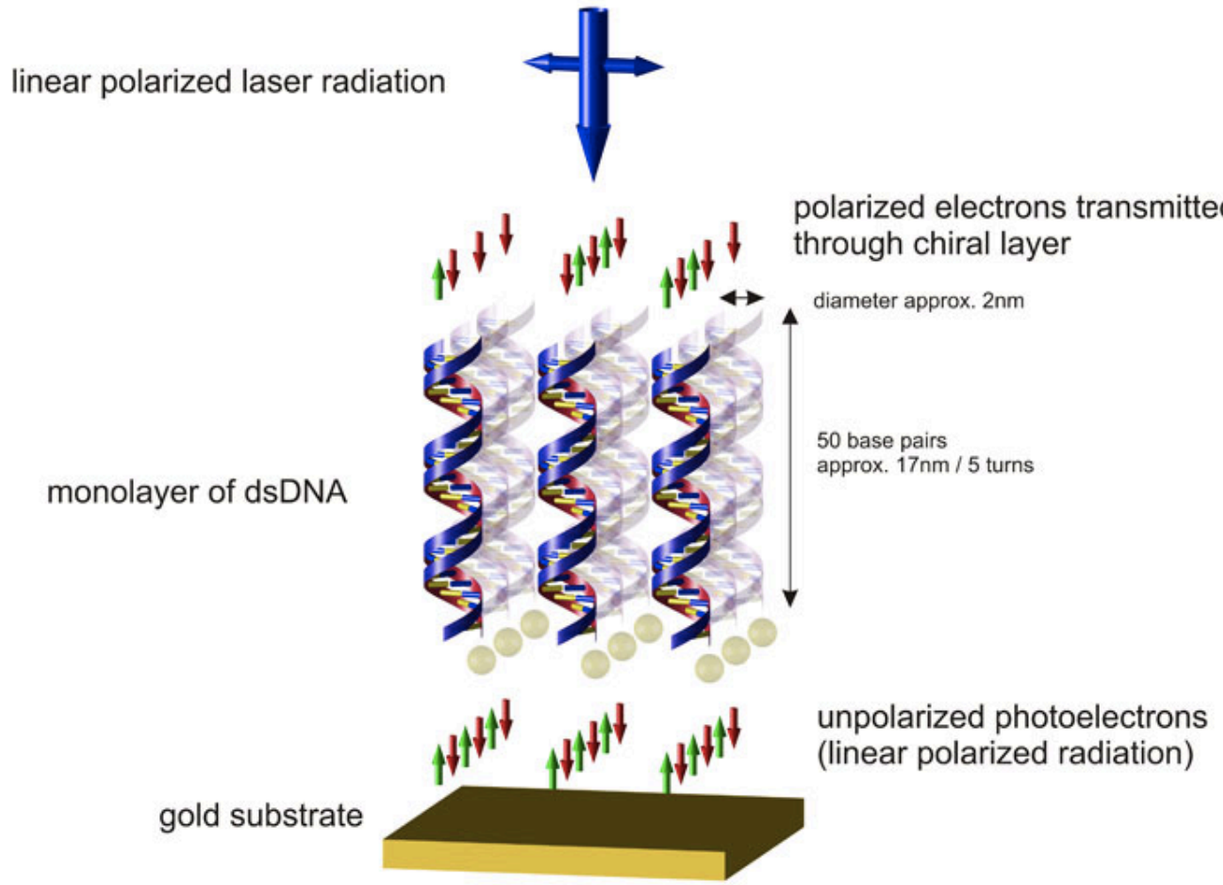

Some open questions!

- Better understanding of the electron transport process (including the spin)
- What is the mechanism for the CISS effect?
- Origin of the high electron and spin transfer, even at room temperature
- Electron and spin-phonon coupling role in modulating and protecting these currents

Chiral Induced Spin Selectivity! (CISS Effect)

Understanding the electron-phonon and spin-phonon interaction is fundamental to understand this effect!

[3] B Göhler, V Hamelbeck, TZ Markus, M Kettner, GF Hanne, Z Vager, R Naaman, and H Zacharias. Spin selectivity in electron transmission through self-assembled monolayers of double-stranded dna. Science, 331(6019):894–897, 2011. [4] D. Aiello *et. al., A Quirality-Based Quantum Leap, https://doi.org/10.1021/acsnano.1c01347, ACS Nano 2022.*

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Introduction: DNA in the context of molecular spintronics

Understanding the electron–phonon and spin–phonon interaction is fundamental to understand this effect!

The importance of theoretical, analytical models in this context

- **DFT. Challenging for the number of atoms in the unit cell. Expensive in time. The effect of spin selectivity is underestimated by these calculations**
- **Analytical methods (Tight Binding). Atomistic derivations that can derive in Hamiltonians with the relevant interactions**

[4] D. Aiello *et. al., A Quirality-Based Quantum Leap, https://doi.org/10.1021/acsnano.1c01347, ACS Nano 2022.*

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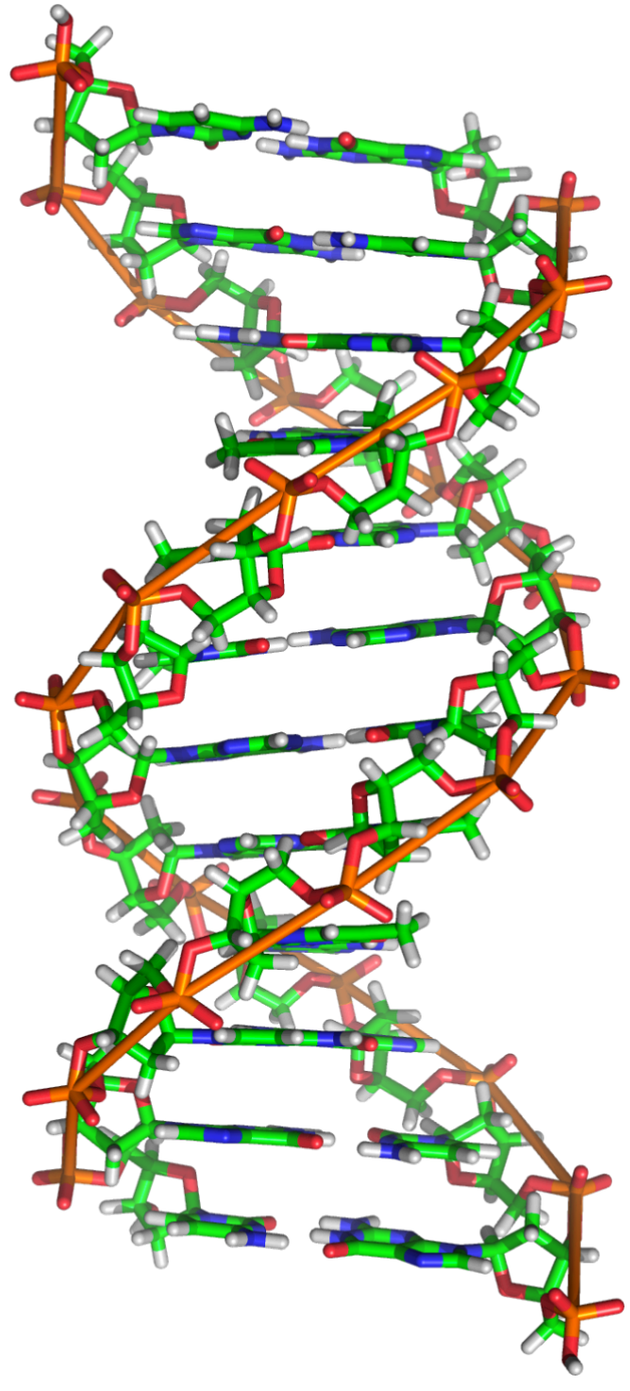
Outline

- Introduction
- The Model
  - DNA structure model
  - The envelope function approximation
  - Inclusion of the vibrations
- Electron–phonon interaction in DNA
- Spin–phonon interaction in DNA
- Conclusions



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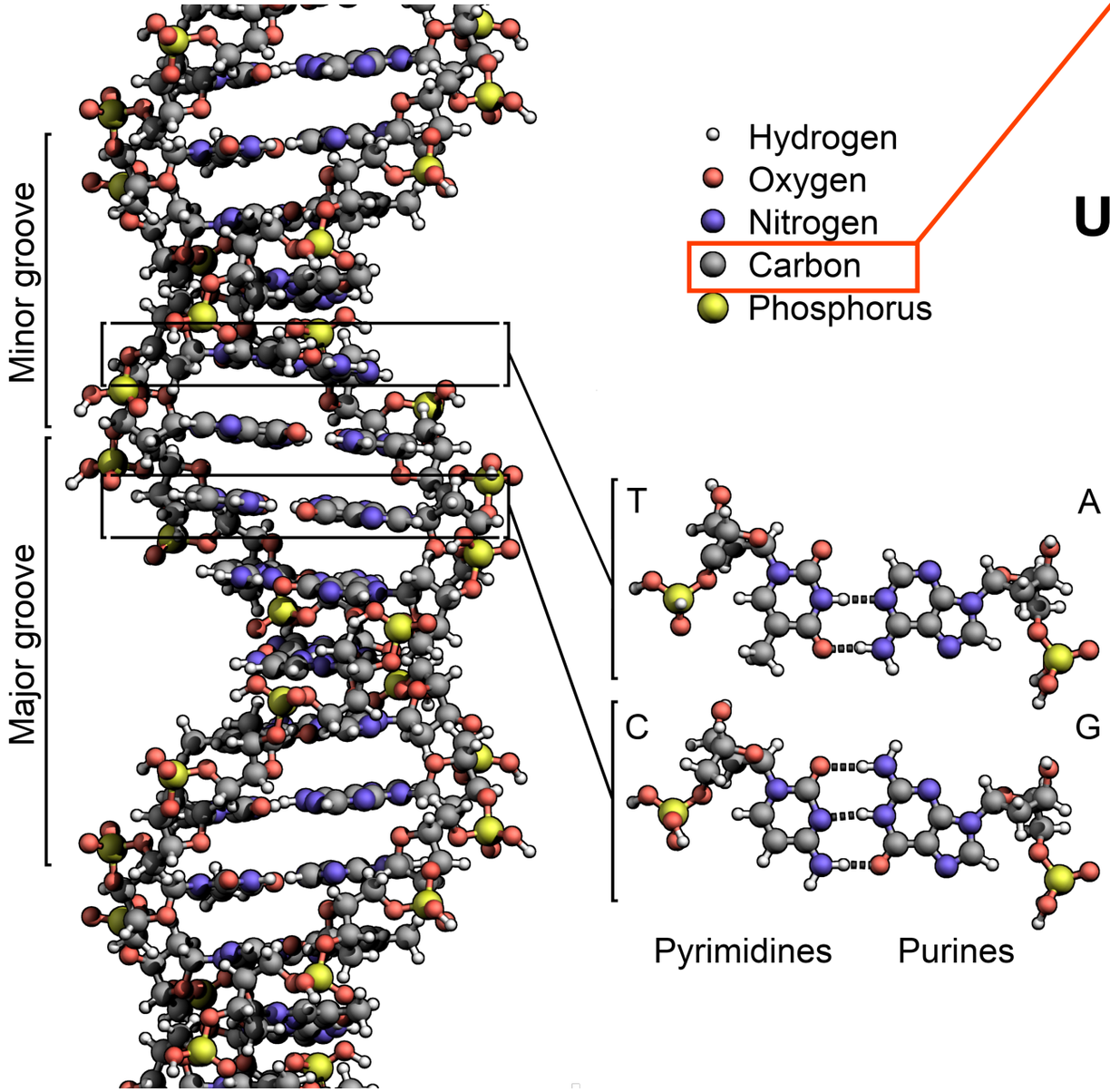
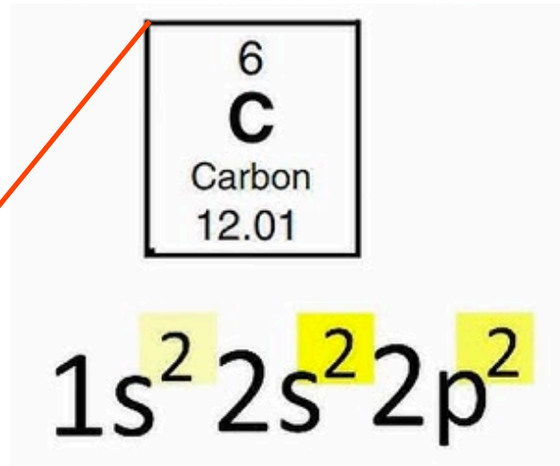
The model: DNA structure model

B-DNA





Unpaired electrons at the pz orbitals

“Simple” analytical model

[5] L.G.D. Hawke, G. Kalosakas, and C. Simserides, Electronic parameters for charge transfer along DNA. Eur. Phys. J. E 32, 291–305 (2010).

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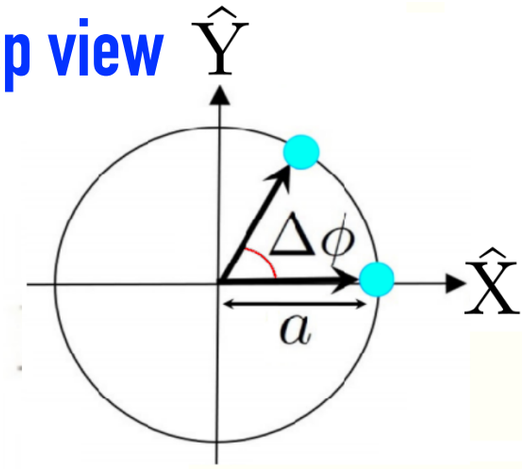
The model: DNA structure model

- B-form DNA with N sites per helix.

Top view



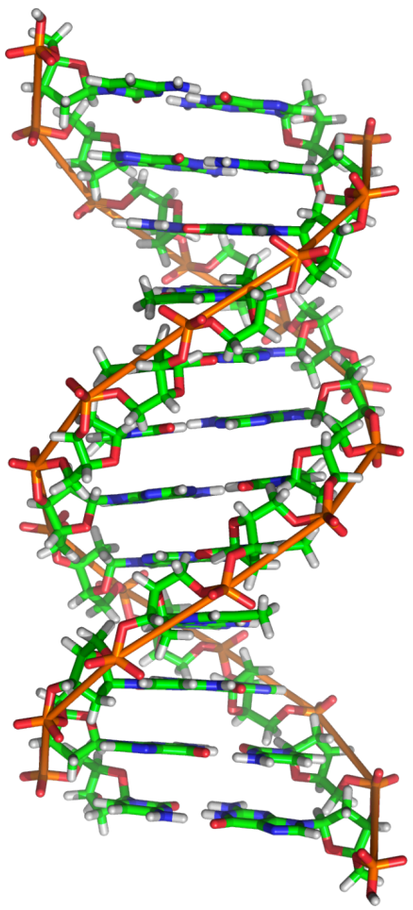
Vectors connecting nearest neighbors

$$\boldsymbol{\tau}_1^{A,B} = a\Delta\phi\hat{y} + \frac{b\Delta\phi}{2\pi}\hat{z},$$

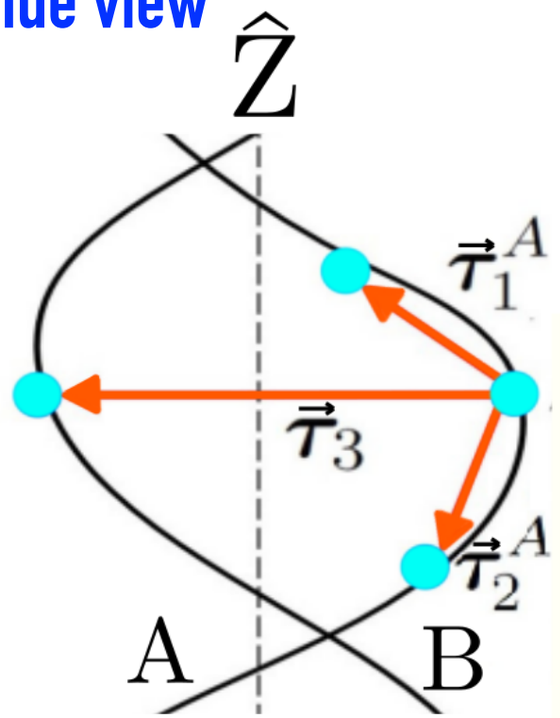
$$\boldsymbol{\tau}_2^{A,B} = -a\Delta\phi\hat{y} - \frac{b\Delta\phi}{2\pi}\hat{z},$$

Intra-helix

B-DNA

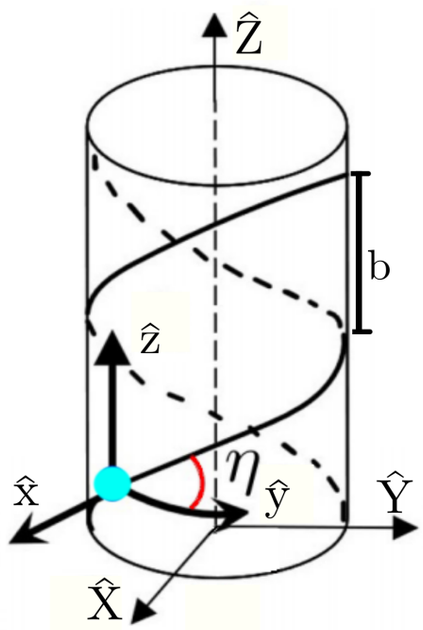


Side view



$$\boldsymbol{\tau}_3 = -2a\hat{x}.$$

Inter-helix



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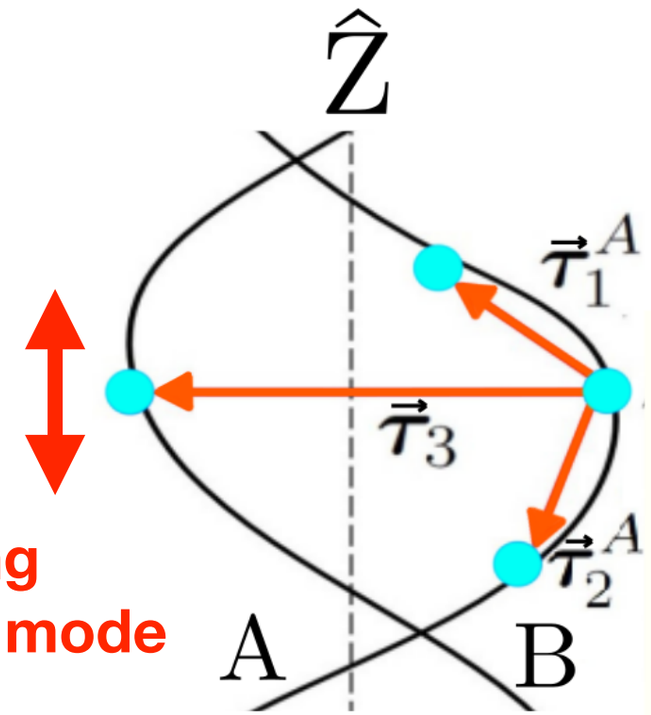
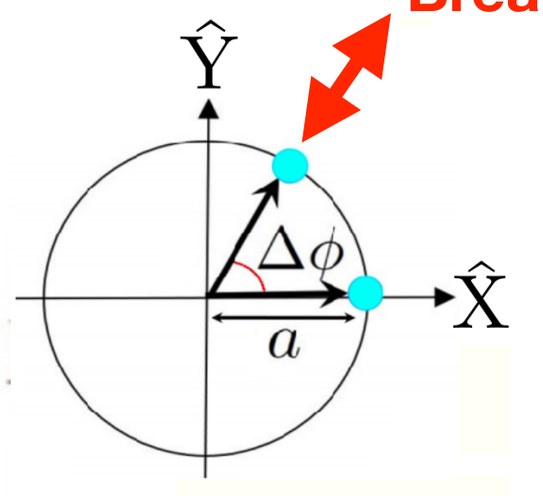
The model: DNA structure model

- Modes in the double-helix DNA model.



Stretching (longitudinal) mode



Breathing (radial) mode

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The model: The envelope function approximation

Wave function

$$\Psi(\mathbf{r}) \approx u_{\mathbf{k}}(\mathbf{r}) F(\mathbf{r}),$$

Fast oscillating wave function

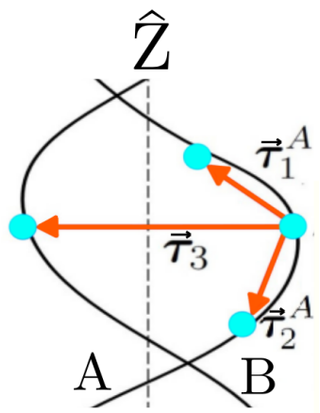
Slowly varying envelope function

Wavefunctions used for the nearest neighbors TB model, in the DNA two-sites system:

$$\Psi_{A\sigma}(\boldsymbol{R}_A) = e^{i\boldsymbol{K}\cdot\boldsymbol{R}_A} F^{\boldsymbol{K}}_{A\sigma}(\boldsymbol{R}_A) + e^{i\boldsymbol{K}'\cdot\boldsymbol{R}_A} F^{\boldsymbol{K}'}_{A\sigma}(\boldsymbol{R}_A),$$

$$\Psi_{B\sigma}(\boldsymbol{R}_B) = e^{i\boldsymbol{K}\cdot\boldsymbol{R}_B} F^{\boldsymbol{K}}_{B\sigma}(\boldsymbol{R}_B) + e^{i\boldsymbol{K}'\cdot\boldsymbol{R}_B} F^{\boldsymbol{K}'}_{B\sigma}(\boldsymbol{R}_B).$$

$$\boldsymbol{K} = \frac{\pi}{2R^2}(0, a\Delta\phi, \frac{b\Delta\phi}{2\pi}), \qquad \boldsymbol{K}' = -\boldsymbol{K}.$$



[6] Mayra Peralta, Steven Feijoo, Solmar Varela, Vladimiro Mujica, and Ernesto Medina. Coherence preservation and electron–phonon interaction in electron transfer in dna. The Journal of Chemical Physics, 153(16):165102, 2020

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The model: The envelope function approximation

$$\varepsilon\Psi_{A\sigma}(\mathbf{R}_A) = \sum_{l=1}^{2} t^{in}_{\mathbf{R}_{A\sigma},(\mathbf{R}_A+\boldsymbol{\tau}_l^A)\sigma}\Psi_{A\sigma}(\mathbf{R}_A+\boldsymbol{\tau}_l^A)$$

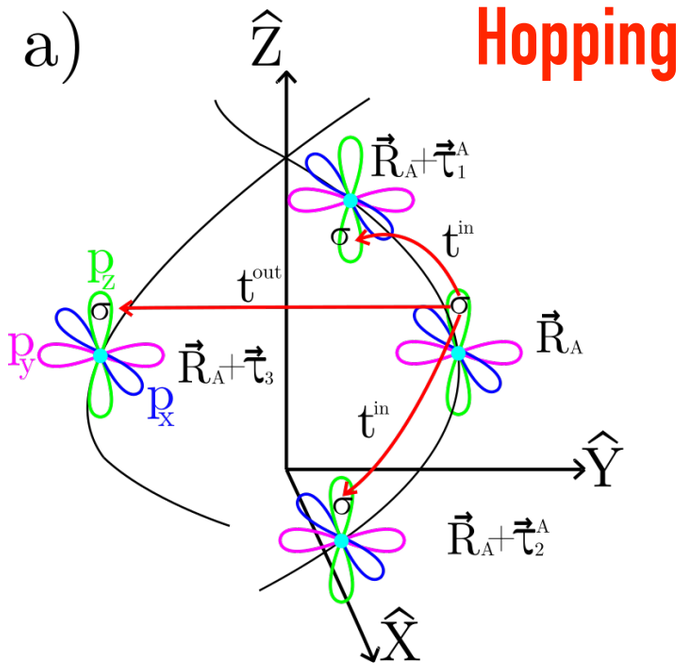
$$+\sum_{l=1}^{2} V^{in}_{\mathbf{R}_{A\sigma},(\mathbf{R}_A+\tau_l^A)\sigma'}\Psi_{A\sigma'}(\mathbf{R}_A+\boldsymbol{\tau}_l^A)$$

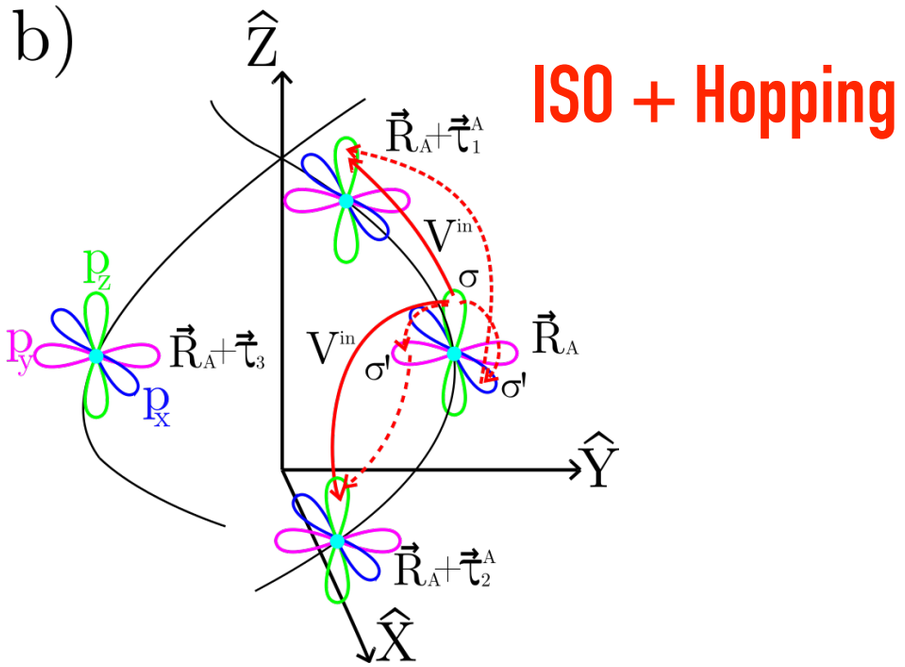
$$+ t^{out}_{\mathbf{R}_{A\sigma},(\mathbf{R}_A+\boldsymbol{\tau}_3)\sigma}\Psi_{B\sigma}(\mathbf{R}_A+\boldsymbol{\tau}_3),$$

$$\varepsilon\Psi_{B\sigma}(\mathbf{R}_B) = \sum_{l=1}^{2} t^{in}_{\mathbf{R}_{B\sigma},(\mathbf{R}_B+\boldsymbol{\tau}_l^B)\sigma}\Psi_{B\sigma}(\mathbf{R}_B+\boldsymbol{\tau}_l^B)$$

$$+\sum_{l=1}^{2} V^{in}_{\mathbf{R}_{B\sigma},(\mathbf{R}_B+\boldsymbol{\tau}_l^B)\sigma'}\Psi_{B\sigma'}(\mathbf{R}_B+\boldsymbol{\tau}_l^B)$$

$$+ t^{out}_{\mathbf{R}_{B\sigma},(\mathbf{R}_B-\boldsymbol{\tau}_3)\sigma}\Psi_{A\sigma}(\mathbf{R}_B-\boldsymbol{\tau}_3).$$





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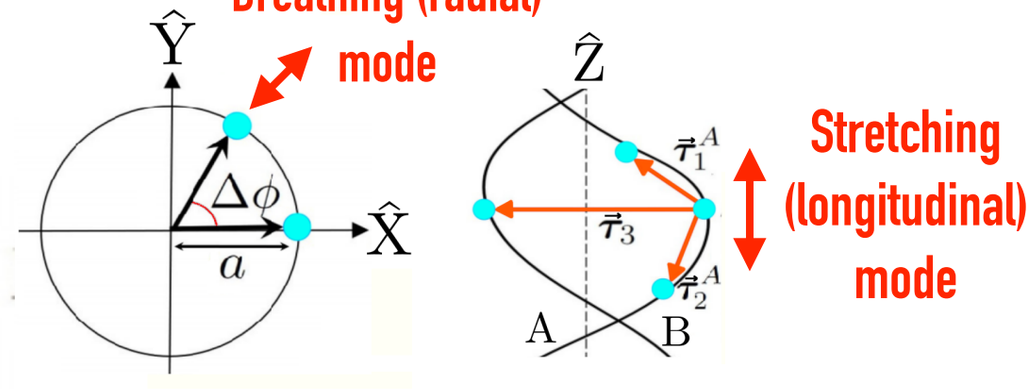
The model: Inclusion of the vibrations

$$\varepsilon\Psi_{A\sigma}(\mathbf{R}_A) = \sum_{l=1}^{2} t^{in}_{\mathbf{R}_{A\sigma},(\mathbf{R}_A+\boldsymbol{\tau}_l^A)\sigma}\Psi_{A\sigma}(\mathbf{R}_A+\boldsymbol{\tau}_l^A)$$
$$+\sum_{l=1}^{2} V^{in}_{\mathbf{R}_{A\sigma},(\mathbf{R}_A+\tau_l^A)\sigma'}\Psi_{A\sigma'}(\mathbf{R}_A+\boldsymbol{\tau}_l^A)$$
$$+t^{out}_{\mathbf{R}_{A\sigma},(\mathbf{R}_A+\boldsymbol{\tau}_3)\sigma}\Psi_{B\sigma}(\mathbf{R}_A+\boldsymbol{\tau}_3),$$

$$\varepsilon\Psi_{B\sigma}(\mathbf{R}_B) = \sum_{l=1}^{2} t^{in}_{\mathbf{R}_{B\sigma},(\mathbf{R}_B+\boldsymbol{\tau}_l^B)\sigma}\Psi_{B\sigma}(\mathbf{R}_B+\boldsymbol{\tau}_l^B)$$
$$+\sum_{l=1}^{2} V^{in}_{\mathbf{R}_{B\sigma},(\mathbf{R}_B+\boldsymbol{\tau}_l^B)\sigma'}\Psi_{B\sigma'}(\mathbf{R}_B+\boldsymbol{\tau}_l^B)$$
$$+t^{out}_{\mathbf{R}_{B\sigma},(\mathbf{R}_B-\boldsymbol{\tau}_3)\sigma}\Psi_{A\sigma}(\mathbf{R}_B-\boldsymbol{\tau}_3).$$



How to include phonons?

These hopping parameters depend on the hybridization between atomic orbitals of different atoms involved in the process, and therefore, they depend on the **distances between atoms**

Atomic vibrations modulate the hopping parameters

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The model: Inclusion of the vibrations

$$\varepsilon\Psi_{A\sigma}(\mathbf{R}_A) = \sum_{l=1}^{2} t^{in}_{\mathbf{R}_{A\sigma},(\mathbf{R}_A+\boldsymbol{\tau}_l^A)\sigma}\Psi_{A\sigma}(\mathbf{R}_A+\boldsymbol{\tau}_l^A)$$
$$+\sum_{l=1}^{2} V^{in}_{\mathbf{R}_{A\sigma},(\mathbf{R}_A+\tau_l^A)\sigma'}\Psi_{A\sigma'}(\mathbf{R}_A+\boldsymbol{\tau}_l^A)$$
$$+t^{out}_{\mathbf{R}_{A\sigma},(\mathbf{R}_A+\boldsymbol{\tau}_3)\sigma}\Psi_{B\sigma}(\mathbf{R}_A+\boldsymbol{\tau}_3),$$

$$\varepsilon\Psi_{B\sigma}(\mathbf{R}_B) = \sum_{l=1}^{2} t^{in}_{\mathbf{R}_{B\sigma},(\mathbf{R}_B+\boldsymbol{\tau}_l^B)\sigma}\Psi_{B\sigma}(\mathbf{R}_B+\boldsymbol{\tau}_l^B)$$
$$+\sum_{l=1}^{2} V^{in}_{\mathbf{R}_{B\sigma},(\mathbf{R}_B+\boldsymbol{\tau}_l^B)\sigma'}\Psi_{B\sigma'}(\mathbf{R}_B+\boldsymbol{\tau}_l^B)$$
$$+t^{out}_{\mathbf{R}_{B\sigma},(\mathbf{R}_B-\boldsymbol{\tau}_3)\sigma}\Psi_{A\sigma}(\mathbf{R}_B-\boldsymbol{\tau}_3).$$

Atomic vibrations modulate the hopping parameters

$$t^{in,out}_{\mathbf{R}_I,\mathbf{R}_I+\boldsymbol{\tau}_l^I} = t_0^{in,out} - \frac{\beta^{in,out}t_0^{in,out}}{c^2}\boldsymbol{\tau}_l^I \cdot[\mathbf{u}_I(\mathbf{R}_I)-\mathbf{u}_I(\mathbf{R}_I+\boldsymbol{\tau}_l^I)],$$

$$V^{in}_{\mathbf{R}_I,\mathbf{R}_I+\boldsymbol{\tau}_l^I} = V_0^{in} - \frac{\eta^{in}V_0^{in}}{c^2}\boldsymbol{\tau}_l^I \cdot[\mathbf{u}_I(\mathbf{R}_I)-\mathbf{u}_I(\mathbf{R}_I+\boldsymbol{\tau}_l^I)],$$

$c = |\boldsymbol{\tau}_l^I|$ **Equilibrium distance between atoms**

$$\beta^{in,out} = -\frac{c}{t_0^{in,out}}\frac{\partial}{\partial c}t_0^{in,out} \qquad \eta^{in} = -\frac{c}{V_0^{in}}\frac{\partial}{\partial c}V_0^{in},$$

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The model: Inclusion of the vibrations

$$t^{in,out}_{\mathbf{R}_I,\mathbf{R}_I+\boldsymbol{\tau}_l^I} = t_0^{in,out} - \frac{\beta^{in,out} t_0^{in,out}}{c^2}\boldsymbol{\tau}_l^I \cdot [\mathbf{u}_I(\mathbf{R}_I) - \mathbf{u}_I(\mathbf{R}_I + \boldsymbol{\tau}_l^I)],$$

$$V^{in}_{\mathbf{R}_I,\mathbf{R}_I+\boldsymbol{\tau}_l^I} = V_0^{in} - \frac{\eta^{in} V_0^{in}}{c^2}\boldsymbol{\tau}_l^I \cdot [\mathbf{u}_I(\mathbf{R}_I) - \mathbf{u}_I(\mathbf{R}_I + \boldsymbol{\tau}_l^I)],$$

$c = |\boldsymbol{\tau}_l^I|$ **Equilibrium distance between atoms**

$$\beta^{in,out} = -\frac{c}{t_0^{in,out}}\frac{\partial}{\partial c} t_0^{in,out} \qquad \eta^{in} = -\frac{c}{V_0^{in}}\frac{\partial}{\partial c} V_0^{in},$$

t^{in} V^{in}

$$\mathbf{u}_A(\mathbf{R}_A) - \mathbf{u}_A(\mathbf{R}_A + \boldsymbol{\tau}_l^A) \approx -(\boldsymbol{\tau}_l^A \cdot \boldsymbol{\nabla}) \times (\alpha^{ac}\mathbf{u}(\mathbf{r}) + \alpha^{op}\mathbf{v}(\mathbf{r})),$$

Intra-helix displacement

t^{out}

$$\mathbf{u}_A(\mathbf{R}_A) - \mathbf{u}_B(\mathbf{R}_A + \boldsymbol{\tau}_3) \approx 2\alpha^{op}\mathbf{v}(\mathbf{r}) - (\boldsymbol{\tau}_3 \cdot \boldsymbol{\nabla})(\alpha^{ac}\mathbf{u}(\mathbf{r}) - \alpha^{op}\mathbf{v}(\mathbf{r})).$$

Inter-helix displacement

Optical and acoustical amplitudes

$$\alpha^{ac}\mathbf{u}(\mathbf{r}) = \mathbf{u}_A(\mathbf{r}) + \mathbf{u}_B(\mathbf{r}),$$
$$\alpha^{op}\mathbf{v}(\mathbf{r}) = \mathbf{u}_A(\mathbf{r}) - \mathbf{u}_B(\mathbf{r}),$$

$$\begin{aligned}
\varepsilon\Psi_{A\sigma}(\mathbf{R}_A) &= \sum_{l=1}^{2} t^{in}_{\mathbf{R}_{A\sigma},(\mathbf{R}_A+\boldsymbol{\tau}_l^A)\sigma}\Psi_{A\sigma}(\mathbf{R}_A+\boldsymbol{\tau}_l^A) \\
&+ \sum_{l=1}^{2} V^{in}_{\mathbf{R}_{A\sigma},(\mathbf{R}_A+\tau_l^A)\sigma'}\Psi_{A\sigma'}(\mathbf{R}_A+\boldsymbol{\tau}_l^A) \\
&+ t^{out}_{\mathbf{R}_{A\sigma},(\mathbf{R}_A+\boldsymbol{\tau}_3)\sigma}\Psi_{B\sigma}(\mathbf{R}_A+\boldsymbol{\tau}_3), \\
\varepsilon\Psi_{B\sigma}(\mathbf{R}_B) &= \sum_{l=1}^{2} t^{in}_{\mathbf{R}_{B\sigma},(\mathbf{R}_B+\boldsymbol{\tau}_l^B)\sigma}\Psi_{B\sigma}(\mathbf{R}_B+\boldsymbol{\tau}_l^B) \\
&+ \sum_{l=1}^{2} V^{in}_{\mathbf{R}_{B\sigma},(\mathbf{R}_B+\boldsymbol{\tau}_l^B)\sigma'}\Psi_{B\sigma'}(\mathbf{R}_B+\boldsymbol{\tau}_l^B) \\
&+ t^{out}_{\mathbf{R}_{B\sigma},(\mathbf{R}_B-\boldsymbol{\tau}_3)\sigma}\Psi_{A\sigma}(\mathbf{R}_B-\boldsymbol{\tau}_3).
\end{aligned}$$

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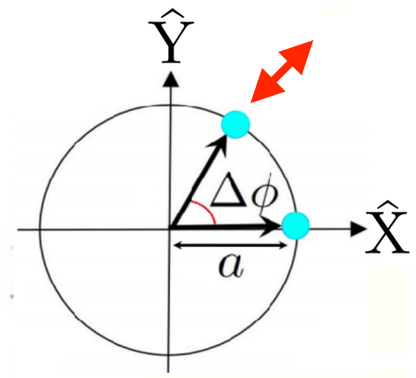
Electron–Phonon Interaction in DNA

- The stretching modes are decoupled from the electron transmission (at 1st order)
- Breathing modes are predominant



$$\epsilon F_A(\mathbf{r})\mathbb{1} = -t_o^{in} 2R\nu k_y F_A(\mathbf{r})$$
$$+ t_o^{out}\left(1 - 2aik_x + \frac{4\beta^{out}}{c^2}(a^2\partial_x(\alpha^{ac}u_x - \alpha^{op}v_x) + a\alpha^{op}v_x)\right)\mathbb{1}F_B(\mathbf{r})$$

$$\epsilon F_B(\mathbf{r})\mathbb{1} = -t_o^{in} 2R\nu k_y F_B(\mathbf{r})$$
$$+ t_o^{out}\left(1 + 2aik_x + \frac{4\beta^{out}}{c^2}(a^2\partial_x(\alpha^{ac}u_x - \alpha^{op}v_x) + a\alpha^{op}v_x)\right)\mathbb{1}F_A(\mathbf{r})$$

$$\mathcal{H}\mathbf{F}(\mathbf{r}) = \varepsilon\mathbf{F}(\mathbf{r}) \qquad \mathbf{F}(\mathbf{r}) = (\mathbf{F}^{\mathbf{K}}(\mathbf{r}), \mathbf{F}^{\mathbf{K}'}(\mathbf{r}))$$

No coupling with phonons in the intra helix elements of the Hamiltonian!

$$\mathcal{H} = \begin{pmatrix} \mathcal{H}^{\mathbf{K}} & \mathbf{0} \\ \mathbf{0} & \mathcal{H}^{\mathbf{K}'} \end{pmatrix} \quad \mathcal{H}^{\mathbf{K},\mathbf{K}'} = \begin{array}{c} \\ \mathbf{A} \\ \mathbf{B} \end{array} \begin{array}{c} \begin{array}{cc} \mathbf{A} & \mathbf{B} \end{array} \\ \begin{pmatrix} -t_o^{in} 2R\nu k_y & t_o^{out}\gamma_A \\ t_o^{out}\gamma_B & -t_o^{in} 2R\nu k_y \end{pmatrix} \end{array}$$

[6] Mayra Peralta, Steven Feijoo, Solmar Varela, Vladimiro Mujica, and Ernesto Medina. Coherence preservation and electron–phonon interaction in electron transfer in dna. The Journal of Chemical Physics, 153(16):165102, 2020

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Spin–Phonon Interaction in DNA

$$\mathcal{H}^{\mathbf{K},\mathbf{K}'} = \begin{array}{c} \begin{array}{cccc} \mathbf{A}\uparrow & \mathbf{A}\downarrow & \mathbf{B}\uparrow & \mathbf{B}\downarrow \end{array} \\ \begin{pmatrix} -2t_0^{in} f^{in}(\mathbf{k})\nu & 2i\lambda_{SO}^{in}\gamma^{in}\nu & t_0^{out} f^{out}(\mathbf{k}) & 0 \\ -2i\lambda_{SO}^{in}\gamma^{in}\nu & -2t_0^{in} f^{in}(\mathbf{k})\nu & 0 & t_0^{out} f^{out}(\mathbf{k}) \\ t_0^{out}(f^{out}(\mathbf{k}))^* & 0 & -2t_0^{in} f^{in}(\mathbf{k}) & 2i\lambda_{SO}^{in}\gamma^{in}\nu \\ 0 & t_0^{out}(f^{out}(\mathbf{k}))^* & -2i\lambda_{SO}^{in}\gamma^{in}\nu & -2t_0^{in} f^{in}(\mathbf{k})\nu \end{pmatrix} \end{array}$$

$$\gamma^{in} \equiv 1 + \frac{\eta^{in}\Delta\phi^2}{c^2}[a^2(\alpha^{ac}\partial_y u_y + \alpha^{op}\partial_y v_y) + \frac{ab}{2\pi}(\alpha^{ac}\partial_y u_z + \alpha^{op}\partial_y v_z + \alpha^{ac}\partial_z u_y + \alpha^{op}\partial_z v_y) + \frac{b^2}{4\pi^2}(\alpha^{ac}\partial_z v_z + \alpha^{op}\partial_z v_z)],$$

$$\gamma^{out} \equiv \frac{2\beta^{out}}{c^2}(a(\alpha^{ac}\partial_x u_x - \alpha^{op}\partial_x v_x) + \alpha^{op} v_x),$$

$$f^{in}(\mathbf{k}) \equiv \Delta\phi(ak_y + \frac{b}{2\pi}k_z),$$

$$f^{out}(\mathbf{k}) \equiv 1 - 2iak_x + 2a\gamma_A^{out}.$$

At this order we can see that the spin is coupled to the stretching modes, while breathing modes are coupled to the non-spin-flipping elements of the Hamiltonian

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Conclusions

- ☑ Intra-helix non spin-flip coupling only includes a second order kinetic term.
- ☑ Electron-phonon interaction is only present between helices (In the breading modes)
- ☑ Spin-phonon interaction appears for inter helix elements
- ☑ Breathing and stretching modes participating in ET

Future work

- To include the Rashba spin orbit interaction in the model
- Calculate transport properties including the electron and spin phonon interactions
- This model can be used to describe electron transfer in other organic molecules

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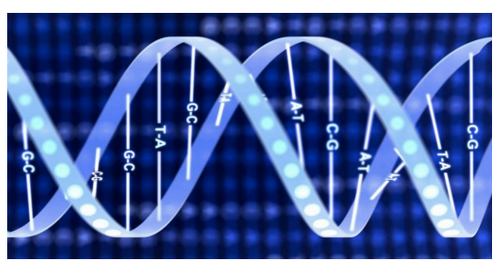
TB description of the electron–phonon and spin-phonon interactions in electron transfer in DNA



TIC to be presented on April 2022. Article Published: Coherent Preservation and Electron Phonon Interaction in Electron Transfer in DNA, J. Chem. Phys. **153**, 165102 (2020). 2nd Article in preparation: Spin phonon interaction in DNA (in writing process)

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Electronic Properties of Li and K on Graphene: Top, Hollow and Bridge Configurations

Dennis Alejandro Freire

Analytical Tight Binding Hamiltonian for 2D Black Phosphorus

Cristina Vaca

Quantum capacitance in graphene with adsorbed Alkali metals

Andrés Feijoo

TB description of the electron–phonon and spin-phonon interactions in electron transfer in DNA

Ricardo Vera

Calculation of the differential conductance of a Graphene based Superlattice/superconductor junction using Green's functions