# Improved effective equation for the Rashba spin-orbit coupling in semiconductor nanowires

Samuel D. Escribano

Theoretical Condensed Matter Physics Department
Universidad Autónoma de Madrid

# Introduction



Reference – Samuel D. Escribano, Alfredo Levy Yeyati and Elsa Prada, *Improved effective equation for the Rashba spin-orbit coupling in semiconductor nanowires*, arXiv:2001.04375 (2020).

(Accepted in Phys. Rev. Research)

Samuel D. Escribano

Alfredo Levy Yeyati

Elsa Prada

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$$\vec{\alpha} \sim \vec{\nabla}\phi$$
$$\vec{\alpha} = \vec{\alpha}_D + \vec{\alpha}_R$$

R. Winkler *et al.*, *Spin-Orbit Coupling in Two-Dimensional Electron and Hole Systems*, Vol. **41** (Springer, 2003).

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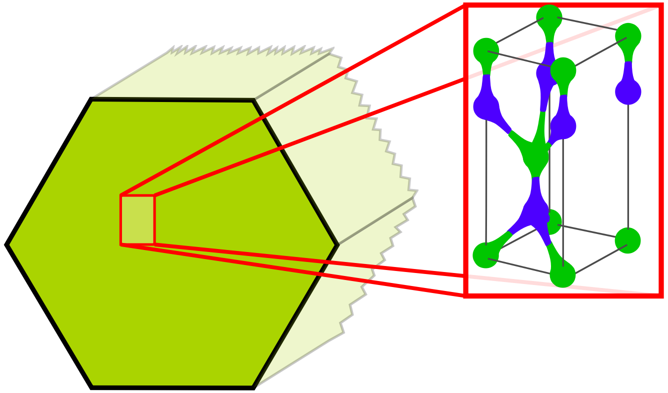
## Dresselhaus SOC

$\vec{\alpha}_D$ is the result of a bulk inversion asymmetry

The unit cell itself is not symmetric



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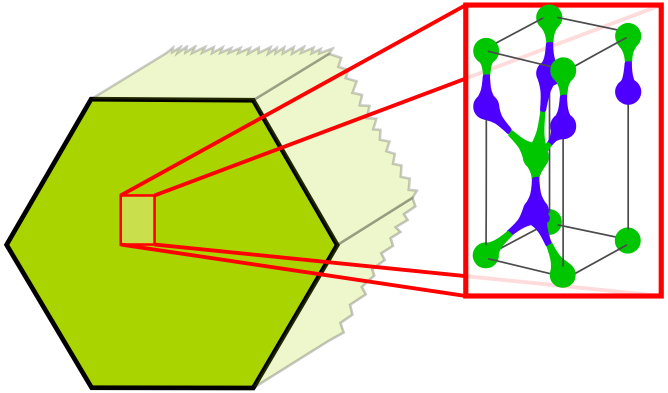
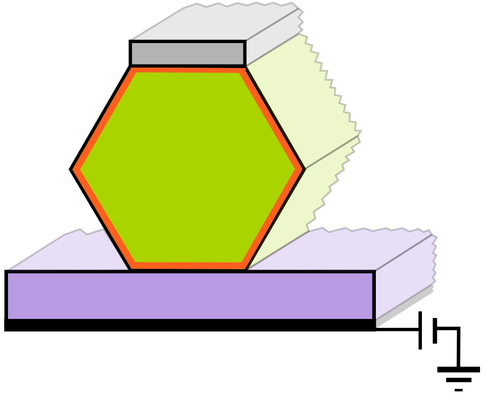


## Rashba SOC

$\vec{\alpha}_R$ is the result of a structural inversion asymmetry

Interfaces and the electrostatic surrounding break the symmetry



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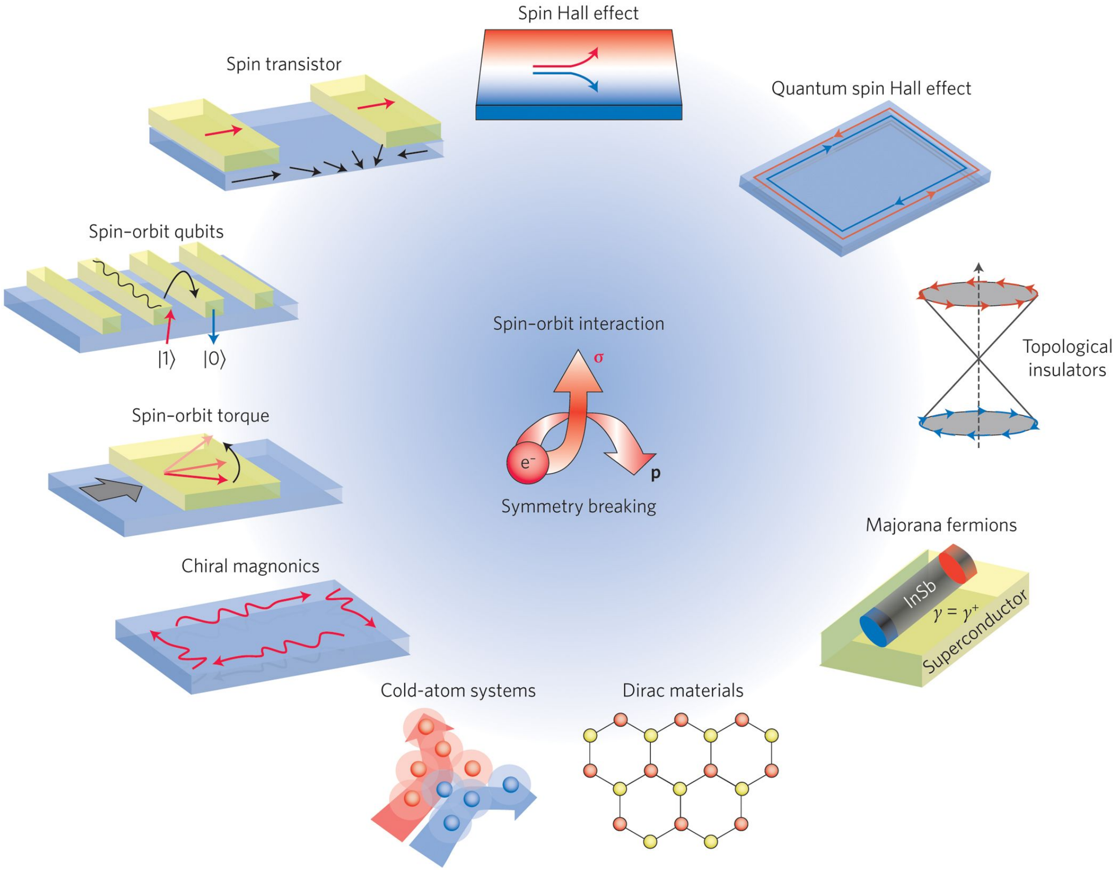


A. Manchon *et al.* Nat. Mat. **14**, 871 (2015).

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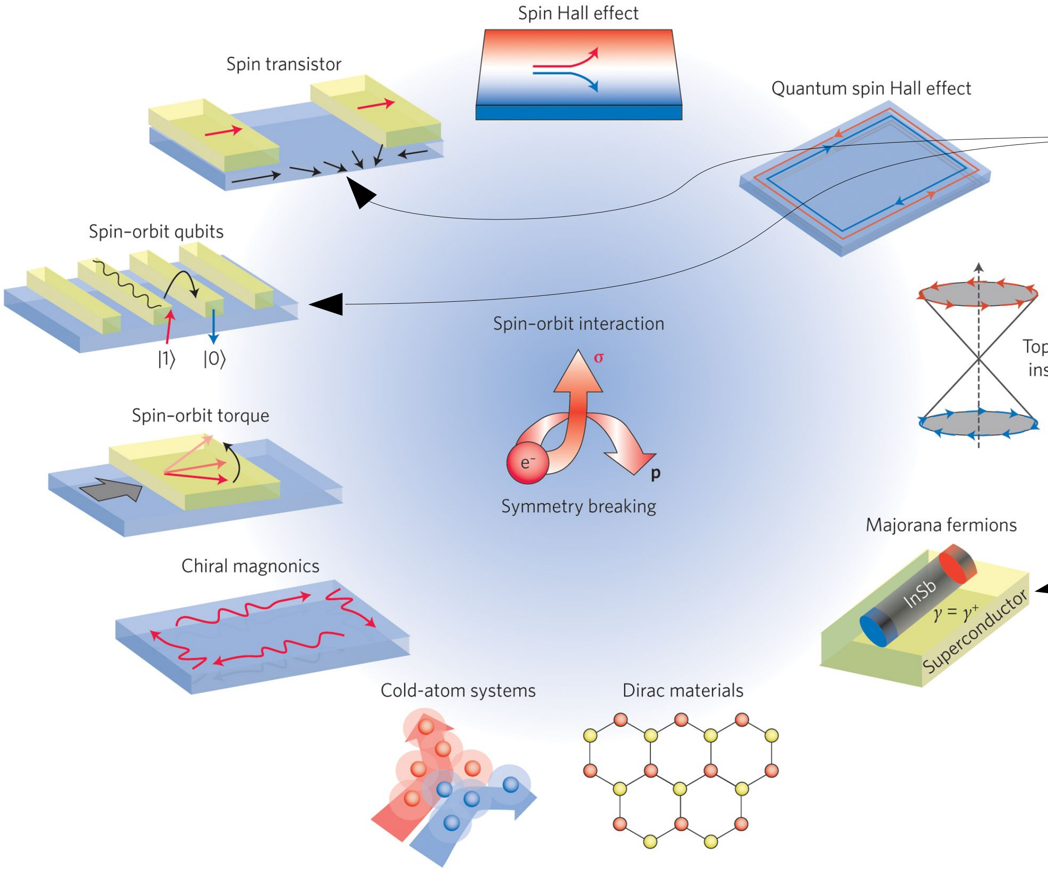


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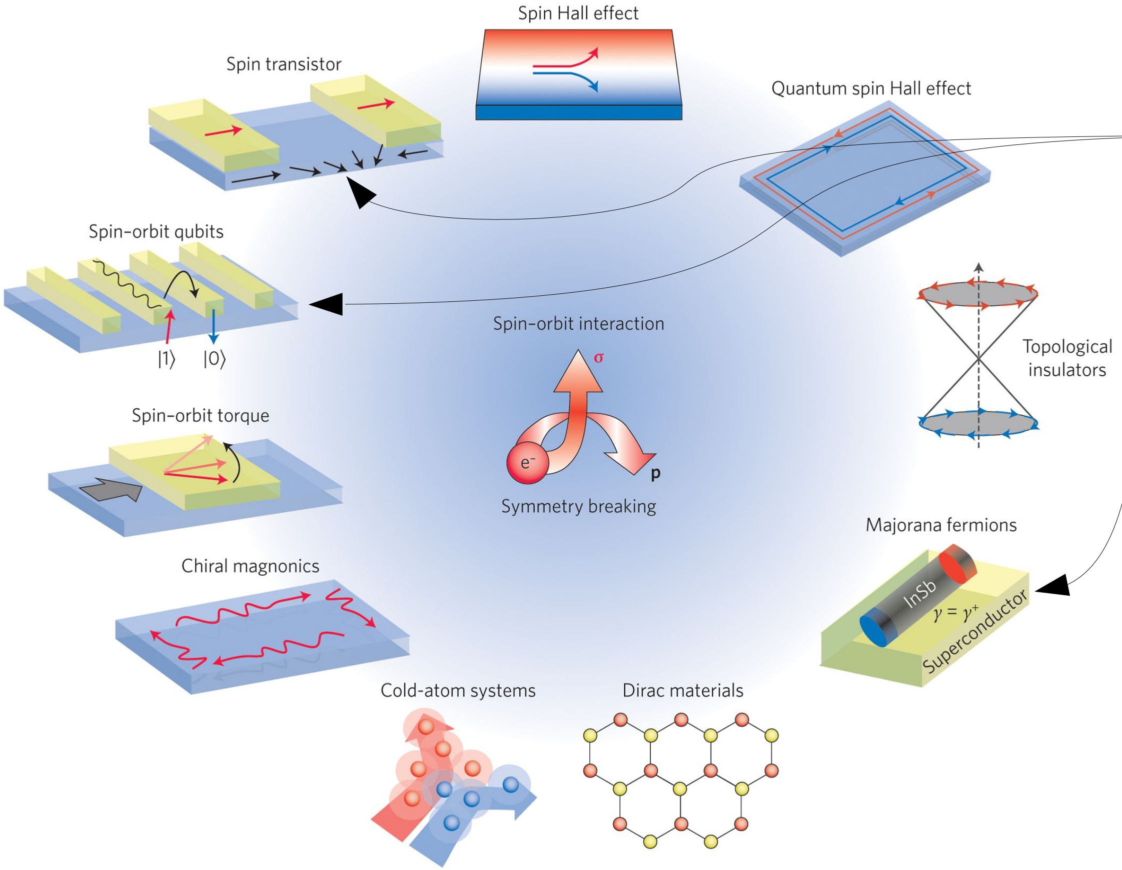


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The precise value of the SOC is crucial in all these systems!!!

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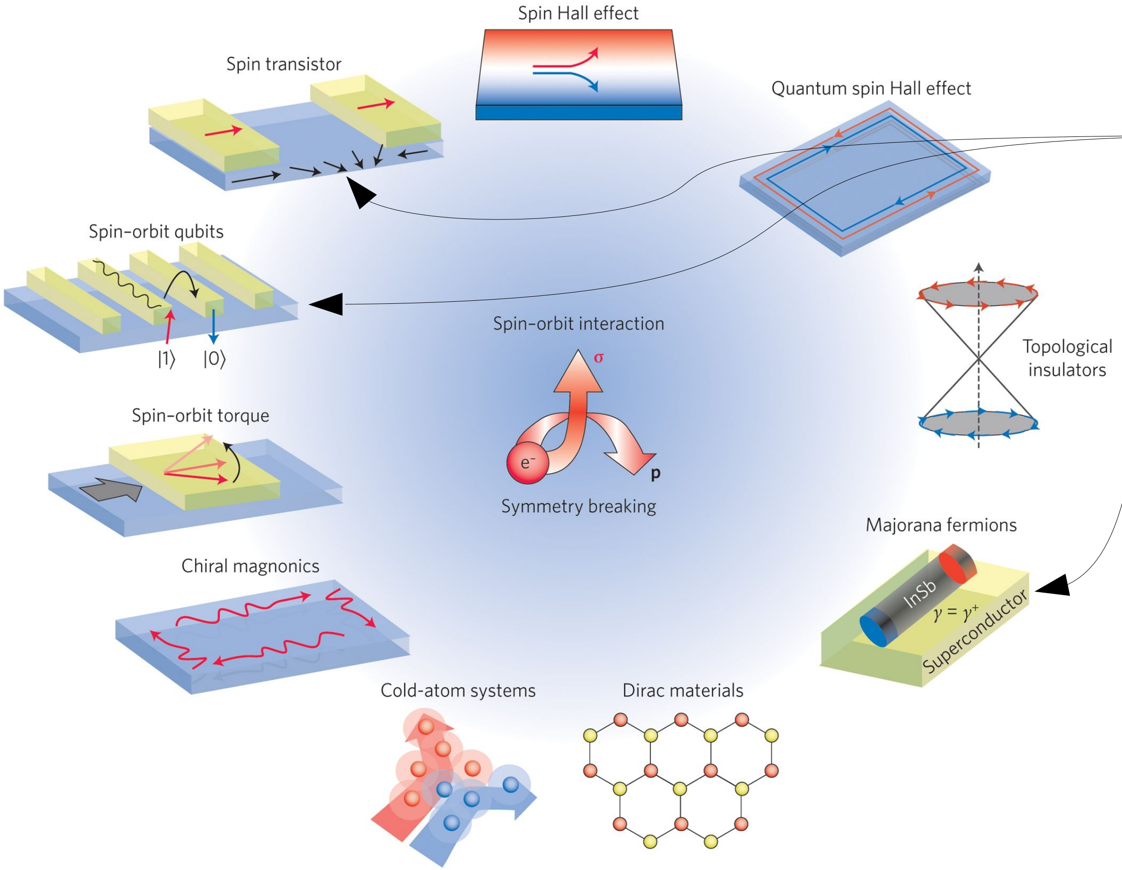


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↓

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We look for a simple equation which describes the Rashba SOC in this kind of nanowires

A. Manchon *et al.* Nat. Mat. **14**, 871 (2015).

# Models



Description of the Rashba SOC in several works:

- Rough constant extracted from experiments.
- Extracted from numerical calculations of effective multiband k·p Hamiltonians.

R. Winkler *et al.*, *Spin-Orbit Coupling in Two-Dimensional Electron and Hole Systems*, Vol. **41** (Springer, 2003).

T. Campos *et al.* PRB **97**, 245402 (2018).

- **Simplified** effective equation extracted from simplified multiband k·p Hamiltonians.

T. Darnhofer *et al.* PRB **47**, 16020 (1993).

P. Wójcik *et al.* PRB **97**, 165401 (2018).

- **Improved** effective equation extracted from simplified multiband k·p Hamiltonians.

**Our work**
S. D. Escribano *et al.*, arXiv:2001.04375

# Models

**8-band k·p model**
Conduction band approximation
Improved equation

Multiband k·p models are known to successfully reproduce the energy-band structure of III-V compound semiconductors. Because the SO coupling can be directly extracted from the shape of the energy spectrum, they are a reliable source of information about the SOC.

$$
\begin{array}{cc}
\text{Basis} \longrightarrow & \begin{array}{cccccccc} |c\uparrow\rangle & |c\downarrow\rangle & |lh\uparrow\rangle & |hh\uparrow\rangle & |hh\downarrow\rangle & |lh\downarrow\rangle & |so\uparrow\rangle & |so\downarrow\rangle \end{array} \\
H = & \begin{pmatrix}
T_{\mathrm{c}} & 0 & \frac{1}{\sqrt{6}}Pk_+ & 0 & \frac{1}{\sqrt{2}}Pk_- & -\sqrt{\frac{2}{3}}Pk_z & -\frac{1}{\sqrt{3}}Pk_z & \frac{1}{\sqrt{3}}Pk_+ \\
0 & T_{\mathrm{c}} & -\sqrt{\frac{2}{3}}Pk_z & -\frac{1}{\sqrt{2}}Pk_+ & 0 & -\frac{1}{\sqrt{6}}Pk_- & \frac{1}{\sqrt{3}}Pk_- & \frac{1}{\sqrt{3}}Pk_z \\
\frac{1}{\sqrt{6}}Pk_- & -\sqrt{\frac{2}{3}}Pk_z & T_{\mathrm{lh}} & -\Omega_2^\dagger & \Omega_1 & 0 & \sqrt{\frac{3}{2}}\Omega_2 & -\sqrt{2}\Omega_3 \\
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\end{pmatrix}
\end{array}
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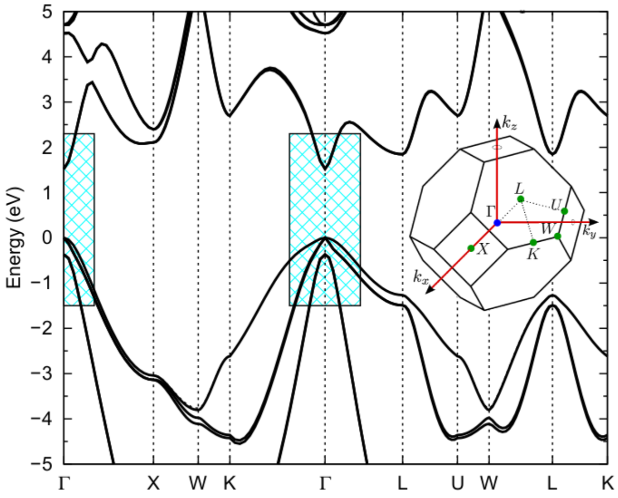

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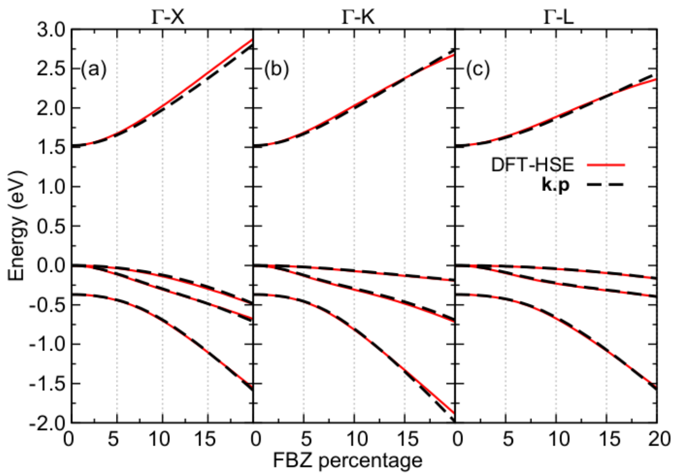

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0 & T_c & -\sqrt{\frac{2}{3}}Pk_z & -\frac{1}{\sqrt{2}}Pk_+ & 0 & -\frac{1}{\sqrt{6}}Pk_- & \frac{1}{\sqrt{3}}Pk_- & \frac{1}{\sqrt{3}}Pk_z \\
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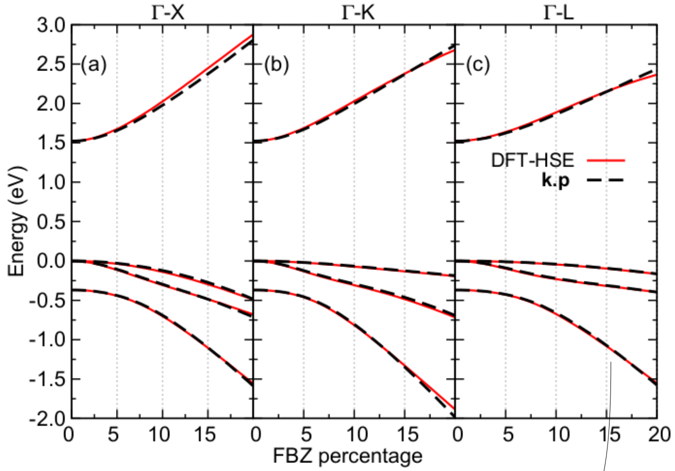


$$E_\pm^{(j)}(k_z) = \frac{\hbar^2 k_z^2}{2m_{\mathrm{eff}}^{(j)}} + E^{(j)} \pm \sqrt{(\alpha_{\mathrm{eff}}^{(j)} k_z)^2 + (\beta_{\mathrm{eff}}^{(j)} k_z^2)^2}$$

The SOC is extracted from the shape of the energy bands using an effective equation

# Models

**8-band k·p model**
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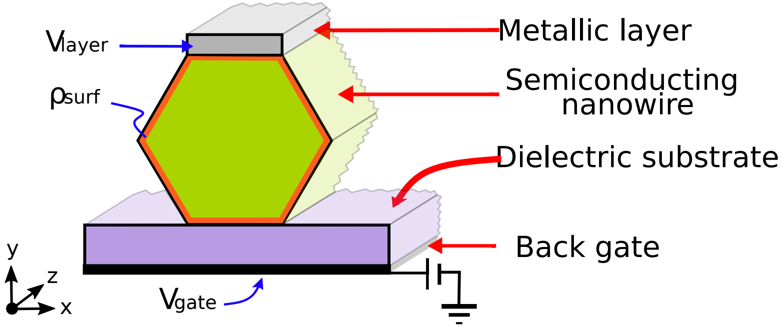
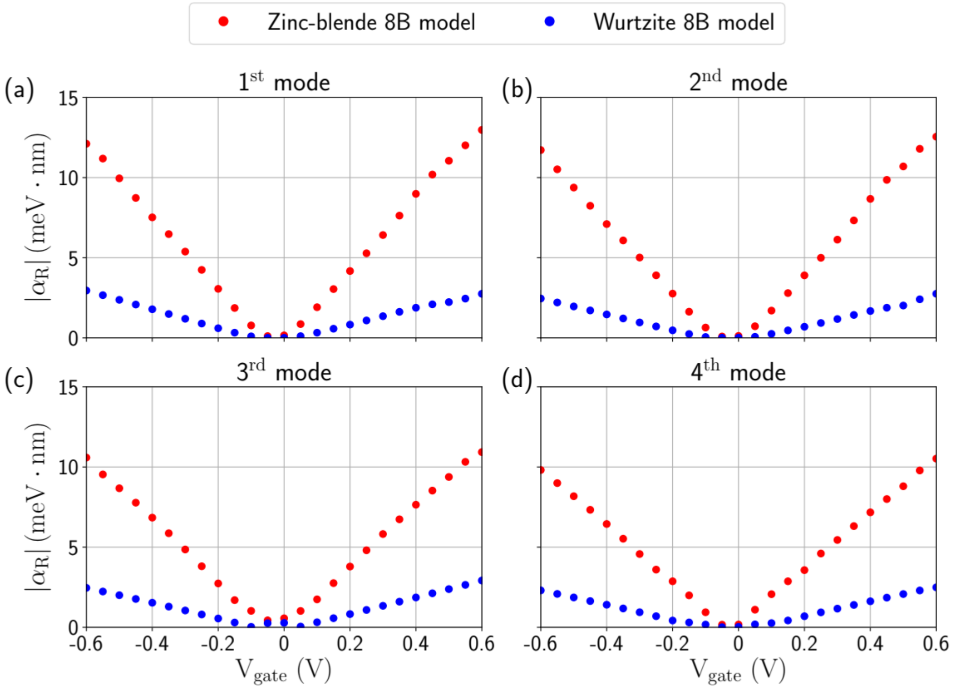
Results for the conduction band of an InAs nanowire embedded in an electrostatic environment:



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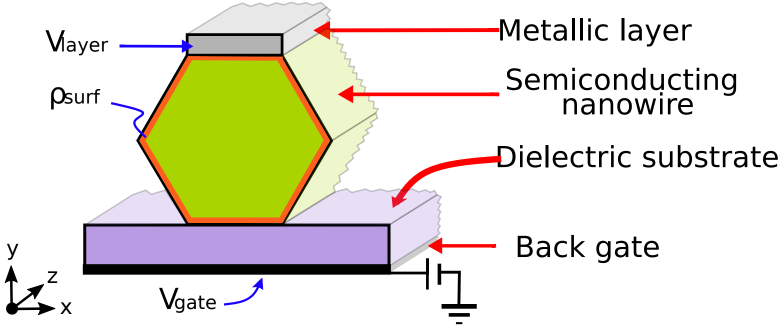


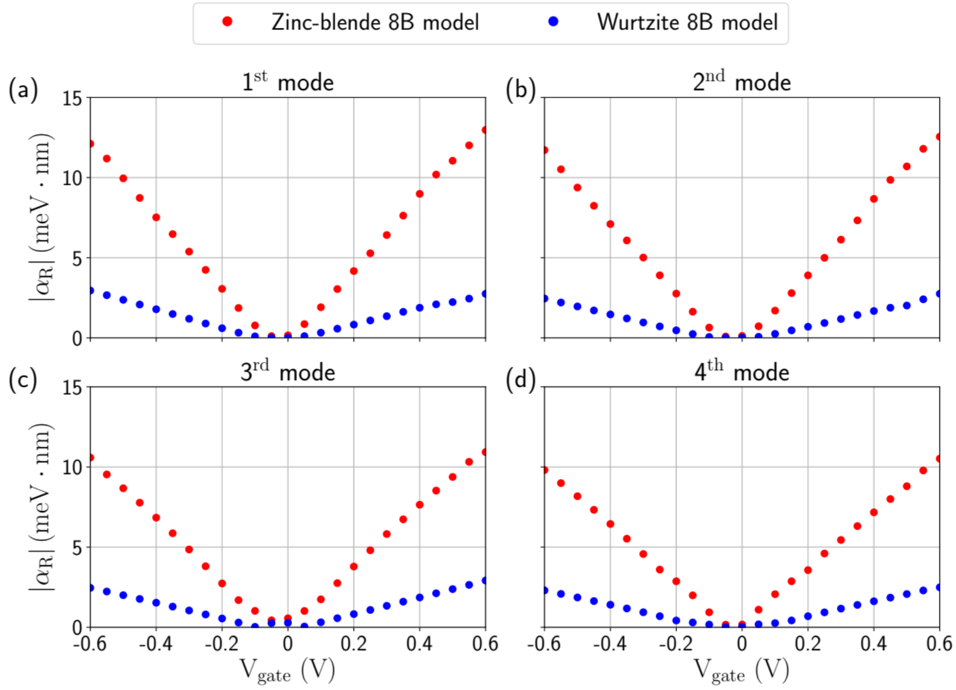


For low-dimensional materials, these multiband Hamiltonians are **computationally expensive**. They also have some further limitations.

# Models



To overcome this problem, one would like to find an effective analytical equation for a Hamiltonian which only involves the conduction band. In order to obtain this Hamiltonian:

$H_{\mathrm{c}}$ $\qquad$ $H_{\mathrm{cv}}$ $\qquad$ $H_{\mathrm{v}}$

$$H = \begin{pmatrix} T_{\mathrm{c}} & 0 & \frac{1}{\sqrt{6}}Pk_+ & 0 & \frac{1}{\sqrt{2}}Pk_- & -\sqrt{\frac{2}{3}}Pk_z & -\frac{1}{\sqrt{3}}Pk_z & \frac{1}{\sqrt{3}}Pk_+ \\ 0 & T_{\mathrm{c}} & -\sqrt{\frac{2}{3}}Pk_z & -\frac{1}{\sqrt{2}}Pk_+ & 0 & -\frac{1}{\sqrt{6}}Pk_- & \frac{1}{\sqrt{3}}Pk_- & \frac{1}{\sqrt{3}}Pk_z \\ \frac{1}{\sqrt{6}}Pk_- & -\sqrt{\frac{2}{3}}Pk_z & T_{\mathrm{lh}} & -\Omega_2^\dagger & \Omega_1 & 0 & \sqrt{\frac{3}{2}}\Omega_2 & -\sqrt{2}\Omega_3 \\ 0 & -\frac{1}{\sqrt{2}}Pk_- & -\Omega_2 & T_{\mathrm{hh}} & 0 & \Omega_1 & -\sqrt{2}\Omega_1^\dagger & \frac{1}{\sqrt{2}}\Omega_2 \\ \frac{1}{\sqrt{2}}Pk_+ & 0 & \Omega_1^\dagger & 0 & T_{\mathrm{hh}} & \Omega_2^\dagger & \frac{1}{\sqrt{2}}\Omega_2^\dagger & \sqrt{2}\Omega_1^\dagger \\ -\sqrt{\frac{2}{3}}Pk_z & -\frac{1}{\sqrt{6}}Pk_+ & 0 & \Omega_1^\dagger & \Omega_2 & T_{\mathrm{lh}} & \sqrt{2}\Omega_3 & \sqrt{\frac{3}{2}}\Omega_2^\dagger \\ -\frac{1}{\sqrt{3}}Pk_z & \frac{1}{\sqrt{3}}Pk_+ & \sqrt{\frac{3}{2}}\Omega_2^\dagger & -\sqrt{2}\Omega_1 & \frac{1}{\sqrt{2}}\Omega_2 & \sqrt{2}\Omega_3 & T_{\mathrm{soff}} & 0 \\ \frac{1}{\sqrt{3}}Pk_- & \frac{1}{\sqrt{3}}Pk_z & -\sqrt{2}\Omega_3 & \frac{1}{\sqrt{2}}\Omega_2^\dagger & \sqrt{2}\Omega_1 & \sqrt{\frac{2}{3}}\Omega_2 & 0 & T_{\mathrm{soff}} \end{pmatrix}$$

Perform a folding-down:

$$H_{\mathrm{CB}} = H_{\mathrm{c}} + H_{\mathrm{cv}} G_{\mathrm{v}} H_{\mathrm{cv}}^\dagger$$

$$G_{\mathrm{v}} = (E - H_{\mathrm{v}})^{-1}$$

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$\Omega_i \sim k$ $\quad$ $T_i \sim k - e\phi(r)$

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-\sqrt{\frac{2}{3}}Pk_z & -\frac{1}{\sqrt{6}}Pk_+ & 0 & \Omega_1^\dagger & \Omega_2 & T_\mathrm{lh} & \sqrt{2}\Omega_3 & \sqrt{\frac{3}{2}}\Omega_2^\dagger \\
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$$G_\mathrm{v} = (E - H_\mathrm{v})^{-1}$$

Unfortunately, $H_\mathrm{v}$ is not invertible

But one can expand $G_\mathrm{v}$ in Dyson series assuming there is a small parameter.

# Models



Assuming that the intra-valence band coupling are small compared to the other energy scales, one can perform the following Dyson expansion:

$$\Omega_i \sim \gamma_i \frac{\hbar^2 k^2}{2m_0} \ll \Delta_{\mathrm{g}}, \Delta_{\mathrm{soff}}, P \longrightarrow G_{\mathrm{v}} = G_{\mathrm{v}}^{(0)} + G_{\mathrm{v}}^{(0)} V G_{\mathrm{v}}^{(0)} + \ldots$$

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Intra-valence band couplings

$$G_{\mathrm{v}}^{(0)} = (E - H_{\mathrm{v}}^{(0)})^{-1}$$

$$H_{\mathrm{v}}^{(0)} = \begin{pmatrix} E_h - e\phi(\vec{r}) & 0 & 0 & 0 & 0 & 0 \\ 0 & E_h - e\phi(\vec{r}) & 0 & 0 & 0 & 0 \\ 0 & 0 & E_h - e\phi(\vec{r}) & 0 & 0 & 0 \\ 0 & 0 & 0 & E_h - e\phi(\vec{r}) & 0 & 0 \\ 0 & 0 & 0 & 0 & E_{\mathrm{soff}} - e\phi(\vec{r}) & 0 \\ 0 & 0 & 0 & 0 & 0 & E_{\mathrm{soff}} - e\phi(\vec{r}) \end{pmatrix},$$

$$V = \begin{pmatrix} \Omega_0^{\mathrm{lh}} & -\Omega_2^\dagger & \Omega_1 & 0 & \sqrt{\frac{3}{2}}\Omega_2 & -\sqrt{2}\Omega_3 \\ -\Omega_2 & \Omega_0^{\mathrm{hh}} & 0 & \Omega_1 & -\sqrt{2}\Omega_1^\dagger & \frac{1}{\sqrt{2}}\Omega_2 \\ \Omega_1^\dagger & 0 & \Omega_0^{\mathrm{hh}} & \Omega_2^\dagger & \frac{1}{\sqrt{2}}\Omega_2^\dagger & \sqrt{2}\Omega_1^\dagger \\ 0 & \Omega_1^\dagger & \Omega_2 & \Omega_0^{\mathrm{lh}} & \sqrt{2}\Omega_3 & \sqrt{\frac{3}{2}}\Omega_2^\dagger \\ \sqrt{\frac{3}{2}}\Omega_2^\dagger & -\sqrt{2}\Omega_1 & \frac{1}{\sqrt{2}}\Omega_2 & \sqrt{2}\Omega_3 & \Omega_0^{\mathrm{soff}} & 0 \\ -\sqrt{2}\Omega_3 & \frac{1}{\sqrt{2}}\Omega_2^\dagger & \sqrt{2}\Omega_1 & \sqrt{\frac{2}{3}}\Omega_2 & 0 & \Omega_0^{\mathrm{soff}} \end{pmatrix},$$

# Models



Assuming that the intra-valence band coupling are small compared to the other energy scales, one can perform the following Dyson expansion:

$$\Omega_i \sim \gamma_i \frac{\hbar^2 k^2}{2m_0} \ll \Delta_{\mathrm{g}}, \Delta_{\mathrm{soff}}, P \longrightarrow G_{\mathrm{v}} = G_{\mathrm{v}}^{(0)} + \cancel{G_{\mathrm{v}}^{(0)} V G_{\mathrm{v}}^{(0)} + \ldots}$$

Intra-valence band couplings

Performing the folding-down

$$H_{\mathrm{CB}}^{(0)} = H_{\mathrm{c}} + H_{\mathrm{cv}} G_{\mathrm{v}}^{(0)} H_{\mathrm{cv}}^{\dagger} = \left[\vec{k}\frac{\hbar^2}{2m^{(0)}(\vec{r})}\vec{k} + E_c - e\phi(\vec{r})\right]\sigma_0 + \frac{1}{2}\left[\vec{\alpha}_R^{(0)}(\vec{r}) \cdot \left(\vec{\sigma} \times \vec{k}\right) + \left(\vec{\sigma} \times \vec{k}\right) \cdot \vec{\alpha}_R^{(0)}(\vec{r})\right]$$

$$\vec{\alpha}_R^{(0)}(\vec{r}) = \frac{P^2}{3}\vec{\nabla}\left[\frac{1}{E_h - e\phi(\vec{r}) - E} - \frac{1}{E_{\mathrm{soff}} - e\phi(\vec{r}) - E}\right]$$

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Assuming

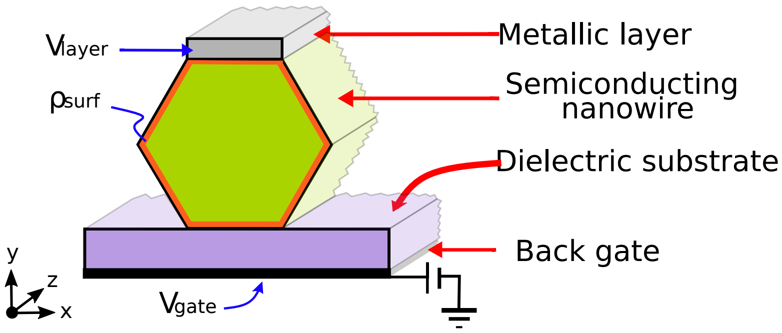
$$|E_h| \gg |e\phi(\vec{r}) - E|$$

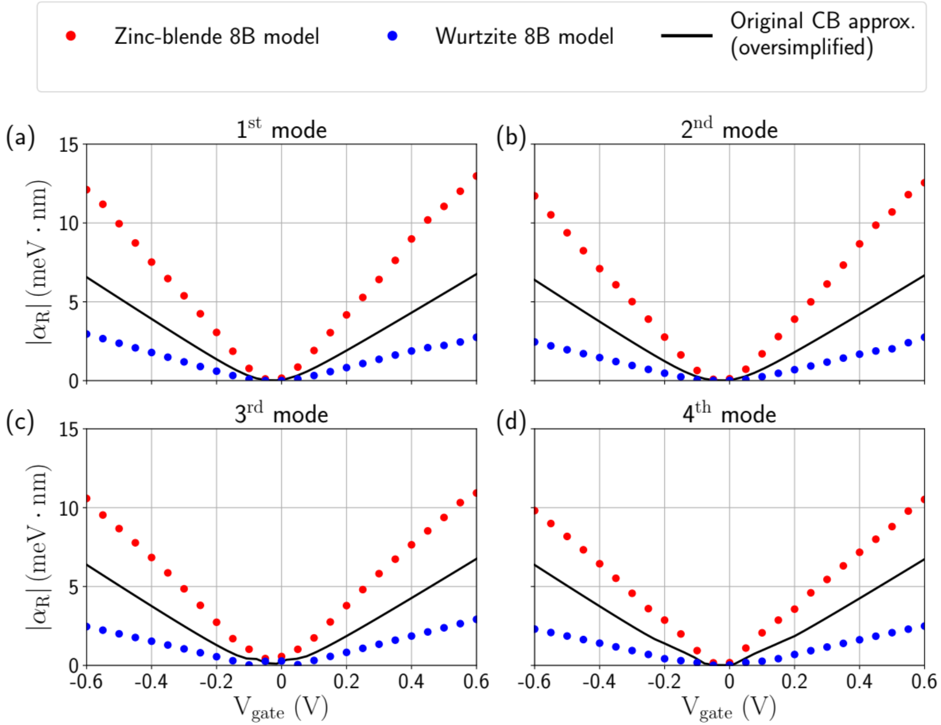
We call to this equation **oversimplified** SOC

$$\boxed{\vec{\alpha}_R^{(0)}(\vec{r}) \simeq -e\frac{P^2}{3}\left[\frac{1}{E_h^2} - \frac{1}{E_\mathrm{soff}^2}\right]\vec{\nabla}\phi(\vec{r})}$$

# Models

Results for the conduction band of an InAs nanowire embedded in an electrostatic environment:



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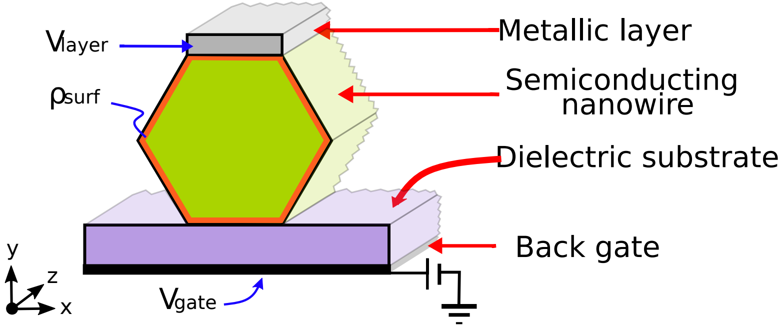


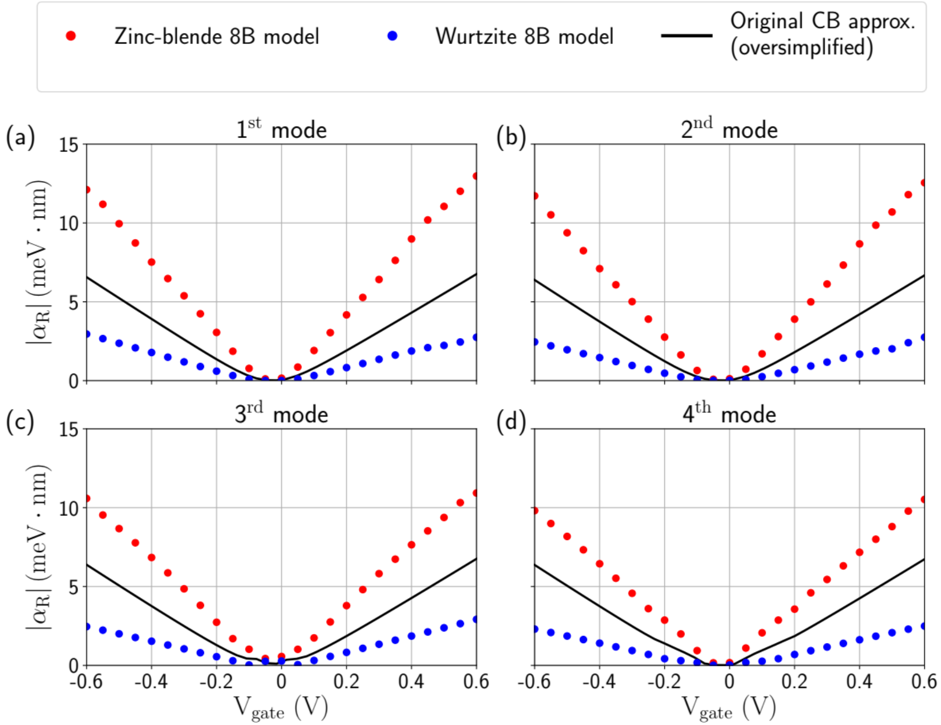


This analytical equation for the SOC fails predicting the numerical behaviour, precisely because the **intra-valence band interactions have been neglected**.

$$k \sim \frac{1}{W}$$

# Models



Because confinement effects become relevant, one has to *improve* the description of the Rashba SOC to include them:

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Hard task

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- **Option 1:** one could go beyond zeroth order in Dyson series. → All terms must be included
Hard task

- **Option 2:** one may find an heuristic equation which reproduces the results of the 8-band model.

  We propose to use the same zeroth-order SOC equation, but substituting the Kane parameter *P*, by another one $P_{\text{fit}}$, chosen so that it reproduces the 8-band model calculations. To this end, we fit this equation to that calculations.

We call to this equation, **improved** SOC

$$\vec{\alpha}_R(\vec{r}) \simeq \frac{P_{\text{fit}}^2}{3} \vec{\nabla} \left( \frac{1}{E_h - E^{(j)} - e\phi(\vec{r})} - \frac{1}{E_{\text{soff}} - E^{(j)} - e\phi(\vec{r})} \right)$$

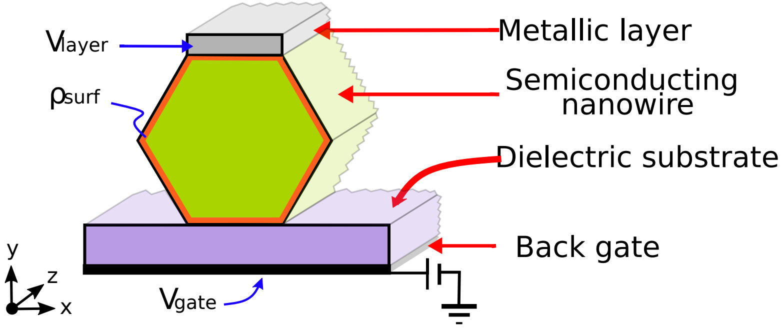
$$E = E^{(j)} + E(k_z)$$

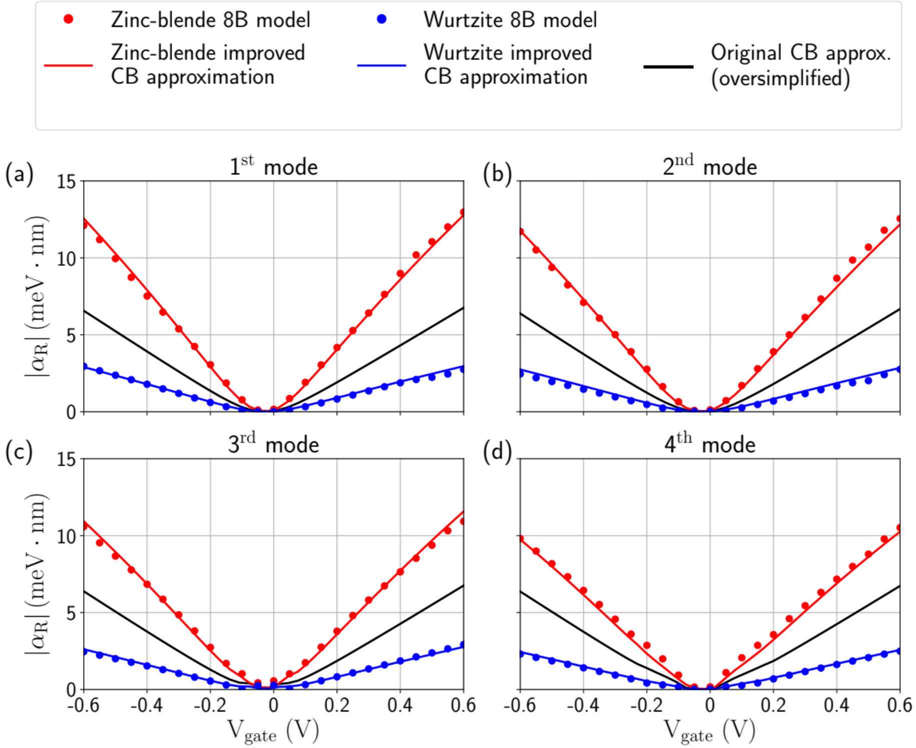
| $P_{\text{fit}}$ | Zinc-blende (111) | Wurtzite (0001) |
|---|---|---|
| InAs | 1252±12 | 723.0±0.1 |
| InSb | 1082±7 | - |
| GaAs | 1912±18 | - |
| GaSb | 1657±35 | - |

# Models



Results for the conduction band of an InAs nanowire embedded in an electrostatic environment:



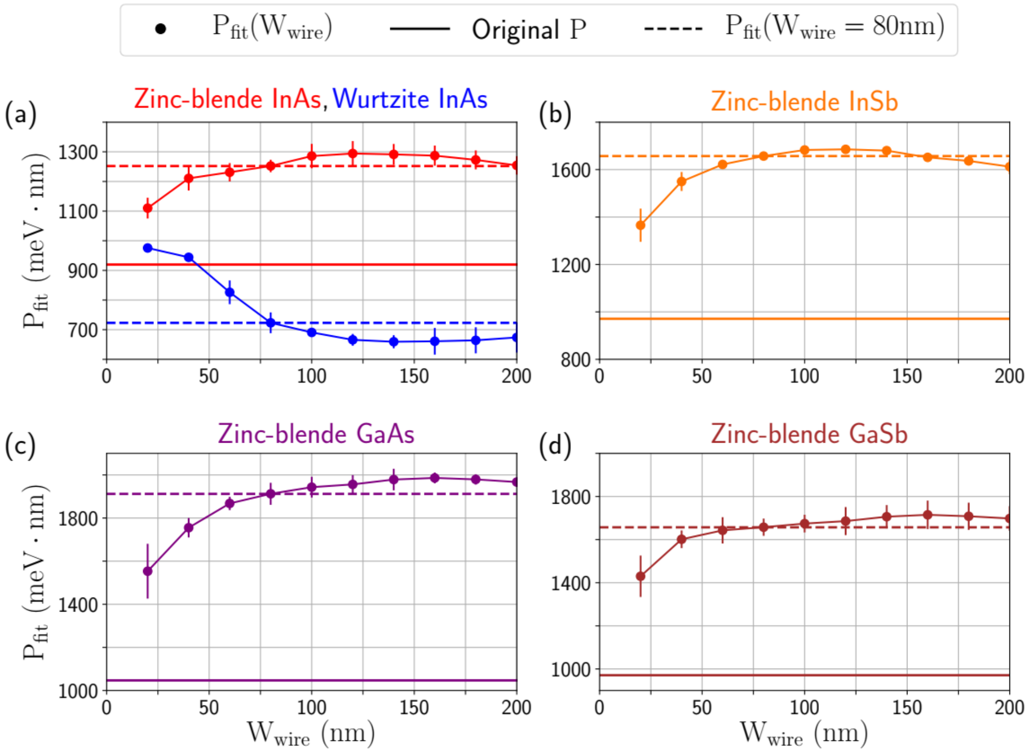

The improved equation predicts correctly the behaviour of the more sophisticated 8-band model with **just one fitting parameter**.

# Models



We show that $P_{fit}$:

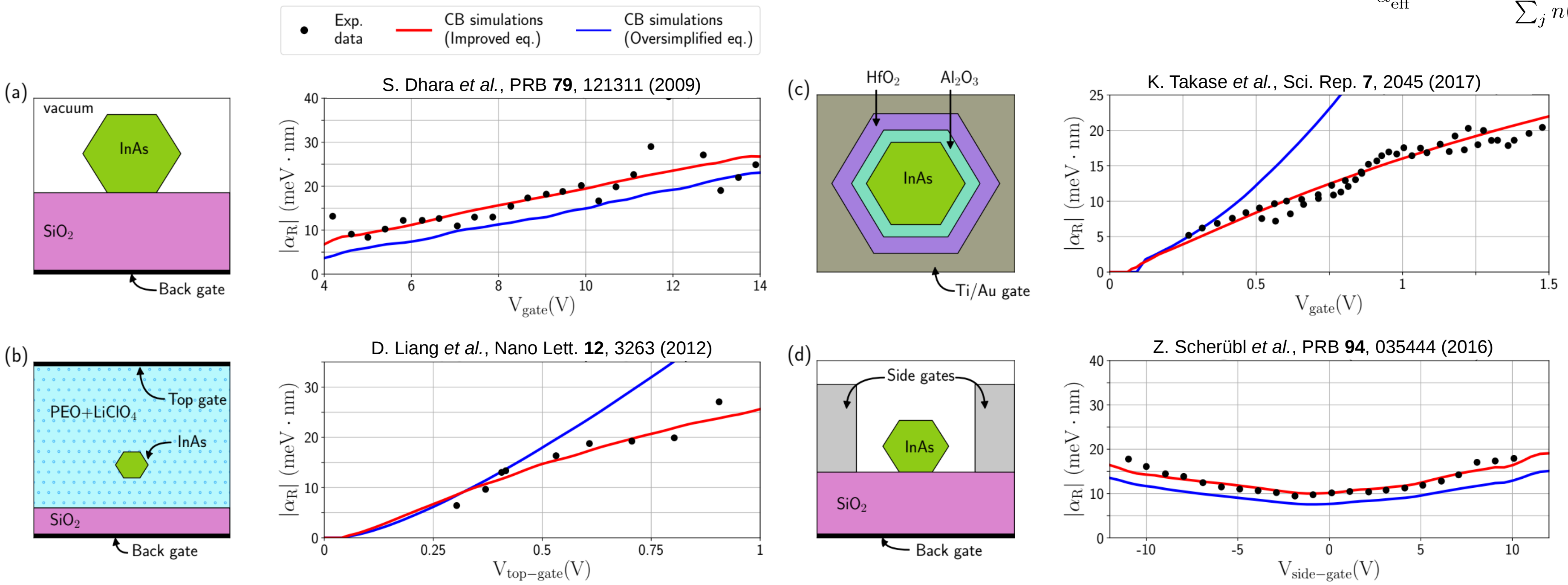
- Is (roughly) independent of the subband, at least for the lowest ones.
- Is (roughly) independent of the electrostatic environment and the electric field.
- Depends on the width of the nanowire, although slightly for a certain range (i.e. [50,200]nm).



# Comparison to experiments

We compare the results provided by the improved equation with data extracted from different magneto-transport experiments. We find an excellent agreement.

$$\vec{\alpha}_{\text{eff}}^{(\text{EV})} = \frac{\sum_j \left\langle \vec{\alpha}_R^{(j)}(\vec{r}) \right\rangle n(E^{(j)})}{\sum_j n(E^{(j)})}$$



# Take-home message

If you want to describe accurately the SOC in nanowires use the improved equation

$$\vec{\alpha}_R(\vec{r}) \simeq \frac{P_{\text{fit}}^2}{3}\vec{\nabla}\left(\frac{1}{E_h - E^{(j)} - e\phi(\vec{r})} - \frac{1}{E_{\text{soff}} - E^{(j)} - e\phi(\vec{r})}\right)$$

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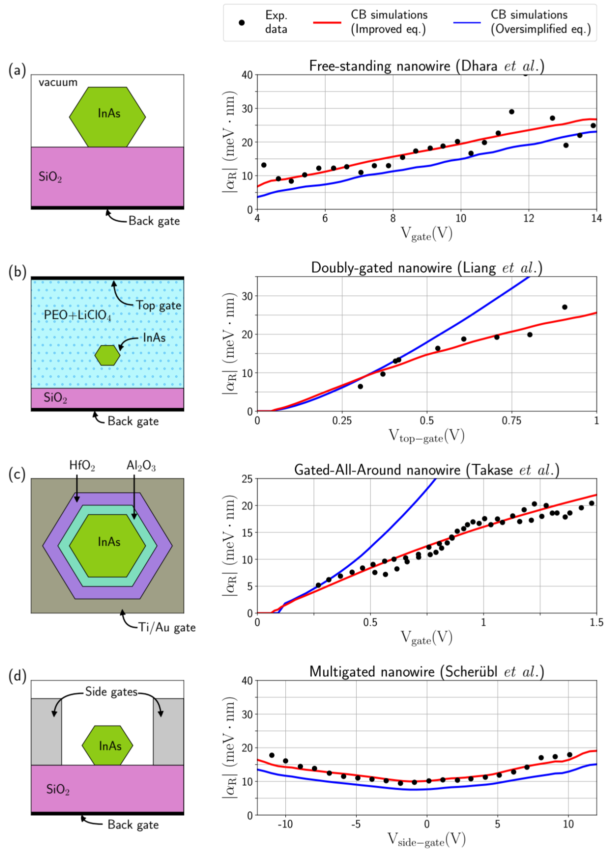


For further details, see: **arXiv:2001.04375**

For any question or inquire, don’t hesitate to contact me: **samuel.diaz@uam.es**