

Realistic multibands $k \cdot p$ from hybrid-DFT

Dr. Carlos Maciel O. Bastos

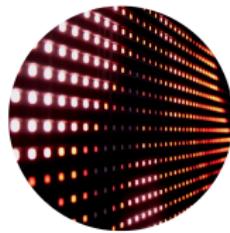
International Center of Physics - University of Brasília (UnB)
Institute of Physics - University of Brasília (UnB)

Colaborators: Guilherme M. Sipahi (USP-BR), Juarez L. F. Da Silva (USP-BR),
Fernando Sabino (USP-BR), Paulo E. Faria Junior (UCF-USA), Tiago Campos, Martin
Gmitra (UPJS-SK) , Jaroslav Fabian (UR-GE).

October 18, 2025

Introduction

- Few categories of materials have had a greater impact in the last century than semiconductors.



LED



solar cell



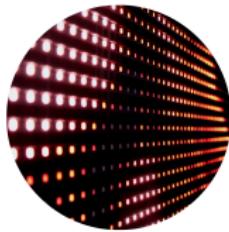
microchip



laser

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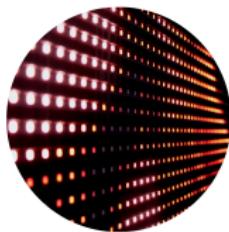


laser

- Modern devices demand increasingly accurate theoretical predictions (e.g., spintronic devices).

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- Modern devices demand increasingly accurate theoretical predictions (e.g., spintronic devices).
- Confined systems require simulations involving a large number of atoms.

Why use the $k \cdot p$ method?

Ab initio methods \Rightarrow Large computational cost and few atoms.

Effective methods \Rightarrow Small computational cost, but it is necessary determine the parameters.

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$k \cdot p$ method:

- Lower computational cost in comparison with ab initio methods.
- Possibility to calculate systems with several atoms (supercells) using the envelope function formalism.
- Potential for identifying the source of effects in the electronic structure.

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- Lower computational cost in comparison with ab initio methods.
- Possibility to calculate systems with several atoms (supercells) using the envelope function formalism.
- Potential for identifying the source of effects in the electronic structure.
- However,
 - It is necessary to determine the parameters independently of the theory.

A brief introduction to $k \cdot p$ method

Electrons moving in the crystal lattice

Solving the Schrödinger equation for many electrons and nuclei.

$$H = - \sum_i^N \frac{\hbar^2}{2m} \nabla_{r_i}^2 - \sum_i^P \frac{\hbar^2}{2M_i} \nabla_{R_i}^2 + \sum_{i < j}^N \frac{e^2}{|r_i - r_j|} - \sum_i^N \sum_j^P \frac{Z_j e}{|r_i - R_j|} + \sum_{i < j}^P \frac{Z_j Z_i}{|R_i - R_j|},$$

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Born-Oppenheimer approximation and single-particle approximation, with spin-orbit potential.

$$H = - \frac{\hbar^2}{2m} \nabla_{r_i}^2 + V_{ef}(r) + \frac{i\hbar^2}{4m_0^2 c^2} (\nabla V_{ef} \times \nabla_{r_i}) \cdot \boldsymbol{\sigma}$$

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Bloch theorem

$$\psi(r) = e^{ik \cdot r} u_{n,k}(r) \quad (1)$$

Electrons moving in the crystal lattice

Therefore, the hamiltonian is

$$\begin{aligned} H(k) = & \frac{p^2}{2m} + \frac{\hbar^2}{2m} k^2 + V_{ef}(r) + \frac{\hbar}{m} \mathbf{k} \cdot \mathbf{p} + \frac{\hbar}{4m_0^2 c^2} (\nabla V_{ef} \times \mathbf{p}) \cdot \boldsymbol{\sigma} \\ & + \frac{\hbar^2}{4m_0^2 c^2} \mathbf{k} \cdot (\boldsymbol{\sigma} \times \nabla V_{ef}) \end{aligned}$$

$$H(k) = H_0 + H_{k.p}(k) + H_{so} + H_{ksso}(k)$$

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Electrons moving in the Crystal lattice

Löwdin method

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Electrons moving in the Crystal lattice

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states are divide in 2 classes

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Electrons moving in the Crystal lattice

Löwdin method

class A: states in the Hamiltonian ($|\alpha\rangle$)

states are divide in 2 classes

class B: all another states ($|\beta\rangle$)

$$|nk\rangle = \sum_{\alpha}^A C_{\alpha n}(k)|\alpha\rangle + \sum_{\beta}^B C_{\beta n}(k)|\beta\rangle$$

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Kane-Luttinger model $\rightarrow H_{k,p}$ to second order and H_{so} to first order.

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$$\begin{aligned} \langle \alpha | H | \alpha' \rangle = & E(k_0) \delta_{\alpha\alpha'} + \frac{\hbar^2 k^2}{2m_0} \delta_{\alpha\alpha'} + \langle \alpha | \frac{\hbar}{m} k \cdot p | \alpha' \rangle + \langle \alpha | \frac{\hbar}{4m_0^2 c^2} (\nabla V_{ef} \times p) \cdot \sigma | \alpha' \rangle \\ & + \sum_{\beta} \frac{\langle \alpha | \frac{\hbar}{m} k \cdot p | \beta \rangle \langle \beta | \frac{\hbar}{m} k \cdot p | \alpha' \rangle}{E_{\alpha} - E_{\beta}} \end{aligned}$$

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Hamiltonian elements are parametrized using group theory

8 × 8 Hamiltonian for zincblend

$$\begin{pmatrix} Q & S & R & 0 & i\frac{S}{\sqrt{2}} & -i\sqrt{2}R & -iP_- & 0 \\ S^\dagger & T & 0 & R & i\frac{(T-Q)}{\sqrt{2}} & i\sqrt{\frac{3}{2}}S & \sqrt{\frac{2}{3}}P_z & -\frac{1}{\sqrt{3}}P_- \\ R^\dagger & 0 & T & -S & -i\sqrt{\frac{3}{2}}S^\dagger & i\frac{(T-Q)}{\sqrt{2}} & -\frac{i}{\sqrt{3}}P_+ & -i\sqrt{\frac{2}{3}}P_z \\ 0 & R^\dagger & -S^\dagger & Q & -i\sqrt{2}R^\dagger & -i\frac{S^\dagger}{\sqrt{2}} & 0 & -P_+ \\ -i\frac{S^\dagger}{\sqrt{2}} & -i\frac{(T-Q)^\dagger}{\sqrt{2}} & i\sqrt{\frac{3}{2}}S & i\sqrt{2}R & \frac{Q+T}{2} + \Delta & 0 & -\frac{i}{\sqrt{3}}P_z & -i\sqrt{\frac{2}{3}}P_- \\ i\sqrt{2}R^\dagger & -i\sqrt{\frac{3}{2}}S^\dagger & -i\frac{(T-Q)^\dagger}{\sqrt{2}} & i\frac{S}{\sqrt{2}} & 0 & \frac{Q+T}{2} + \Delta & \sqrt{\frac{2}{3}}P_+ & -\frac{1}{\sqrt{3}}P_z \\ -iP_- & \sqrt{\frac{2}{3}}P_z & \frac{i}{\sqrt{3}}P_- & 0 & \frac{i}{\sqrt{3}}P_z & \sqrt{\frac{2}{3}}P_- & E_c & 0 \\ 0 & -\frac{1}{\sqrt{3}}P_+ & i\sqrt{\frac{2}{3}}P_z & -P_- & i\sqrt{\frac{2}{3}}P_+ & -\frac{1}{\sqrt{3}}P_z & 0 & E_c \end{pmatrix}$$

$$Q = -(\tilde{\gamma}_1 + \tilde{\gamma}_2)(k_x^2 + k_y^2) - (\tilde{\gamma}_1 - 2\tilde{\gamma}_2)k_z^2$$

$$E_c = E_g + \tilde{e}k^2$$

$$P_- = \frac{1}{\sqrt{2}}Pk_-$$

$$R = \sqrt{3} \left[(2i\tilde{\gamma}_3 k_x k_y) + \tilde{\gamma}_2(k_x^2 - k_y^2) \right]$$

$$S = 2\sqrt{3}i\tilde{\gamma}_3 k_z(k_x - ik_y)$$

$$P_+ = \frac{1}{\sqrt{2}}Pk_+$$

$$T = (\tilde{\gamma}_2 - \tilde{\gamma}_1)(k_x^2 + k_y^2) - (\tilde{\gamma}_1 + 2\tilde{\gamma}_2)k_z^2$$

$$k_{\pm} = k_x \pm ik_y$$

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$$k_\pm = k_x \pm ik_y$$

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Proposed fitting method to calculate the $k \cdot p$

Proposed fitting method

CMO Bastos, FP Sabino, PEF Junior, T Campos, JLF Da Silva, GM Sipahi, Semiconductor Science and Technology 31 (10), 105002, 2016

Consider a general $k \cdot p$ Hamiltonian matrix

$$\begin{pmatrix} \alpha_{11}(k, \{p\}) & \dots & \alpha_{1i}(k, \{p\}) & \dots & \alpha_{1n}(k, \{p\}) \\ \vdots & \ddots & \vdots & \ddots & \vdots \\ \alpha_{1i}^\dagger(k, \{p\}) & \dots & \alpha_{ii}(k, \{p\}) & \dots & \alpha_{in}(k, \{p\}) \\ \vdots & \ddots & \vdots & \ddots & \vdots \\ \alpha_{1n}^\dagger(k, \{p\}) & \dots & \alpha_{in}^\dagger(k, \{p\}) & \dots & \alpha_{nn}(k, \{p\}) \end{pmatrix},$$

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secular equation

$$\det [H - I\epsilon] = 0 \Rightarrow \sum_{i=0}^{n-1} c_i(k, \{p\}) \epsilon^i(k) = -\epsilon^n(k)$$

Proposed fitting method

CMO Bastos, FP Sabino, PEF Junior, T Campos, JLF Da Silva, GM Sipahi, Semiconductor Science and Technology 31 (10), 105002, 2016

We define the analytical functions

$$\sum_{i=0}^{n-1} c_i(k, \{p\}) \epsilon^i(k) = -\epsilon^n(k)$$

$$\begin{cases} c_0^A(k, \{p\}) \\ c_1^A(k, \{p\}) \\ \vdots \\ c_{n-1}^A(k, \{p\}) \end{cases}$$

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CMO Bastos, FP Sabino, PEF Junior, T Campos, JLF Da Silva, GM Sipahi, Semiconductor Science and Technology 31 (10), 105002, 2016

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and numerical functions obtained by solving the linear system of equations.

$$\begin{pmatrix} 1 & \epsilon_1(k) & \dots & \epsilon_1^i(k) & \dots & \epsilon_1^{n-1}(k) \\ \vdots & \vdots & \ddots & \vdots & \ddots & \vdots \\ 1 & \epsilon_i(k) & \dots & \epsilon_i^i(k) & \dots & \epsilon_i^{n-1}(k) \\ \vdots & \vdots & \ddots & \vdots & \ddots & \vdots \\ 1 & \epsilon_n(k) & \dots & \epsilon_n^i(k) & \dots & \epsilon_n^{n-1}(k) \end{pmatrix} \begin{pmatrix} c_0^N(k) \\ c_1^N(k) \\ \vdots \\ c_i^N(k) \\ \vdots \\ c_{n-1}^N(k) \end{pmatrix} = - \begin{pmatrix} \epsilon_1^n(k) \\ \vdots \\ \epsilon_i^n(k) \\ \vdots \\ \epsilon_n^n(k) \end{pmatrix},$$

Proposed fitting method

Therefore,

CMO Bastos, FP Sabino, PEF Junior, T Campos, JLF Da Silva, GM Sipahi, Semiconductor Science and Technology 31 (10), 105002, 2016

$$\left\{ \begin{array}{l} c_0^A(k, \{p\}) = c_0^N[\epsilon_1(k), \epsilon_2(k), \dots, \epsilon_n(k)] \\ c_1^A(k, \{p\}) = c_1^N[\epsilon_1(k), \epsilon_2(k), \dots, \epsilon_n(k)] \\ \vdots \\ c_{n-1}^A(k, \{p\}) = c_{n-1}^N[\epsilon_1(k), \epsilon_2(k), \dots, \epsilon_n(k)] . \end{array} \right.$$

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CMO Bastos, FP Sabino, PEF Junior, T Campos, JLF Da Silva, GM Sipahi, Semiconductor Science and Technology 31 (10), 105002, 2016

$$\begin{cases} c_0^A(k, \{p\}) = c_0^N[\epsilon_1(k), \epsilon_2(k), \dots, \epsilon_n(k)] \\ c_1^A(k, \{p\}) = c_1^N[\epsilon_1(k), \epsilon_2(k), \dots, \epsilon_n(k)] \\ \vdots \\ c_{n-1}^A(k, \{p\}) = c_{n-1}^N[\epsilon_1(k), \epsilon_2(k), \dots, \epsilon_n(k)] \end{cases}$$

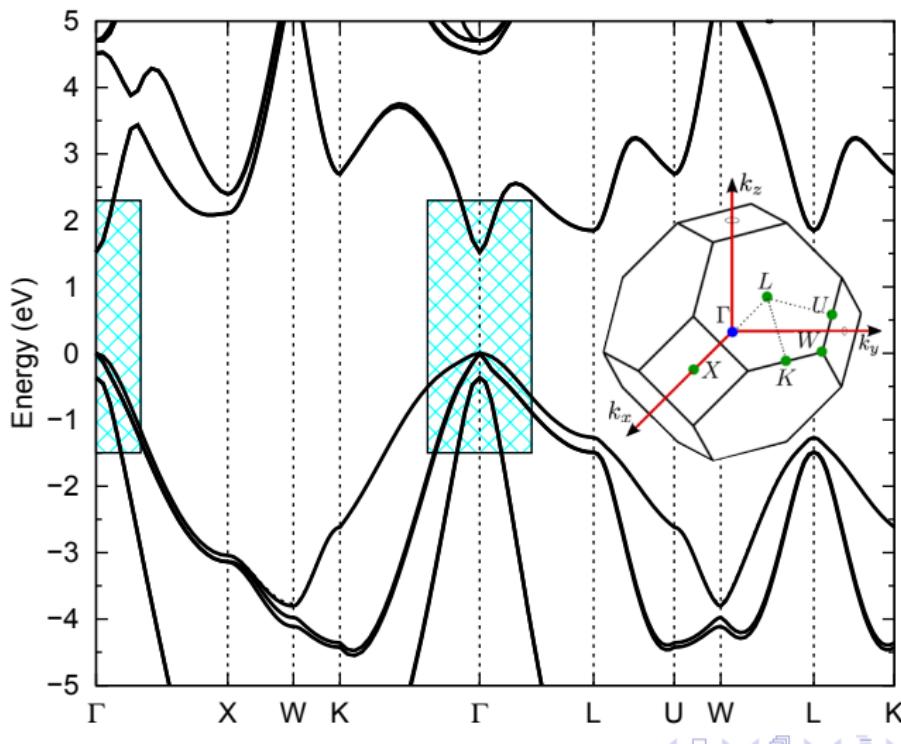
The fittings are performed between analytical and numerical functions, together.

For the numerical function, the band structure has been measured or calculated.

GaAs zincblend example

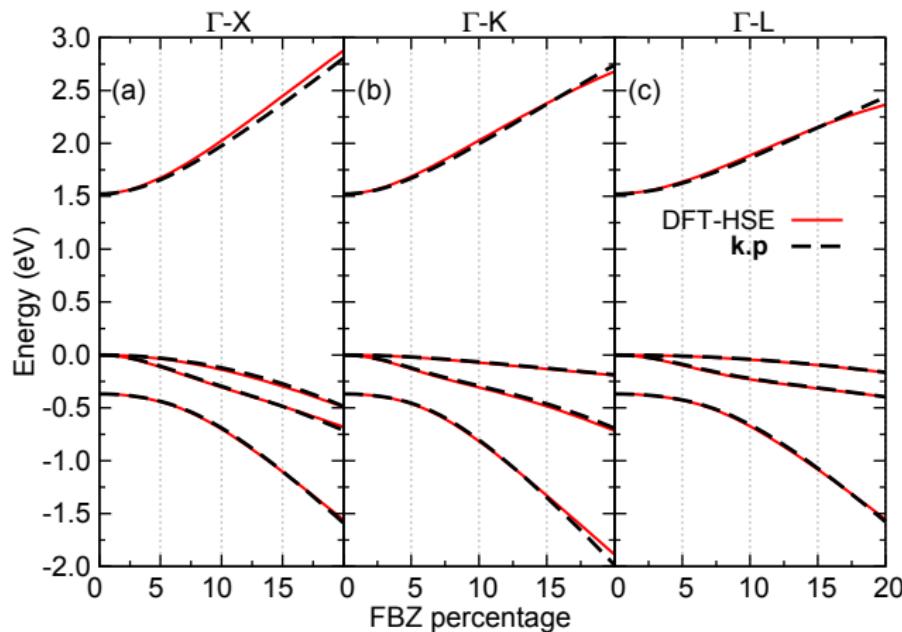
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Band structure calculated from HSE06 using VASP



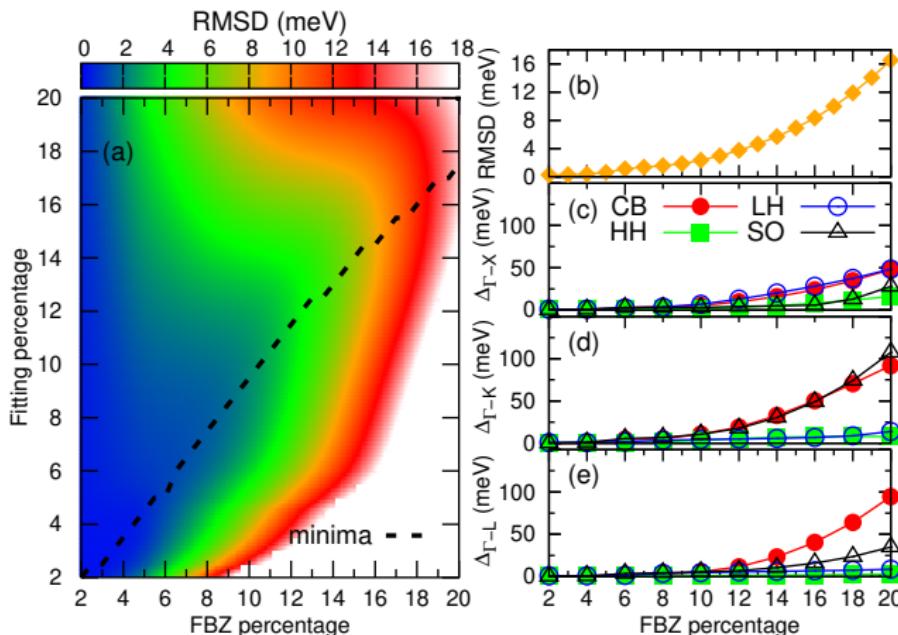
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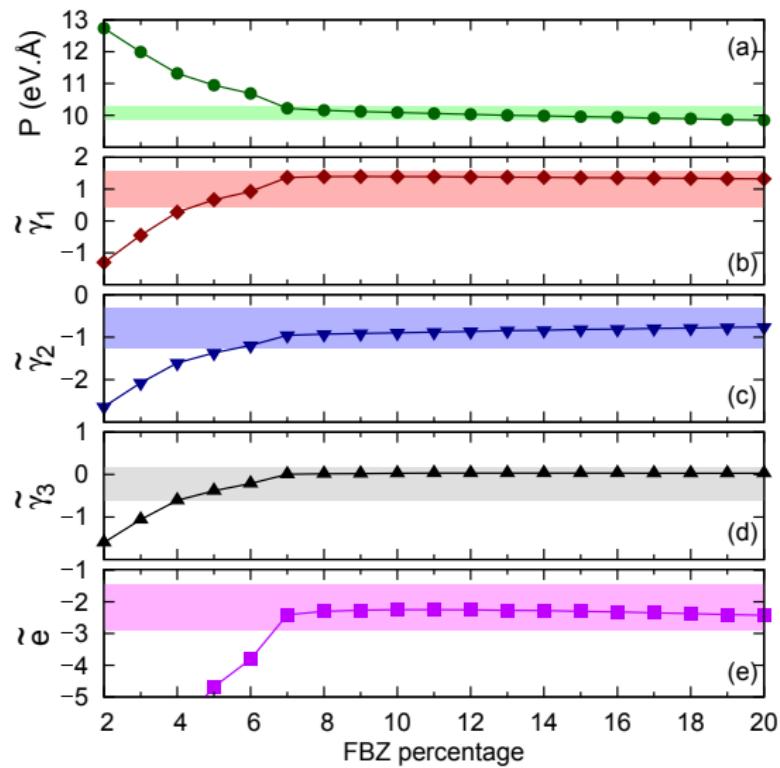
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GaAs zincblend example

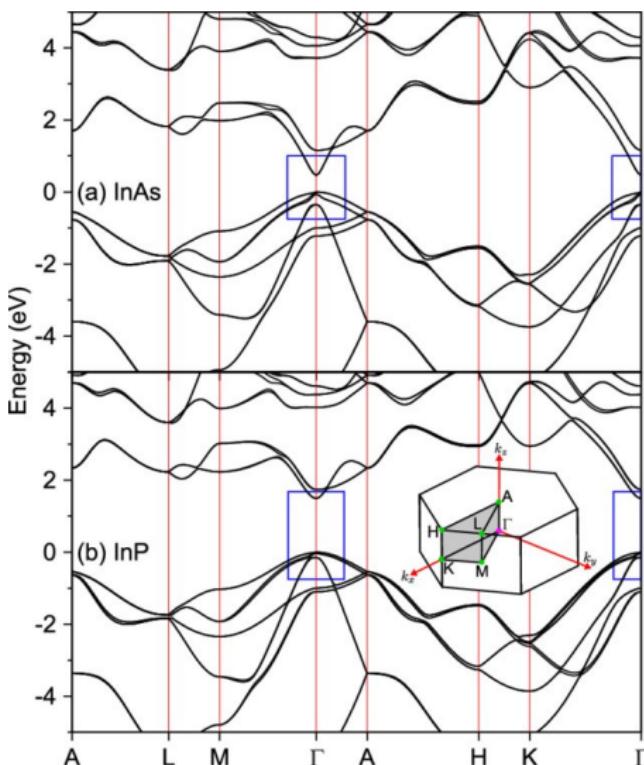
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New $k \cdot p$ models for another structures: InAs and InP wurtzite example

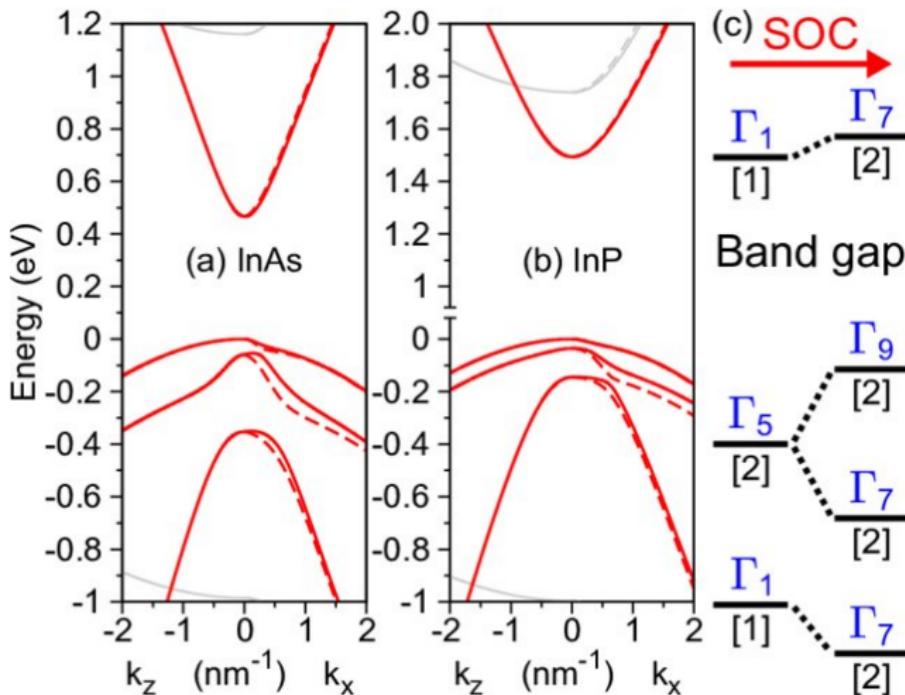
New $k \cdot p$ models

PE Faria Junior, T Campos, CMO Bastos, M Gmitra, J Fabian, GM Sipahi Physical Review B 93 (23), 235204, 2016



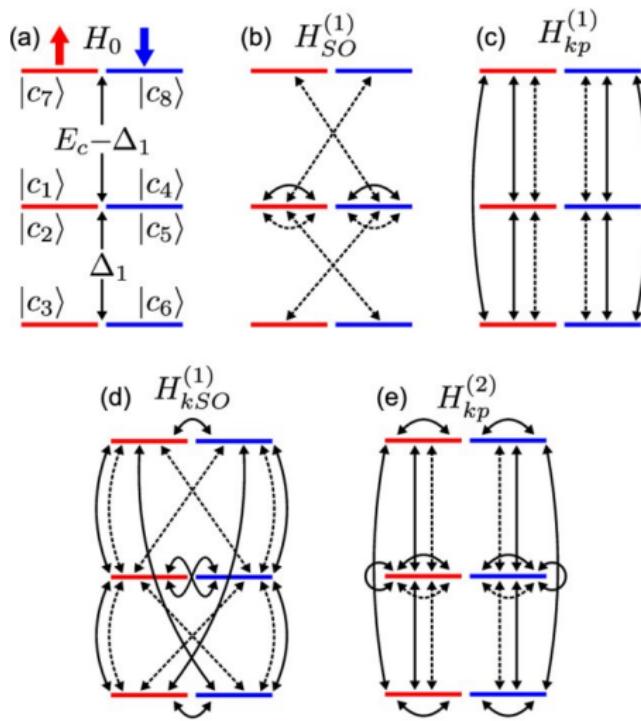
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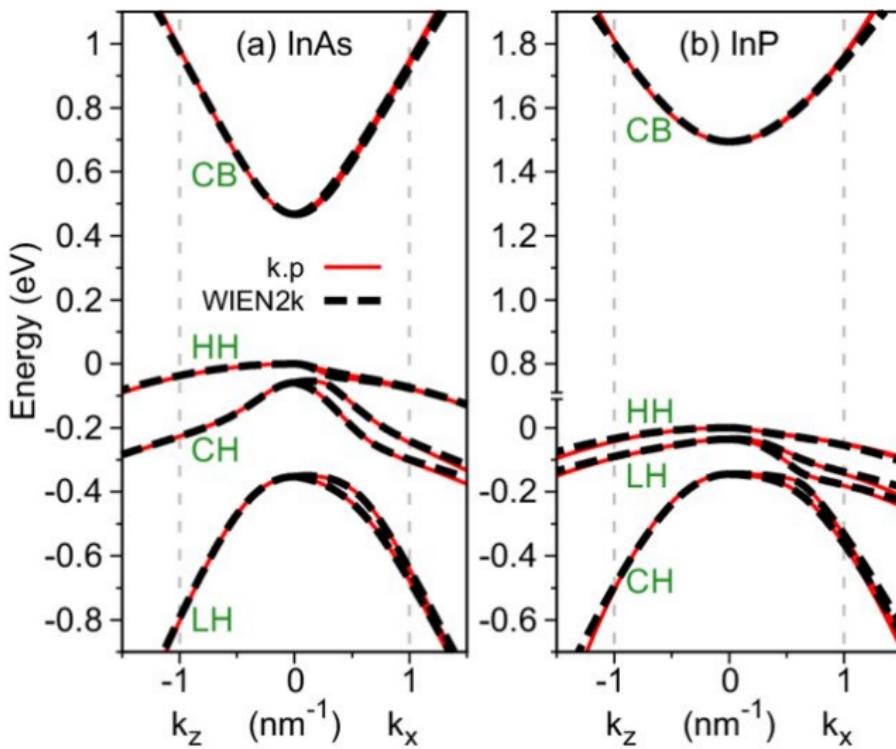
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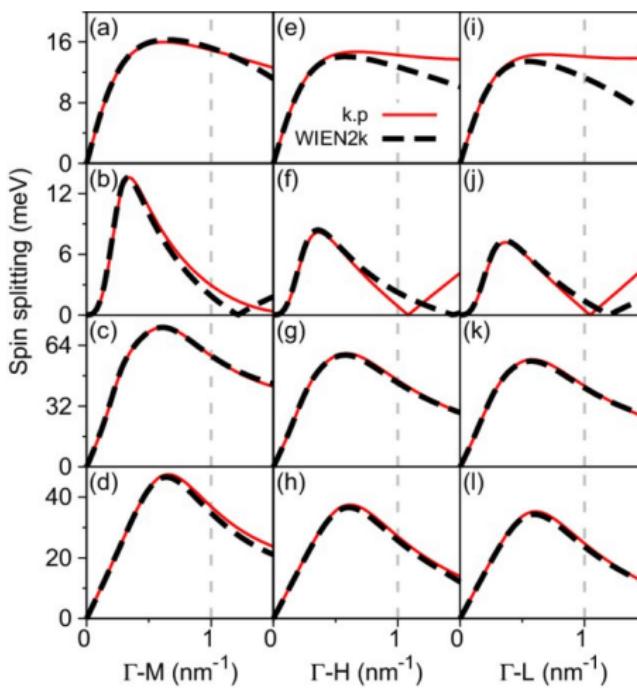
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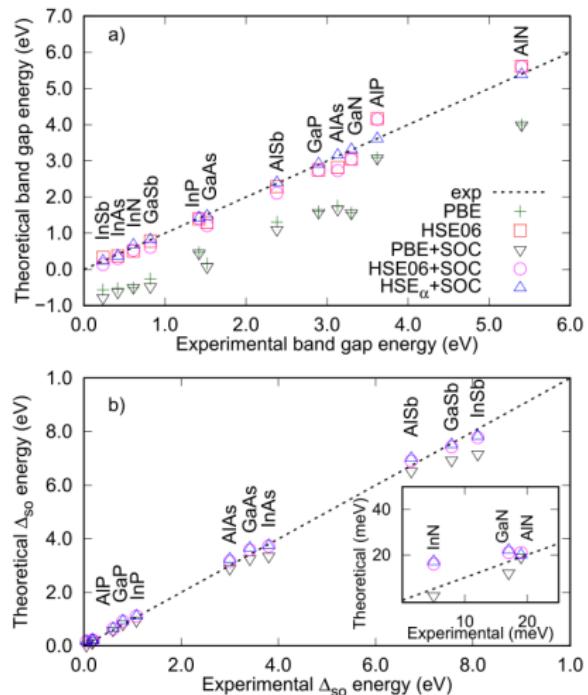
Improve the precision of $k \cdot p$ parameters with hybrid-DFT: HSE $_{\alpha}$

$$E_{XC}^{HSE} = E_c^{PBE} + E_x^{PBE,LR}(\omega) + \alpha E_x^{HF,SR}(\omega) + (1 - \alpha) E_x^{PBE,SR}(\omega)$$

CMO Bastos, FP Sabino, GM Sipahi, JLF
Da Silva Journal of Applied Physics 123
(6), 2018

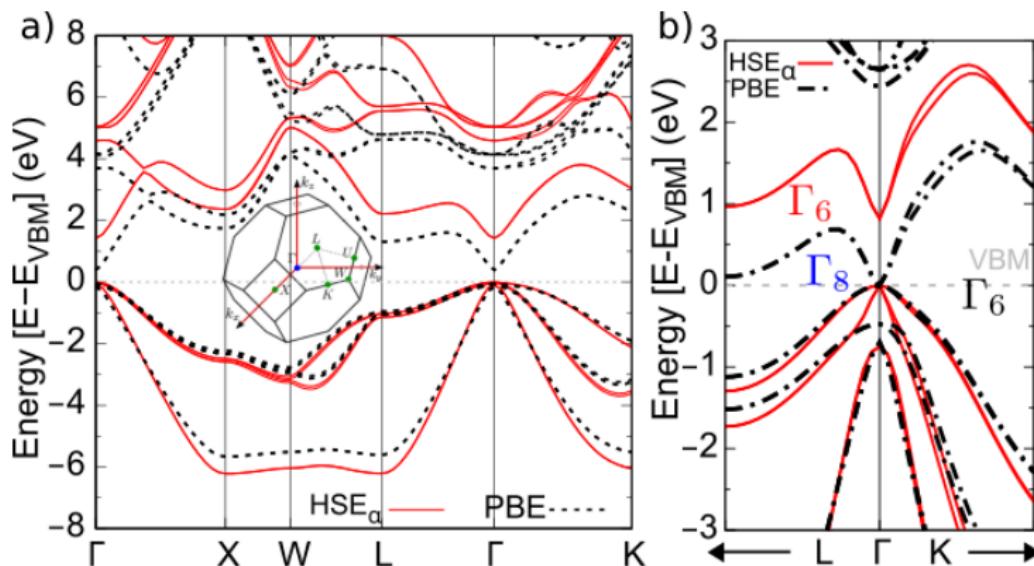
Improve the precision with HSE α

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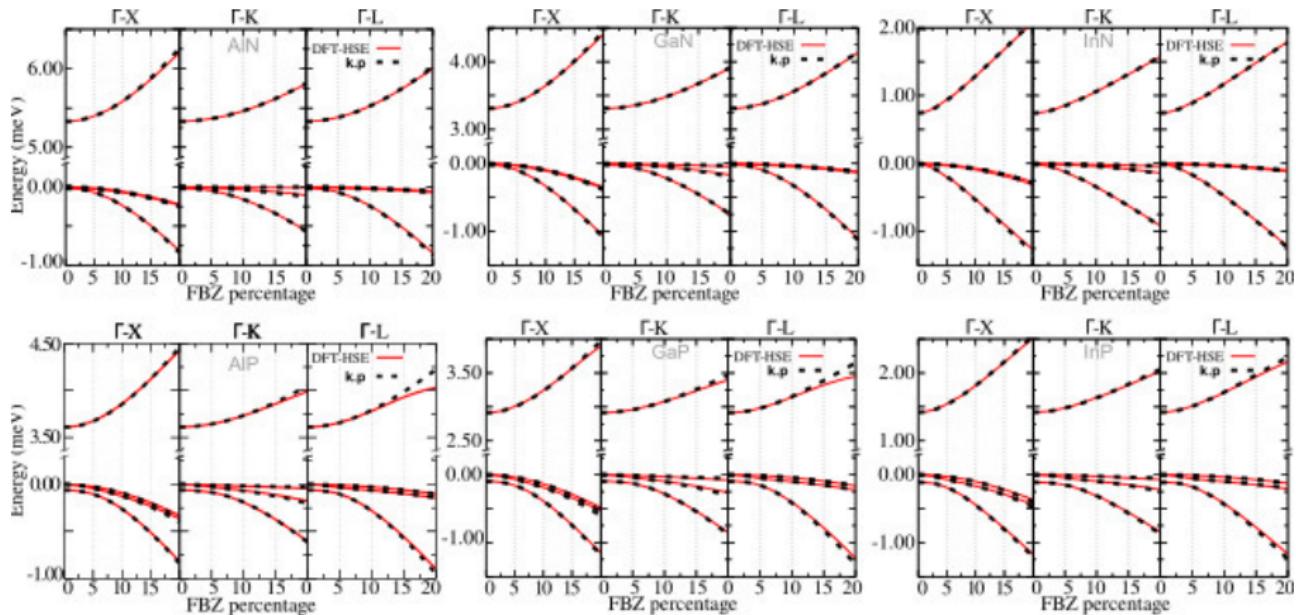
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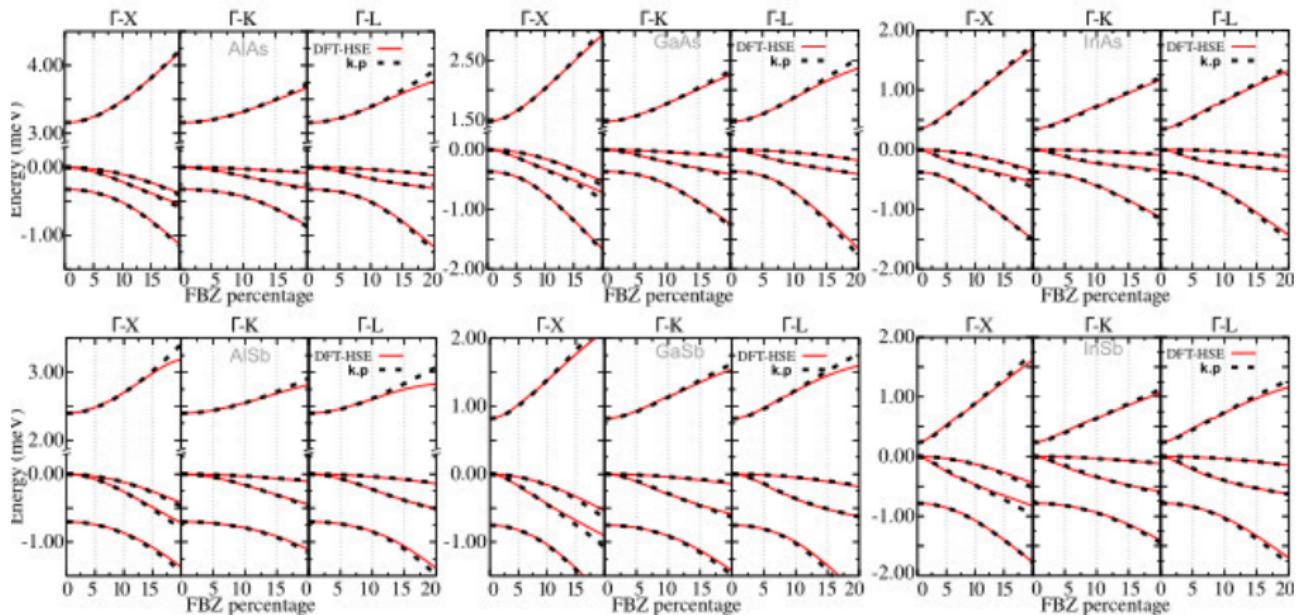
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Conclusions

- A framework combining two main methods in electronic calculations DFT and $k \cdot p$ was established.
- A new $k \cdot p$ model was developed and fitted for wurtzite, capable of describing spin splitting in the bands.
- The HSE_α framework was introduced to improve the description of the band structure.
- By developing a fitting method to extract the $k \cdot p$ model, the approach was extended to potentially study any crystal material.
- Since 2018, the resulting parameters have been successfully used in the literature, producing results comparable with experiments.

Acknowledgments

