Ab initio and full-zone ***k*** ·***p*** computations of the electronic structure of wurtzite BeO

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Outline

- Motivations
- What is full-zone ***k*** **·*p***?
- Application to BeO
- Results and Discussion
- Conclusions

Motivations

- ***k ·p*** electronic structure model is important to study optical and transport properties of bulk semiconductor materials and low dimensional structures.
- Conventional ***k ·p*** may be very accurate in the regions close to the band extrema, but it is not suitable to describe the electronic structure in the whole Brillouin Zone (BZ).
- It is desirable to have a method that maintains the simplicity of the conventional ***k ·p*** but is accurate over the full BZ.
- We have developed a full-zone ***k ·p*** model that attains this objectives and can be used for all those applications where a full-band description is needed.

Why full-zone ***k·p***?

- Traditional approach beyond the basic effective mass approximation: “few-band” ***k ·p*** (usually 6 or 8 bands for WZ, taking into account spin-orbit effects)
- Good representation close to a given point in the Brillouin Zone (usually Γ for direct-gap semiconductors)
- Full-Brillouin-Zone extension: satisfies requirements of accuracy in the entire BZ and for a wide range of energies

Full-zone *k·p*

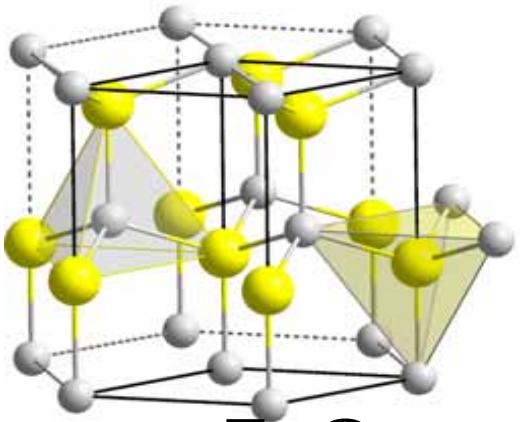
- ***k ·p*** is an empirical method, which needs reliable experimental/ab initio reference data (*optimization targets*)

  ➡ new calculations with ABINIT

- The number of fitting parameters used by ***k ·p*** must be minimized not to undermine its computational efficiency

  ➡ developement of a novel approach for FZ ***k ·p*** in wurtzite crystals

BeO primer



- Very high energy gap (10.6 eV)
- Hexagonal lattice + lattice constant near ZnO

  ➡ alloy with ZnO and BeZnO/ZnO QW

- Recent interest in BeZnO/ZnO light-emitting diodes and lasers

  ➡ several theoretical and experimental works on BeO/BeZnO properties since 2006

[1] Y. R. Ryu, T. S. Lee, J. A. Lubguban, H. W. White, B.-J. Kim, Y.-S. Park, and C.-J. Youn, Appl. Phys. Lett., vol. 88, p. 241108(3), Jun. 2006.
[2] S. F. Ding, G. H. Fan, S. T. Li, K. Chen, and B. Xiao, Physica B, vol. 394, pp. 127–131, 2007.
[3] Y. Duan, H. Shi, and L. Qin, Phys. Lett. A, vol. 372, pp. 2930-2933, 2008.

Full-zone ***k·p***: application to Wurtzite Crystals

- We are interested in studying optical and transport properties of ternary alloy BeZnO
- The first step is the analysis of the electronic structure of the binary compounds: BeO and ZnO
- We need an accurate yet computationally efficient method suitable for inclusion e.g. in laser/LED design tools or in full-band Monte Carlo transport simulation

BeO Full-zone *k·p*

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  ➡ developement of a novel approach for FZ ***k ·p*** in wurtzite crystals

Reference data for ***k·p***: ABINIT

- We have performed DFT calculations on BeO with ABINIT using GGA pseudopotentials (cut-off energy: 40 Ha, 6x6x6 integration grid over the BZ)
- Energy gap = 7.7085 eV (target: 10.6 eV)
- Converged lattice constants and internal parameter:
  - a = 2.6945 Å (exp. [1]: a = 2.698 Å LDA [2]: a = 2.664 Å)
  - c = 4.3751 Å (exp. [1]: c = 4.380 Å LDA [2]: c = 4.337 Å)
  - u = 0.3793 (exp. [1]: u = 0.378 LDA [2]: u = 0.377)

[1] Y.-N. Xu and W. Y. Ching, "Electronic, optical, and structural properties of some wurtzite crystals," *Phys. Rev. B, vol. 48, no. 7, pp. 4335–4351, Aug.* 1993.
[2] B. Baumeier, P. Krüger, and J. Pollmann, "Atomic and electronic structure of BeO and the BeO (1010) surface: An *ab initio* investigation", *Phys. Rev. B, vol. 75, no. 04, pp. 5323–5330, 2007.*

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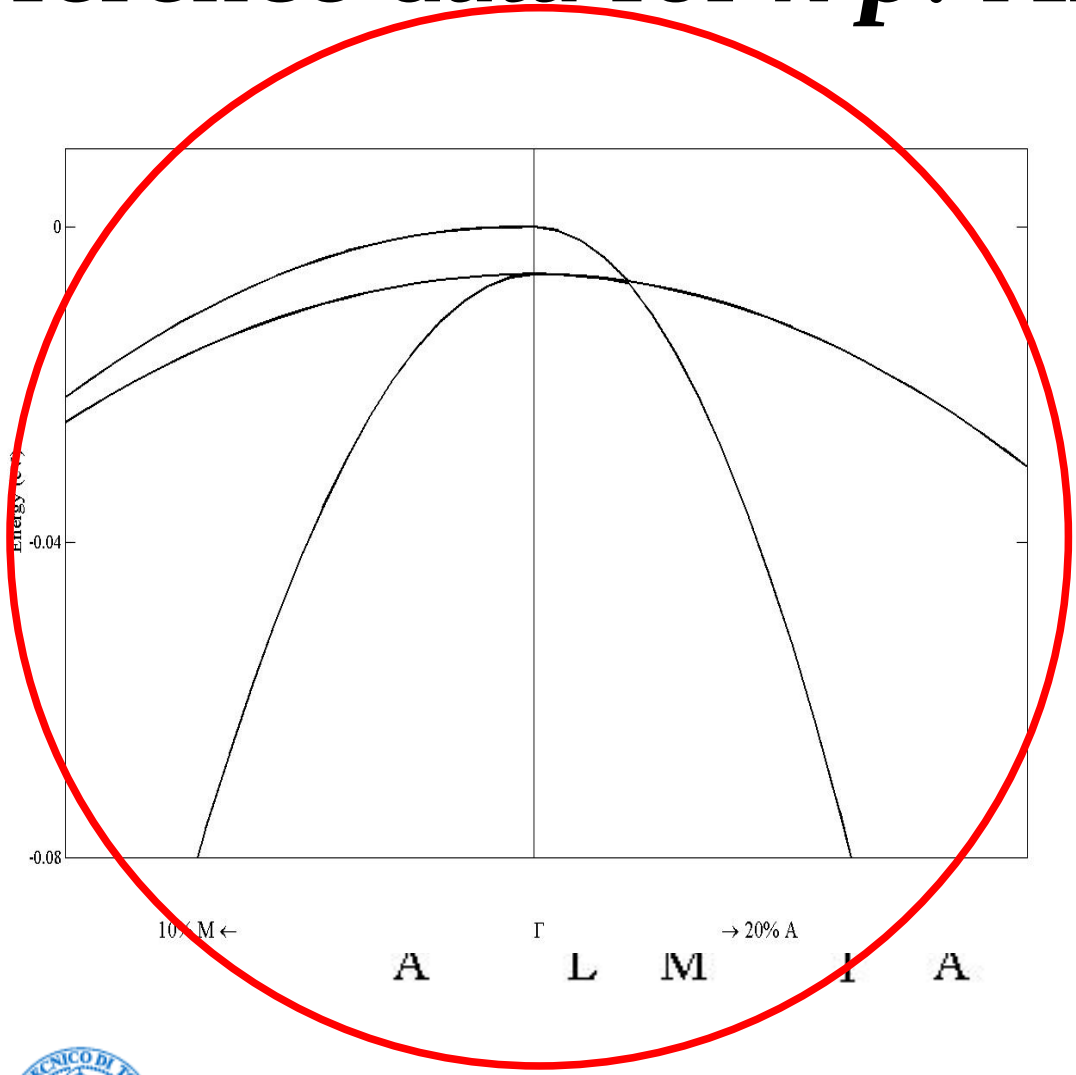
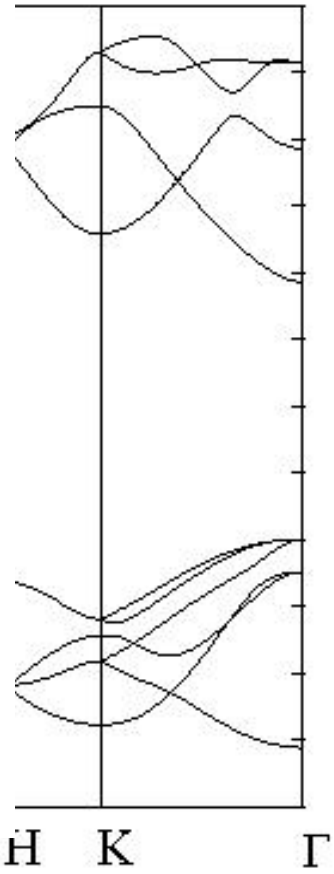
Reference data for ***k·p***: ABINIT

- C
  sp
  sr
  ne
  in





BeO Full-zone *k·p*

- ***k ·p*** is an empirical method, which needs reliable experimental/ab initio reference data (*optimization targets*)

⇨ new calculations with ABINIT

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➡ 2- developement of a novel approach for FZ ***k ·p*** in wurtzite crystals

$k \cdot p$ basics

Based on Bloch theorem to solve Schrödinger equation

$$\psi(\boldsymbol{x}) = e^{i\boldsymbol{k}\cdot\boldsymbol{x}} u(\boldsymbol{x}) \quad + \quad \mathcal{H}\psi(\boldsymbol{x}) = E\,\psi(\boldsymbol{x})$$

$$=$$

$$\left(\frac{\hbar^2 k^2}{2m_0} + \frac{\hbar}{m_0}\boldsymbol{k}\cdot\boldsymbol{p} + \frac{\hbar^2}{2m_0}\boldsymbol{p}^2 + V \right) u_{n,\boldsymbol{k}} = E_n u_{n,\boldsymbol{k}}$$

(with $\boldsymbol{p} = -i\hbar\nabla$)

basis functions

Method: series expansion of u $\quad u_{n,\boldsymbol{k}} = \sum_m c_m^{(n)} u_{m,\boldsymbol{k}_0}$

$\boldsymbol{k \cdot p}$ basics

Final equation: eigenvalues problem

$$H(\boldsymbol{k})\boldsymbol{c}^{(n)} = E_n(\boldsymbol{k})\boldsymbol{c}^{(n)}$$

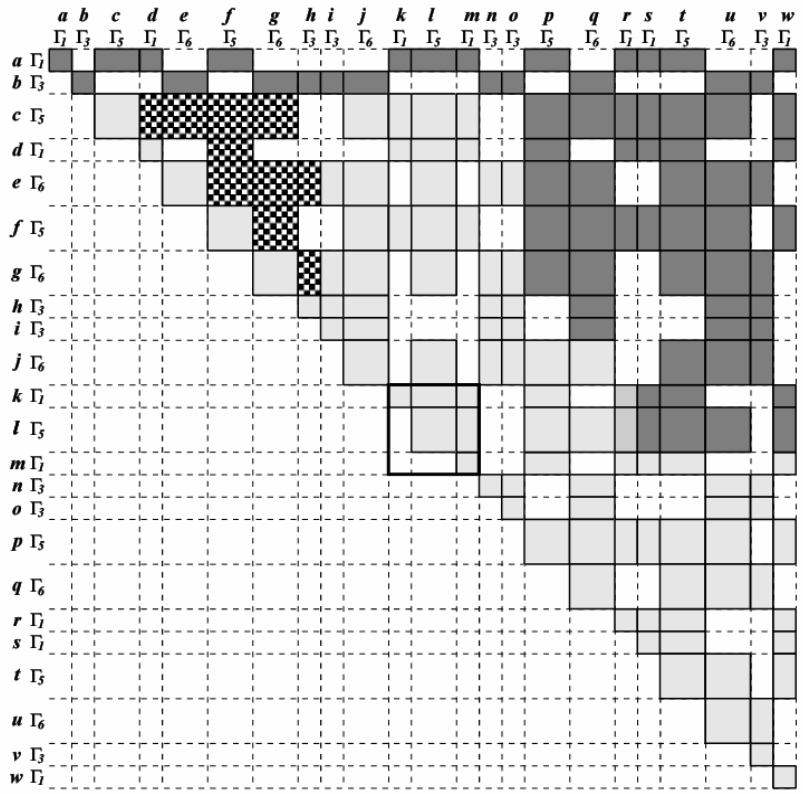
with

$$h_{m'm} = \left(E + \frac{\hbar^2}{2m_0}\|\boldsymbol{k}-\boldsymbol{k}_0\|^2\right)\delta_{m'm} + \frac{\hbar}{m_0}\langle\psi_{m',k}|\,(\boldsymbol{k}-\boldsymbol{k}_0)\cdot\boldsymbol{p}\,|\psi_{m',k}\rangle$$

Determining h coefficients:

- directly from definition (knowing wavefunctions)
- fit (exploiting crystal **simmetries**)

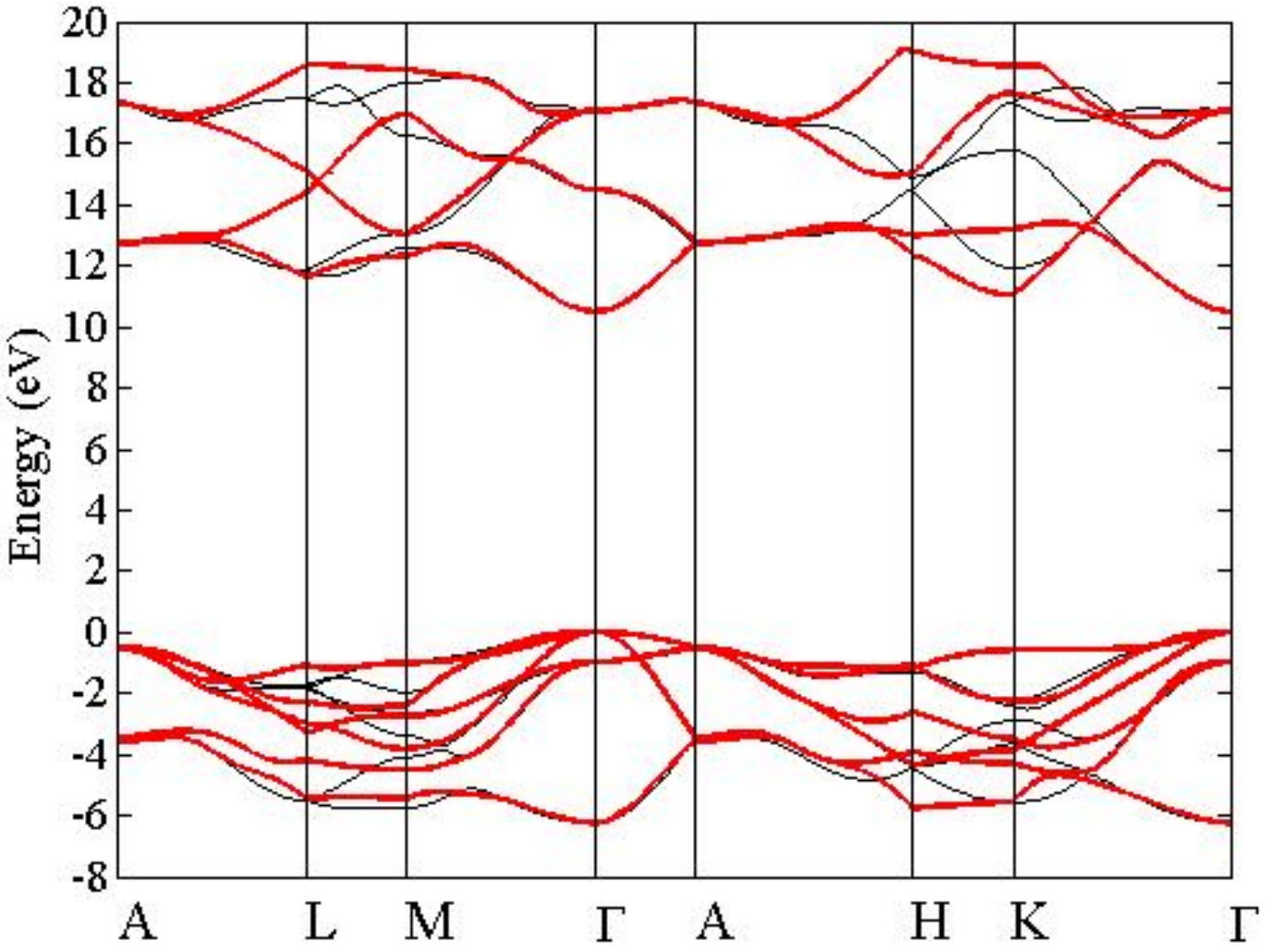
First FZ ***k·p*** improvement: Wurtzite simmetries in Γ



	$E\,(g_0)$	$C_2\,(\tilde{g}_3)$	$2C_3\,(g_2)$	$2C_6\,(\tilde{g}_1)$	$3\sigma_d\,(g_6)$	$3\sigma_d'\,(\tilde{g}_9)$
Γ_1	(1)	(1)	(1)	(1)	(1)	(1)
Γ_3	(1)	(−1)	(1)	(−1)	(1)	(−1)
Γ_5	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}$	$\begin{pmatrix} -1/2 & -\sqrt{3}/2 \\ \sqrt{3}/2 & -1/2 \end{pmatrix}$	$\begin{pmatrix} 1/2 & -\sqrt{3}/2 \\ \sqrt{3}/2 & 1/2 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$	$\begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$
Γ_6	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} -1/2 & -\sqrt{3}/2 \\ -\sqrt{3}/2 & -1/2 \end{pmatrix}$	$\begin{pmatrix} -1/2 & -\sqrt{3}/2 \\ \sqrt{3}/2 & -1/2 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

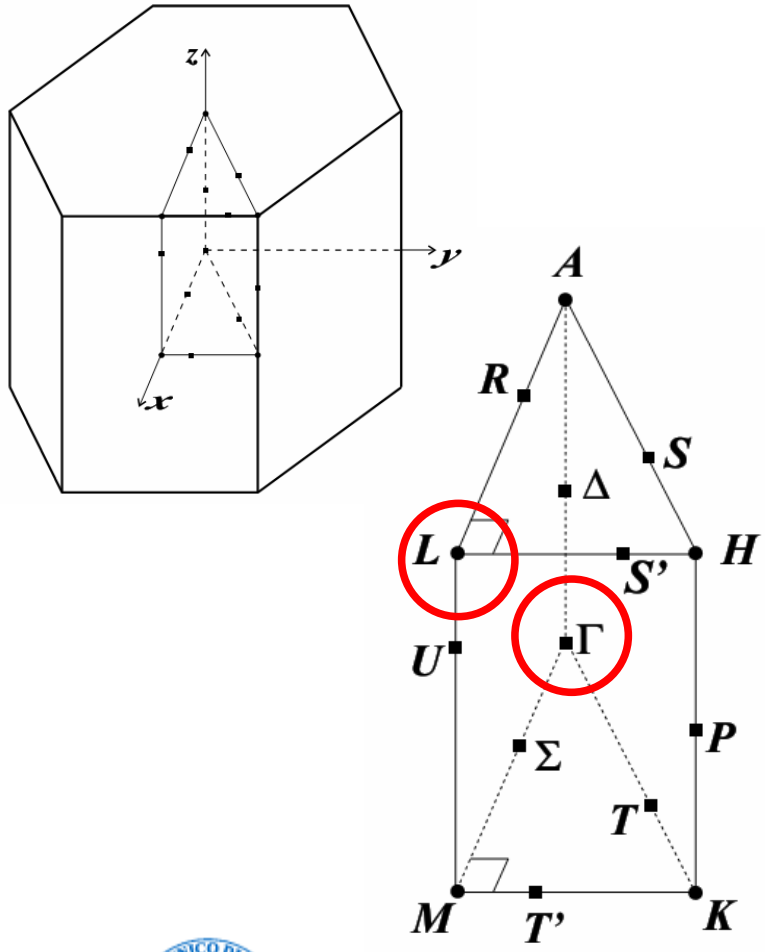
- Periodic functions on Bravais solid (***k*** = ***0***)
- Decomposition in **representations**

Limitations of single-point $\boldsymbol{k \cdot p}$ full-zone



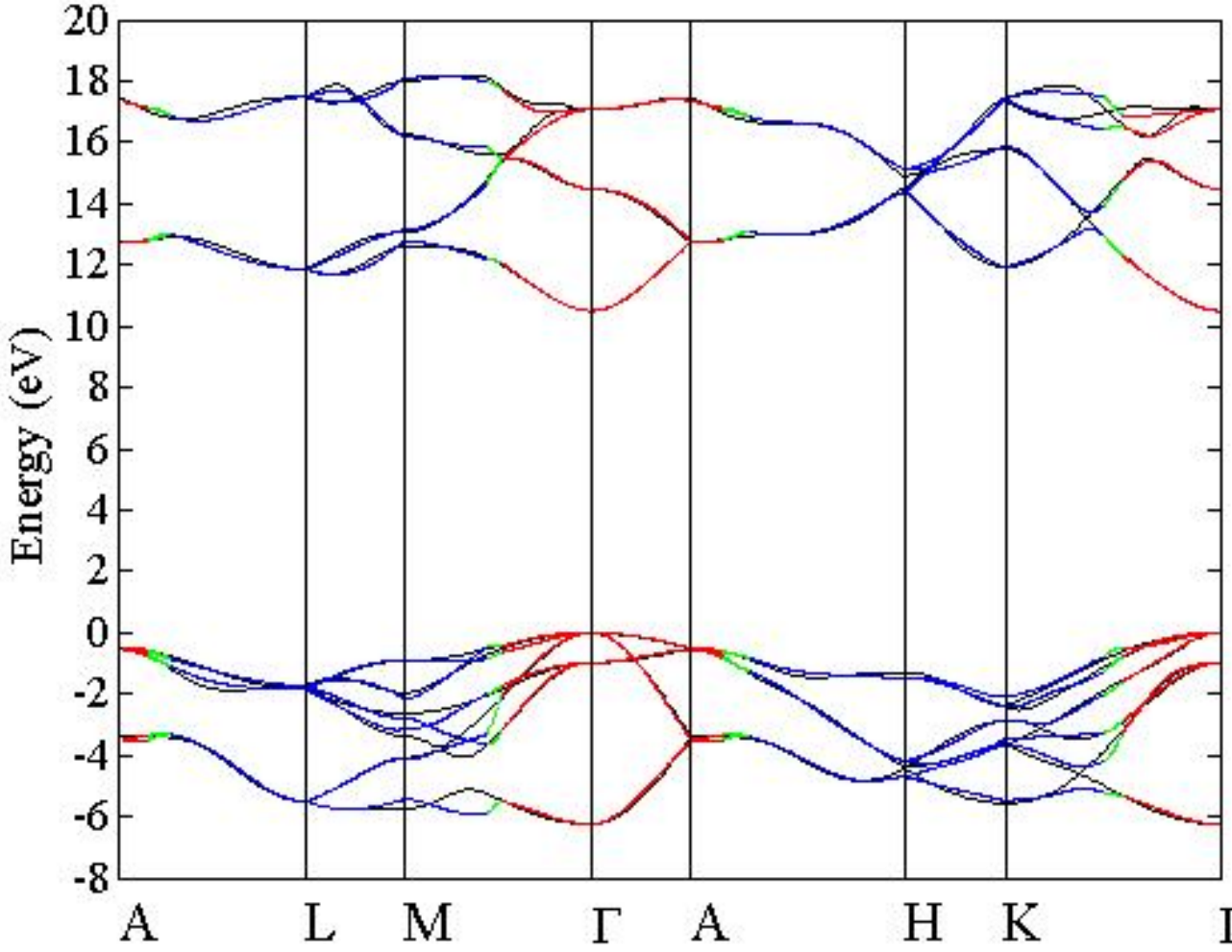
Energy inaccuracies far from Γ when using the standard $\boldsymbol{k \cdot p}$ single point expansion

Second FZ ***k·p*** improvement: Two expansion points



- We have performed two ***k ·p*** calculations using two expansion points: the first in Γ and the second in L
- 6 valence bands and 4 conduction bands

k·p vs. ABINIT



ABINIT
(with the so-called *scissor correction*)

k ·p in Γ

k ·p in L

Two-expansion point k ·p

Conclusions

- We have developed a novel full-zone ***k ·p*** approach for wurtzite crystals based on multi-k-point expansion.
- This approach makes it possible to significantly improve the precision of the conventional ***k ·p*** method over the full BZ.
- We presently applying this technique to several wurtzite materials (III-Nitrides and II-VI Oxides).
- As presented for BeO the novel approach leads to full zone ***k ·p*** electronic structure with overall quality comparable with *ab initio* methods.