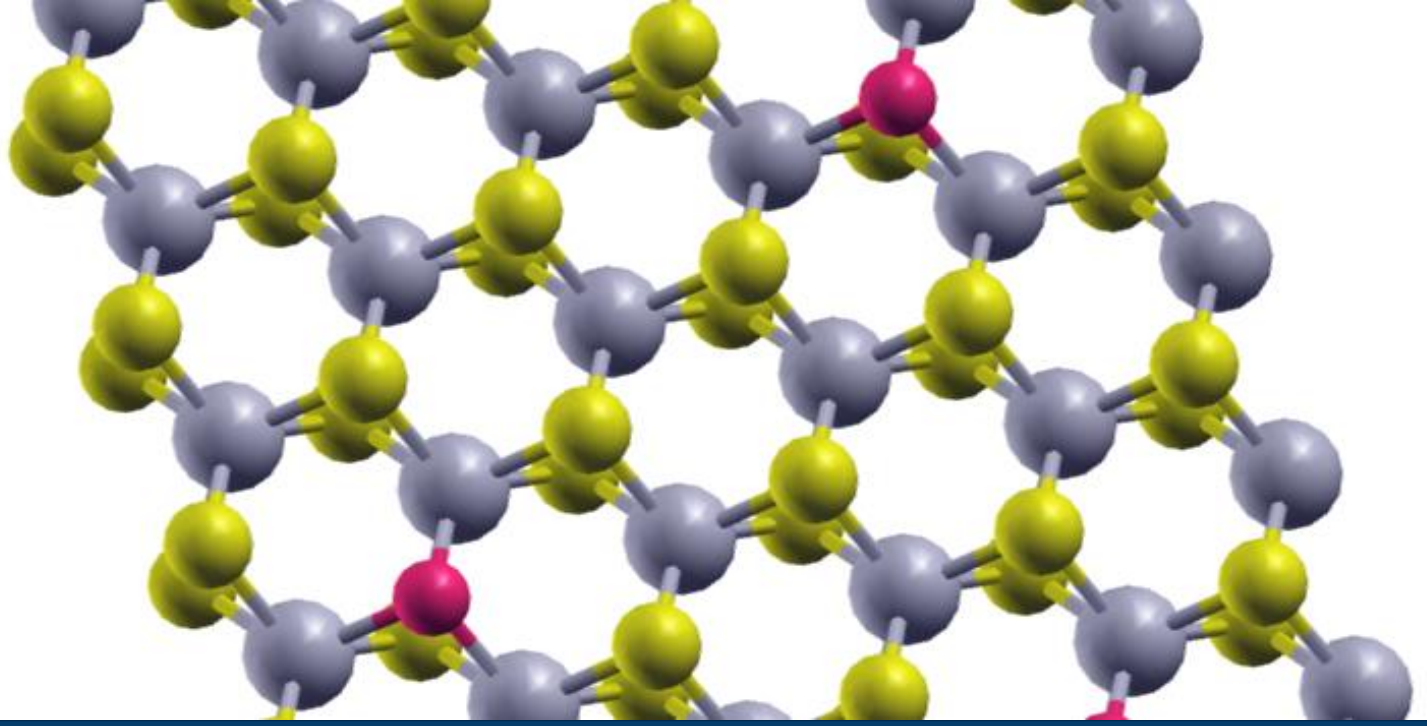


BAND UNFOLDING FOR SUPERCELL CALCULATIONS

SEPTEMBER 10th, 2019 I STEFAN ROST

Peter Grünberg Institut, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

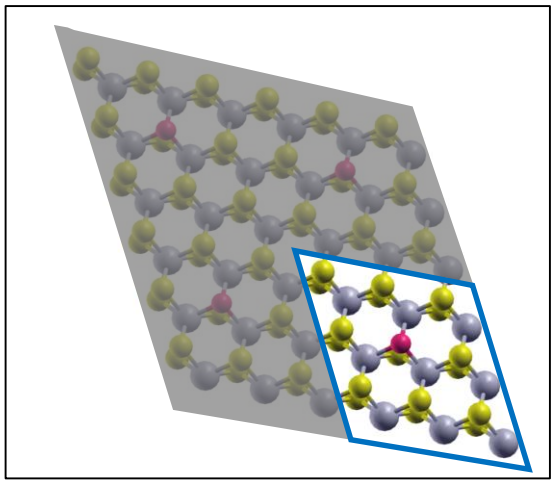
Mitglied der Helmholtz-Gemeinschaft

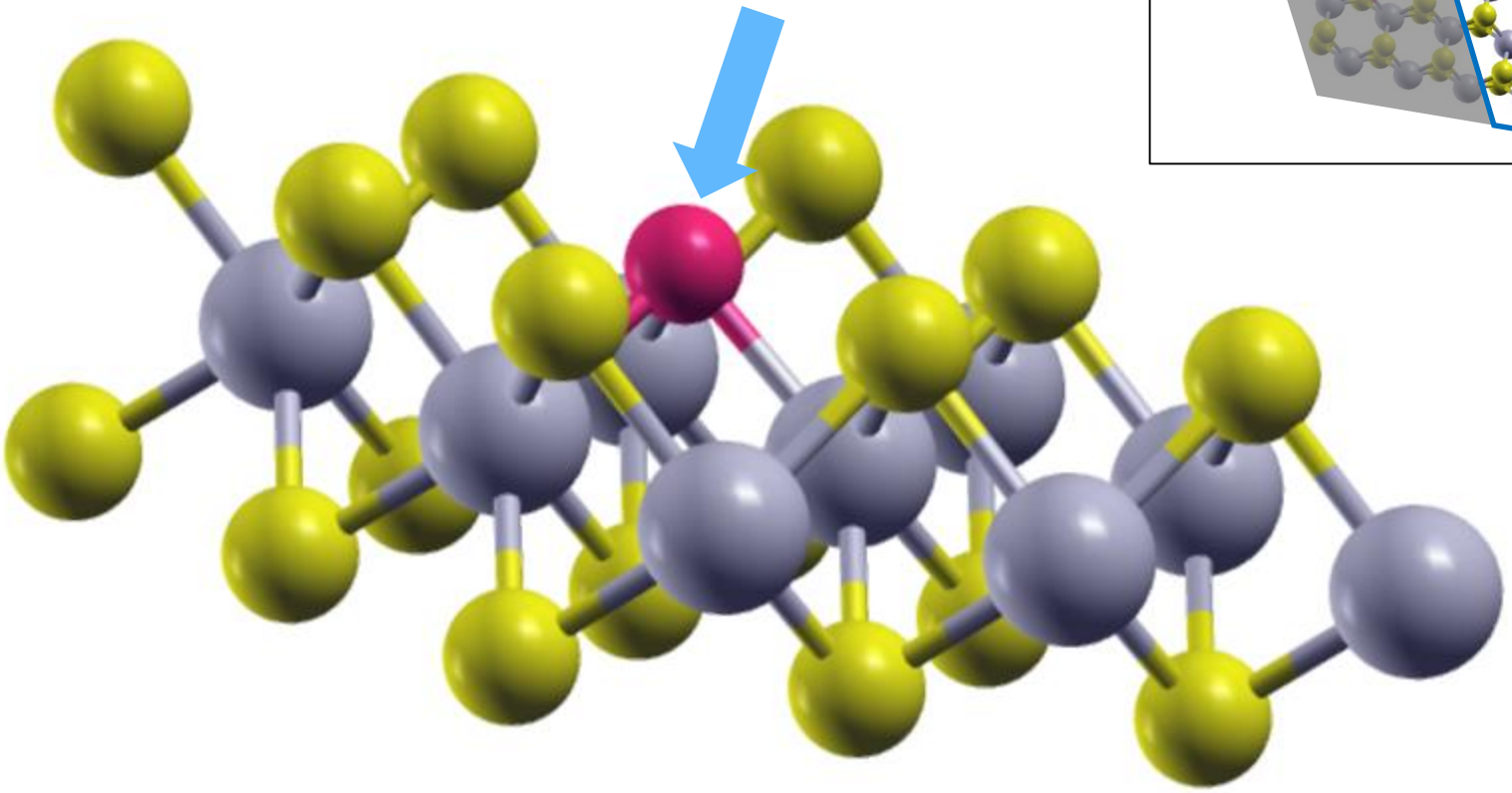
MAX DRIVING THE EXASCALE TRANSITION

JÜLICH Forschungszentrum

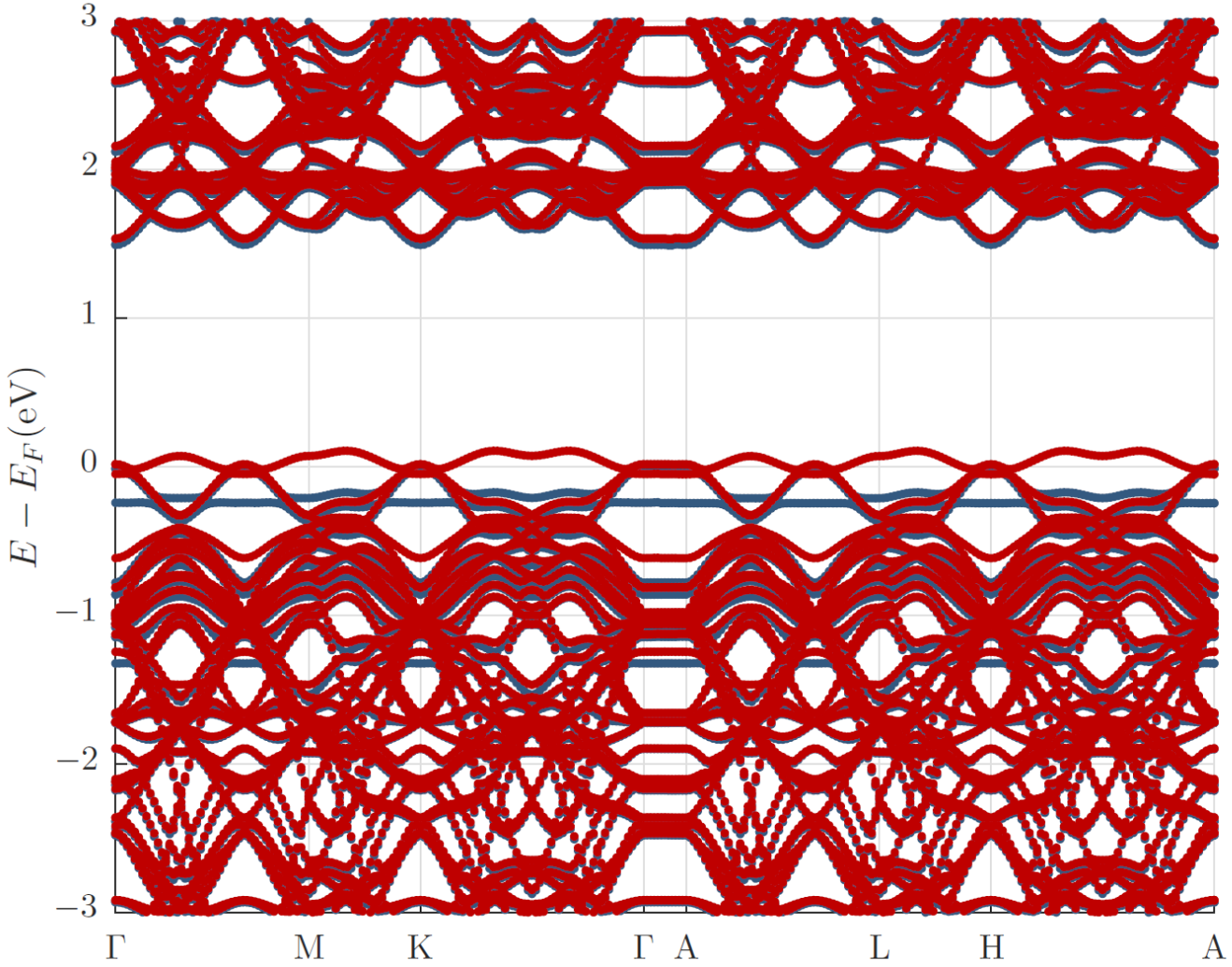
MOTIVATION – DEFECT STATE

phosphorus atom
relaxes inwards





BAND STRUCTURE $MoSe_2 + P$



MAX DRIVING THE EXASCALE TRANSITION

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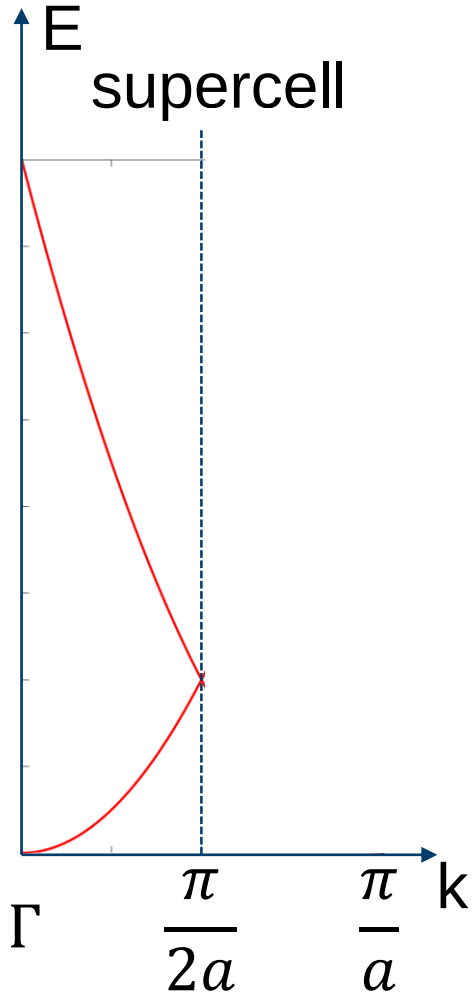
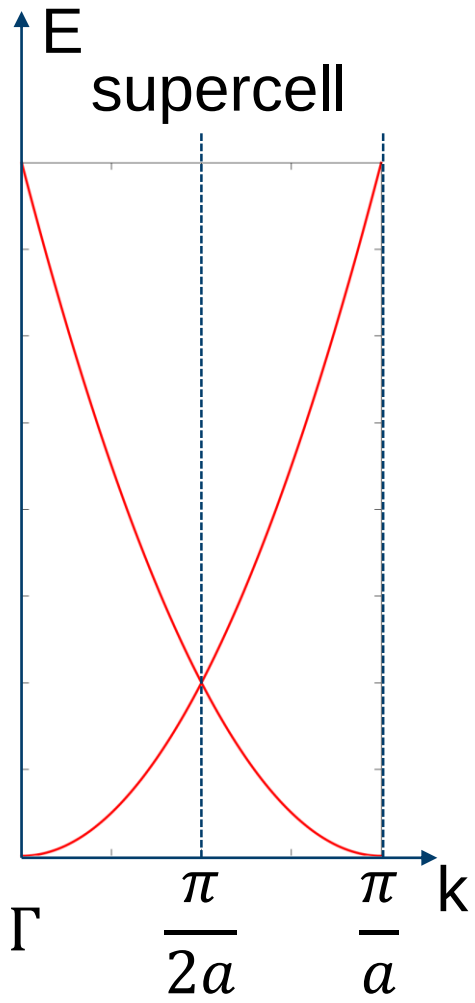
MOTIVATION

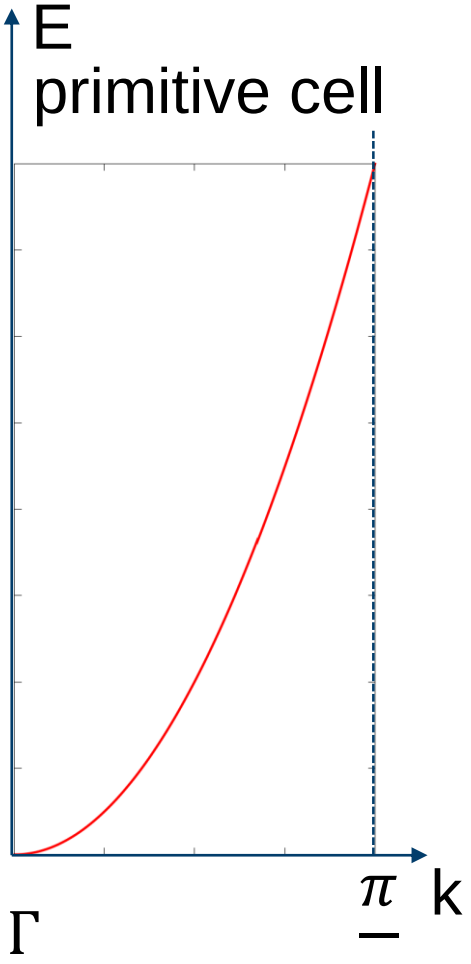


MAX DRIVING THE EXASCALE TRANSITION
JÜLICH Forschungszentrum

MOTIVATION



$\overset{?}{\Rightarrow}$



MAX DRIVING THE EXASCALE TRANSITION
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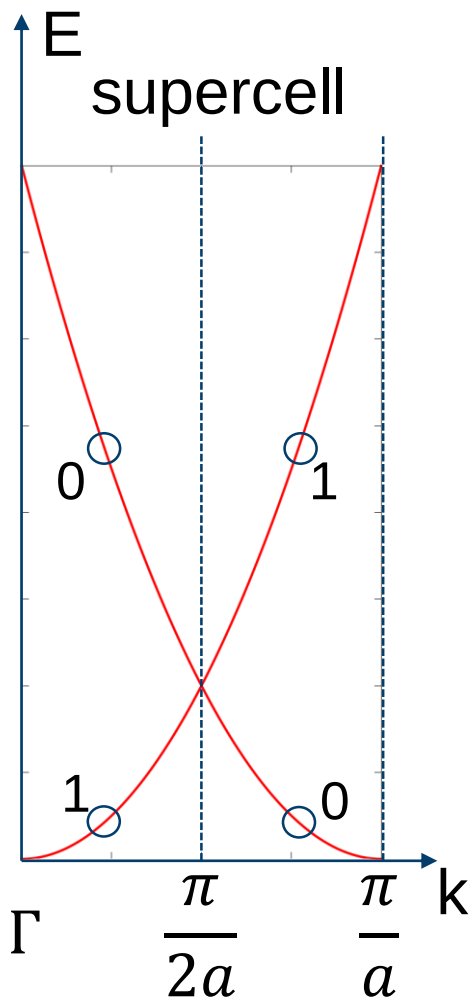
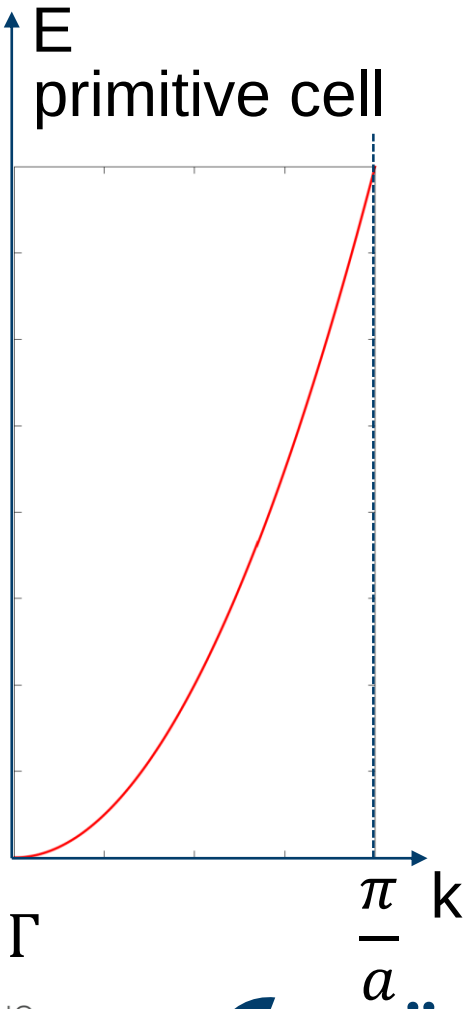
MOTIVATION



spectral weights

$\Rightarrow$



MAX DRIVING THE EXASCALE TRANSITION
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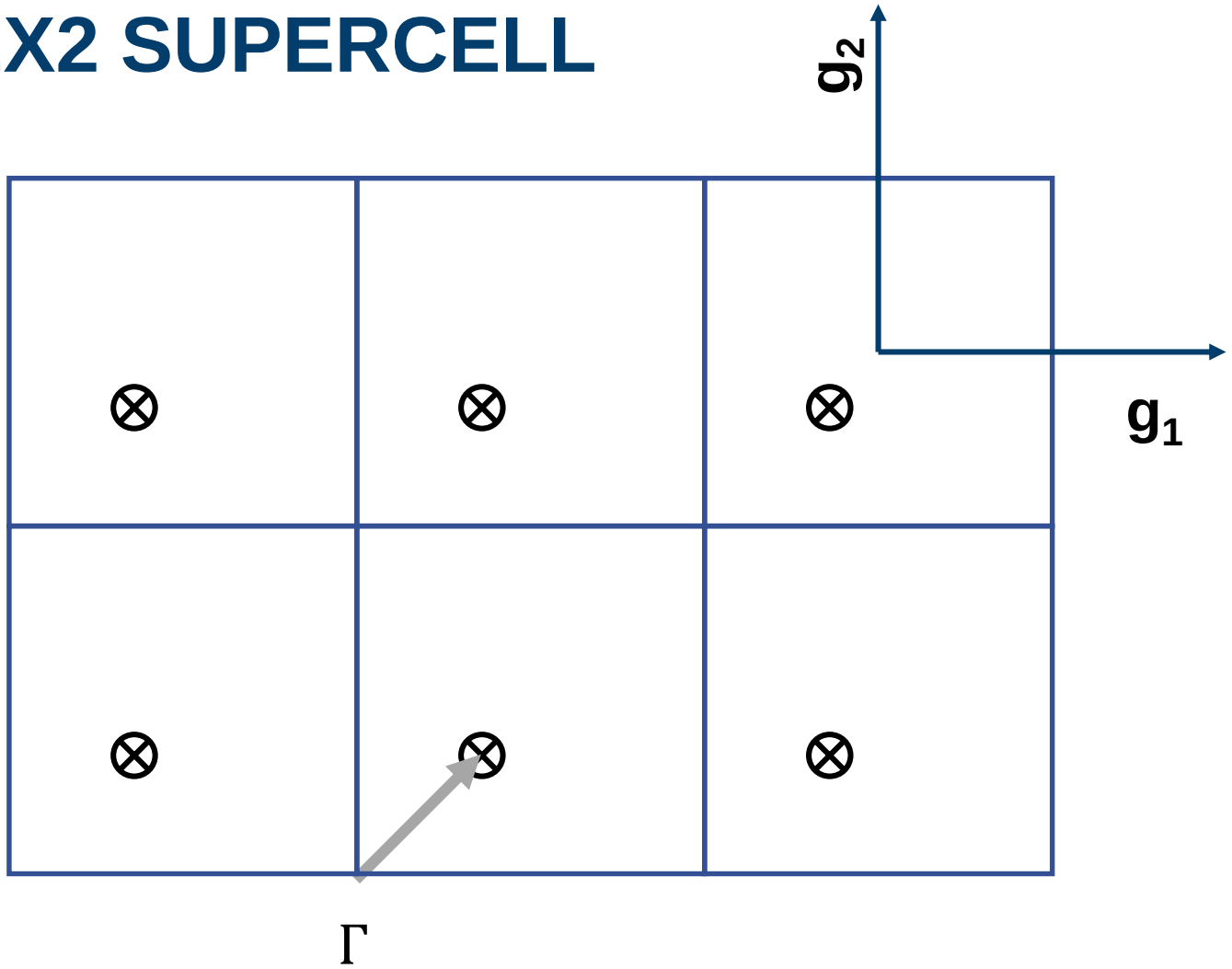
UNFOLDING OF A BAND STRUCTURE
EXAMPLE 2X2 SUPERCELL

$\mathbf{g_1}$, $\mathbf{g_2}$
reciprocal lattice vectors of unit cell



MAX DRIVING THE EXASCALE TRANSITION
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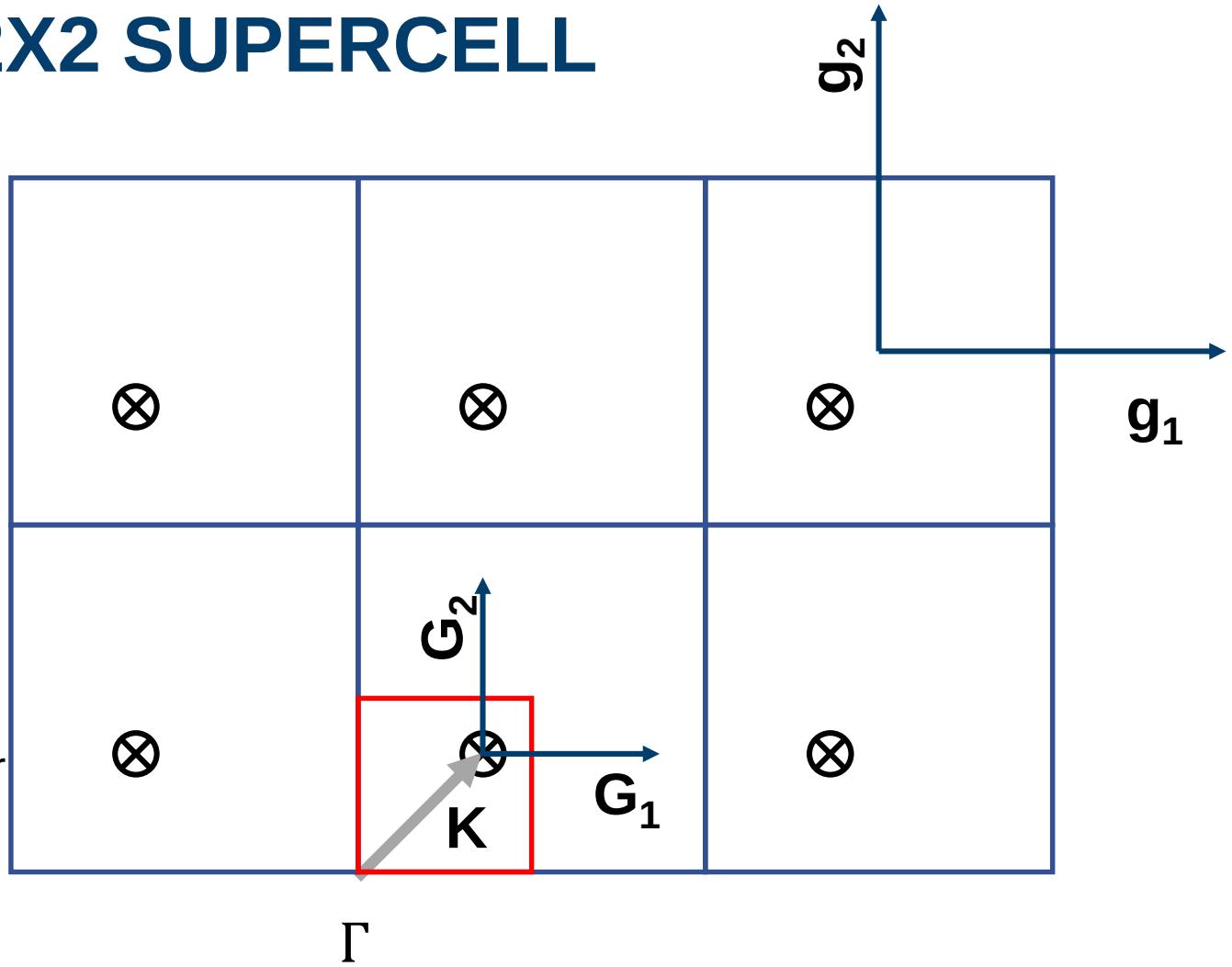
UNFOLDING OF A BAND STRUCTURE
EXAMPLE 2X2 SUPERCELL

g_1, g_2
reciprocal lattice vectors of unit cell

G_1, G_2
reciprocal lattice vectors of 2x2 super cell

K
wave vector in 2x2 super cell



MAX DRIVING THE EXASCALE TRANSITION
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UNFOLDING OF A BAND STRUCTURE
EXAMPLE 2X2 SUPERCELL

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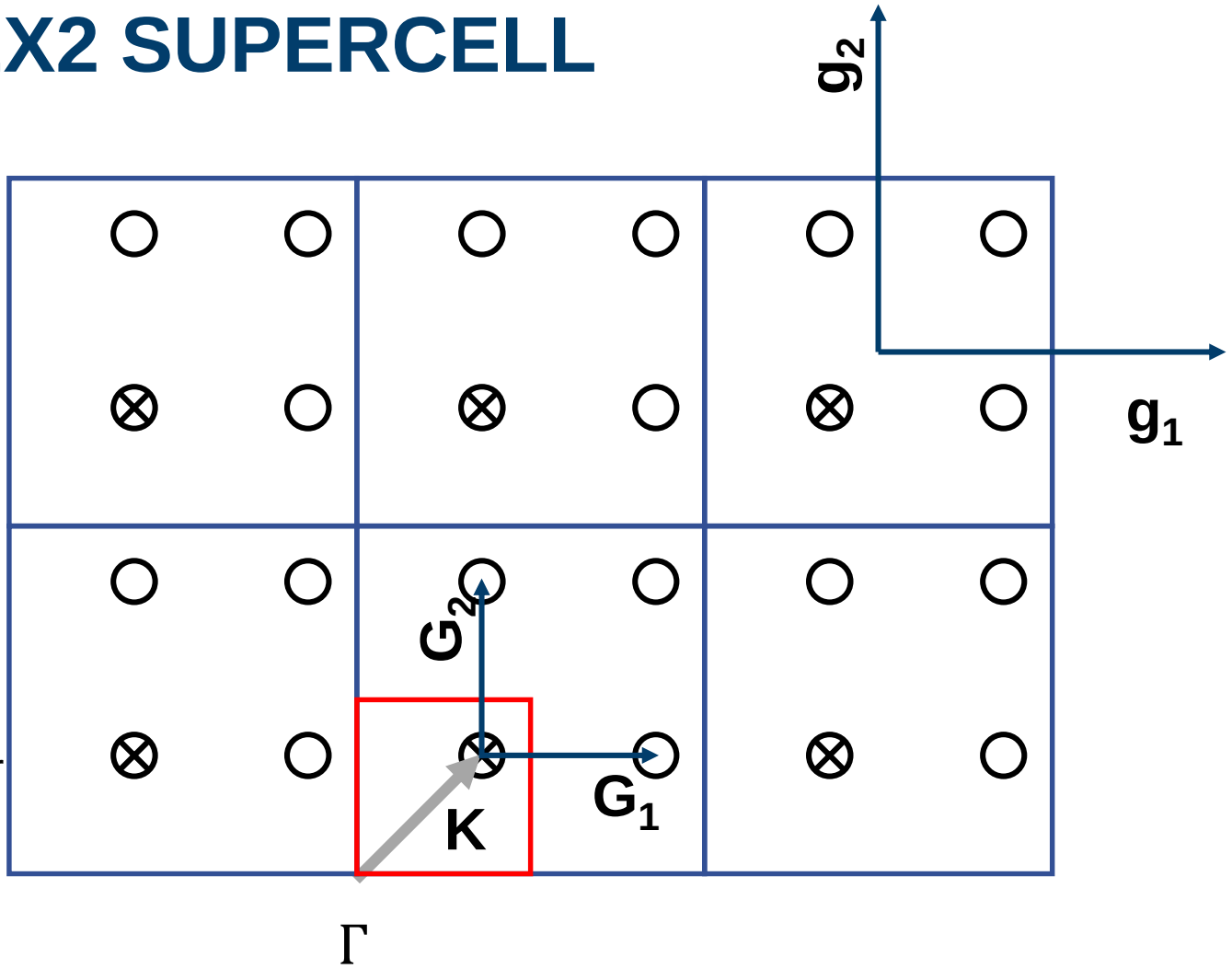

MAX DRIVING THE EXASCALE TRANSITION
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UNFOLDING OF BAND STRUCTURE

$$\mathbf{k} = \mathbf{K} + m_1\mathbf{G}_1 + m_2\mathbf{G}_2$$

using plane waves:

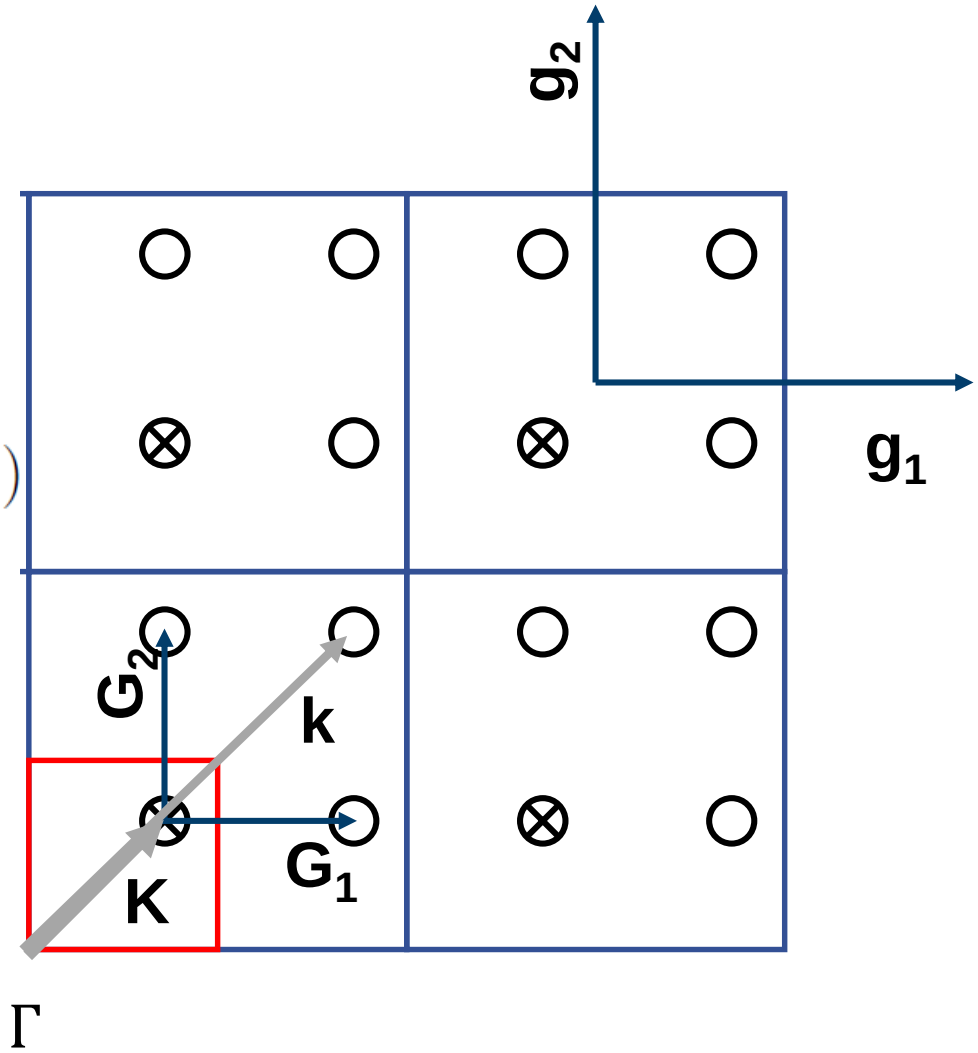
$$\Psi_{n,\mathbf{K}}(\mathbf{r}) = \sum_{\mathbf{G}} C_{n,\mathbf{K}}(\mathbf{G}) e^{i(\mathbf{K}+\mathbf{G})\cdot\mathbf{r}}$$

$$w_n(\mathbf{k}) = \sum_{\mathbf{G}} C_{n,\mathbf{K}}(\mathbf{G}) \cdot C^*_{n,\mathbf{K}}(\mathbf{G})$$

$$w_n(\mathbf{k}) = \sum_{\tilde{\mathbf{G}}} |C_{n,\mathbf{K}}(\tilde{\mathbf{G}})|^2$$

spectral weight

Subset of **G** matching to one **k** and its multiples in the unit cell



MAX DRIVING THE EXASCALE TRANSITION
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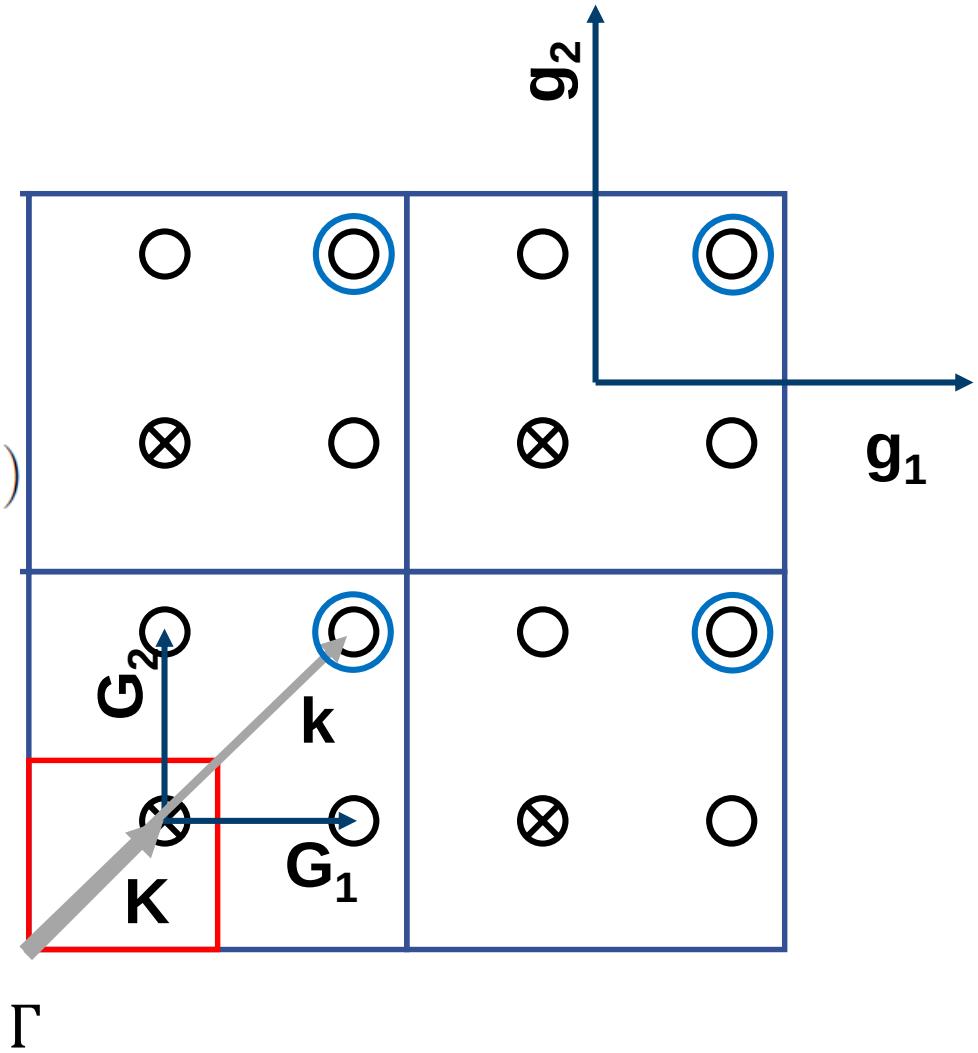

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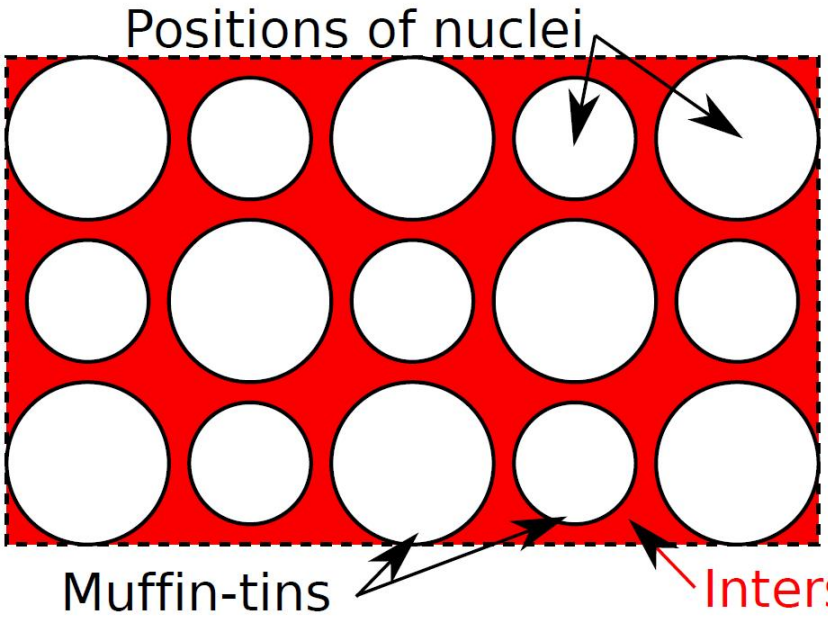
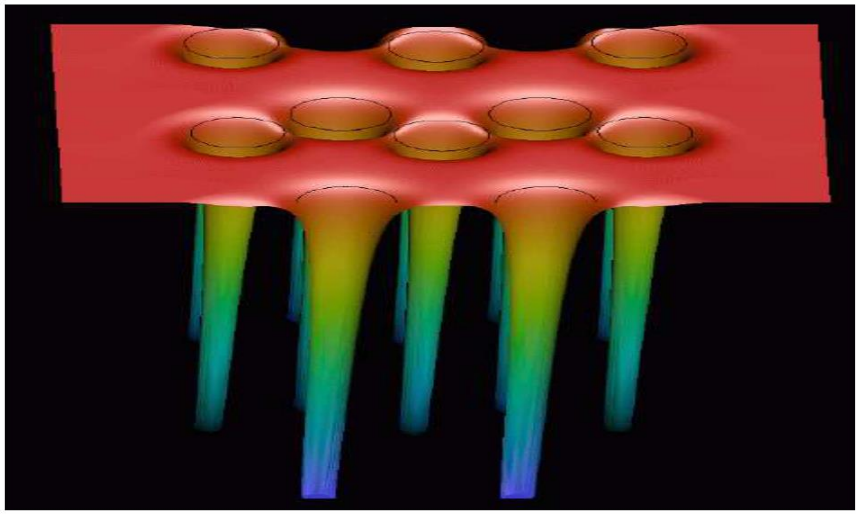
LAPW BASIS





D. Wortmann. “DFT in practice”. In: Computing Solids. Forschungszentrum Jülich GmbH.

$$\chi_{\mathbf{K},\mathbf{G}}(\mathbf{r}) = \begin{cases} e^{i(\mathbf{K}+\mathbf{G})\mathbf{r}} & \text{interstitial region} \\ \sum_{l,m} \left(a_{lm}^{\alpha,\mathbf{G}}(\mathbf{K}) u_l^\alpha(r^\alpha) + b_{lm}^{\alpha,\mathbf{G}}(\mathbf{K}) \dot{u}_l^\alpha(r^\alpha) \right) \mathrm{Y}_{lm} & \text{muffin-tin } \alpha \end{cases}$$

UNFOLDING OF BANDSTRUCTURE (2)

For the LAPW basis:

$$\Psi_{n,\mathbf{K}}(\mathbf{r}) = \sum_{\mathbf{G}} C_{n,\mathbf{K}}(\mathbf{G}) \cdot \chi_{\mathbf{K},\mathbf{G}}(\mathbf{r})$$

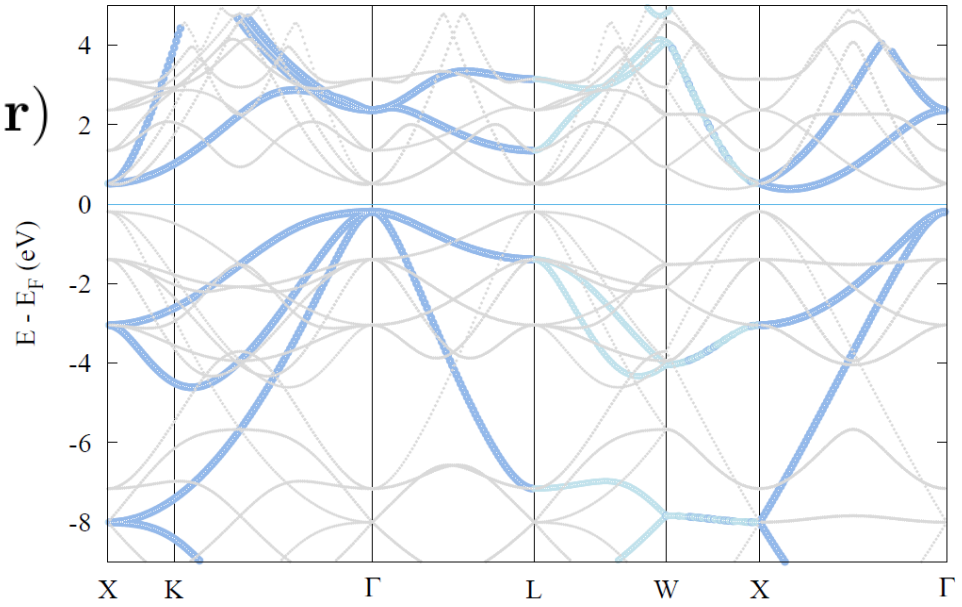
With an overlap matrix:

$$S_{\mathbf{K},\mathbf{G},\mathbf{G}'} = \left\langle \chi_{\mathbf{K},\mathbf{G}} \middle| \chi_{\mathbf{K},\mathbf{G}'} \right\rangle$$

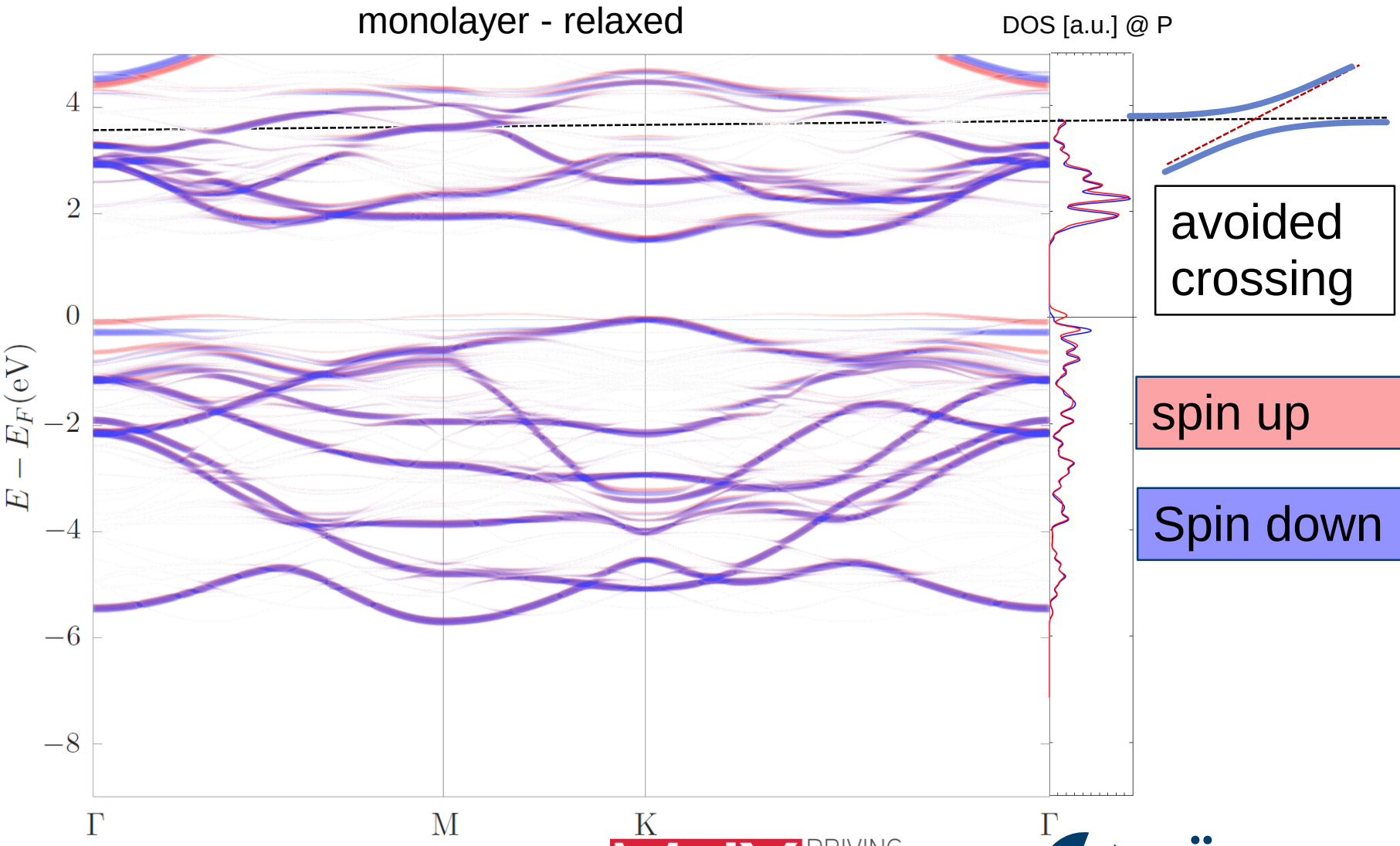
Spectral weight:

$$w_n(\mathbf{k}) = \sum_{\tilde{\mathbf{G}}(\mathbf{k})} \sum_{\mathbf{G}'} C^*_{n,\mathbf{K}(\mathbf{k})}(\tilde{\mathbf{G}}(\mathbf{k})) \cdot C_{n,\mathbf{K}(\mathbf{k})}(\mathbf{G}') \cdot S_{\mathbf{K}(\mathbf{k}),\tilde{\mathbf{G}}(\mathbf{k}),\mathbf{G}'}$$

Test case - Si bulk



UNFOLDED BANDSTRUCTURE $MoSe_2 + P$



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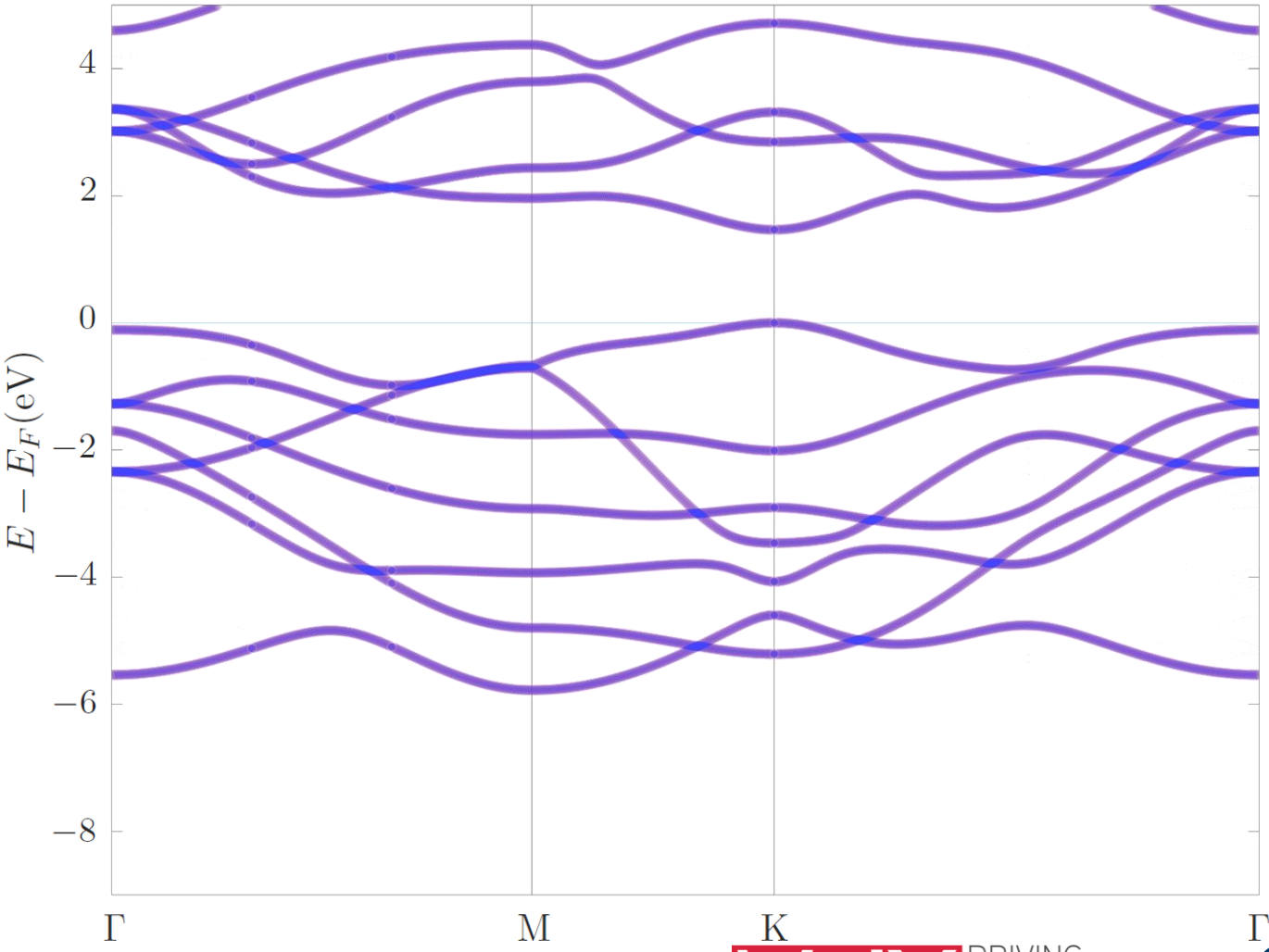
UNFOLDED BANDSTRUCTURE $MoSe_2$

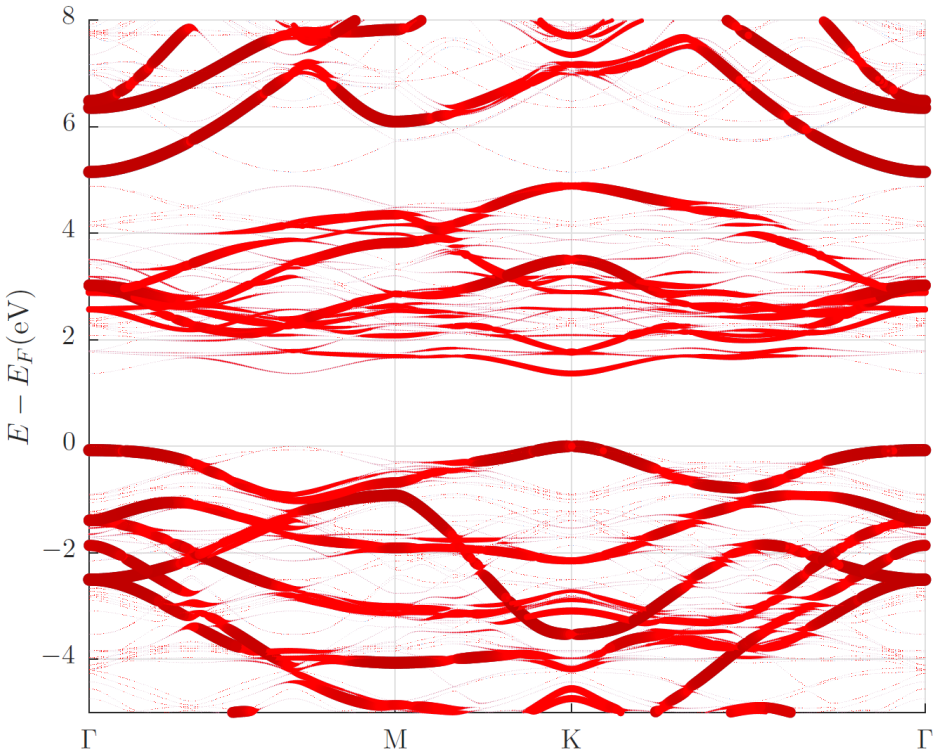
monolayer

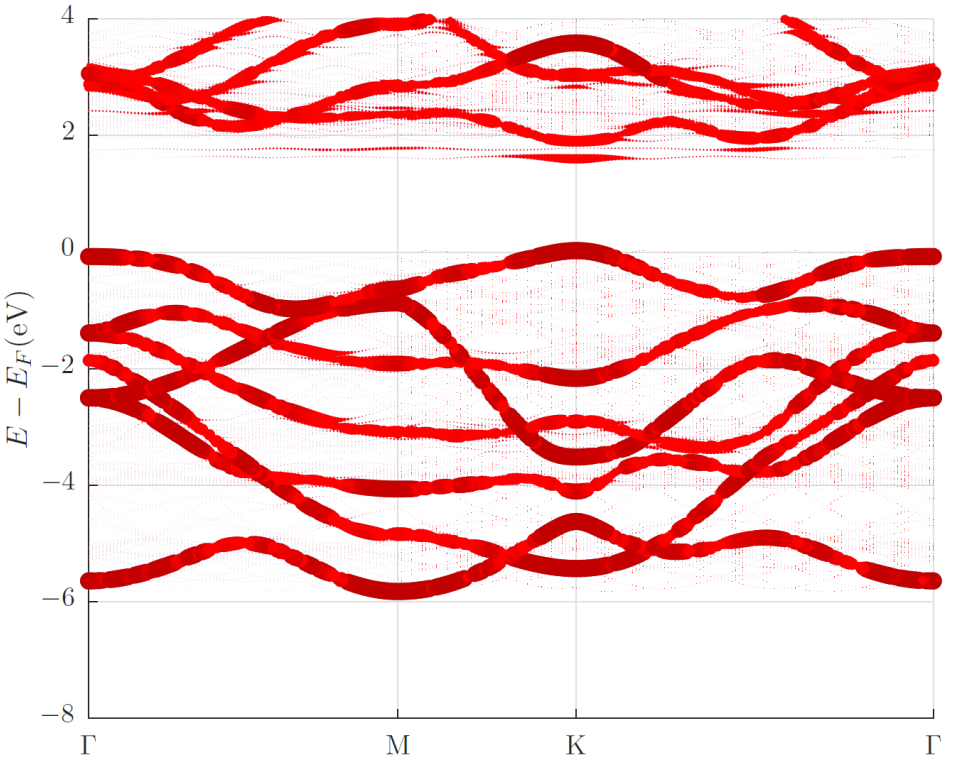


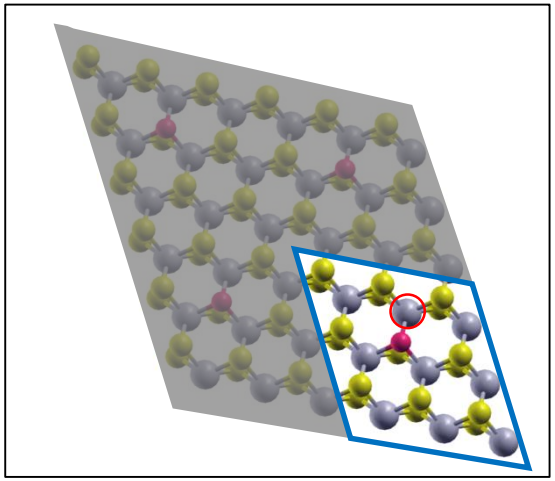
spin up

Spin down

3X3 VS 5X5 - MoS_2 + Cr DEFECT SYSTEM







MAX DRIVING THE EXASCALE TRANSITION

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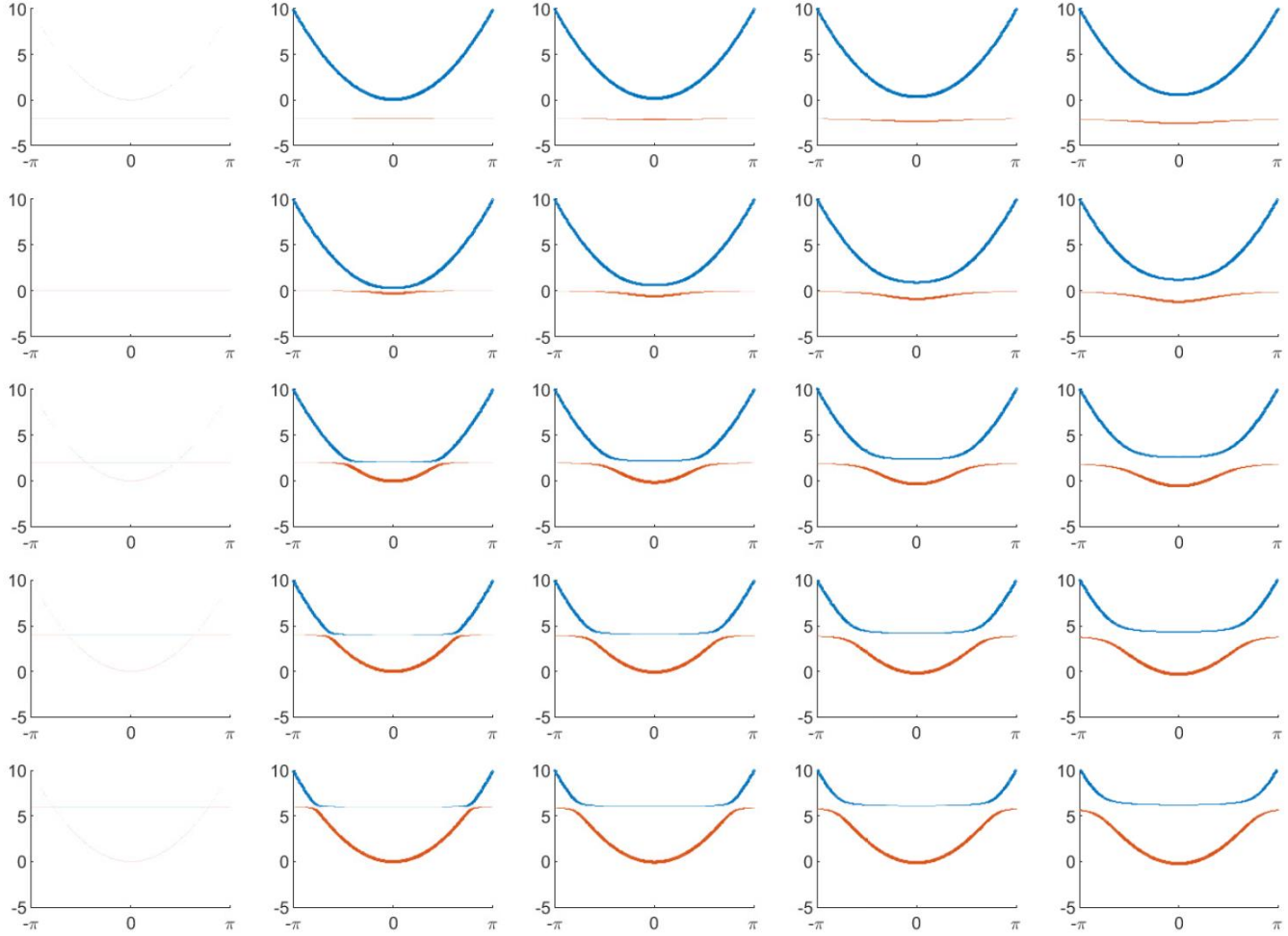
INFLUENCE OF COUPLING AND DEFECT LEVEL ENERGIES



MAX DRIVING THE EXASCALE TRANSITION
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IMPLEMENTATION IN FLEUR

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="0" tworkf=".00"/>
      <unfoldingBand unfoldBand="F" supercellX="1" supercellY="1" supercellZ="1"/>
      <plotting iplot="F" score="F" plplot="F"/>
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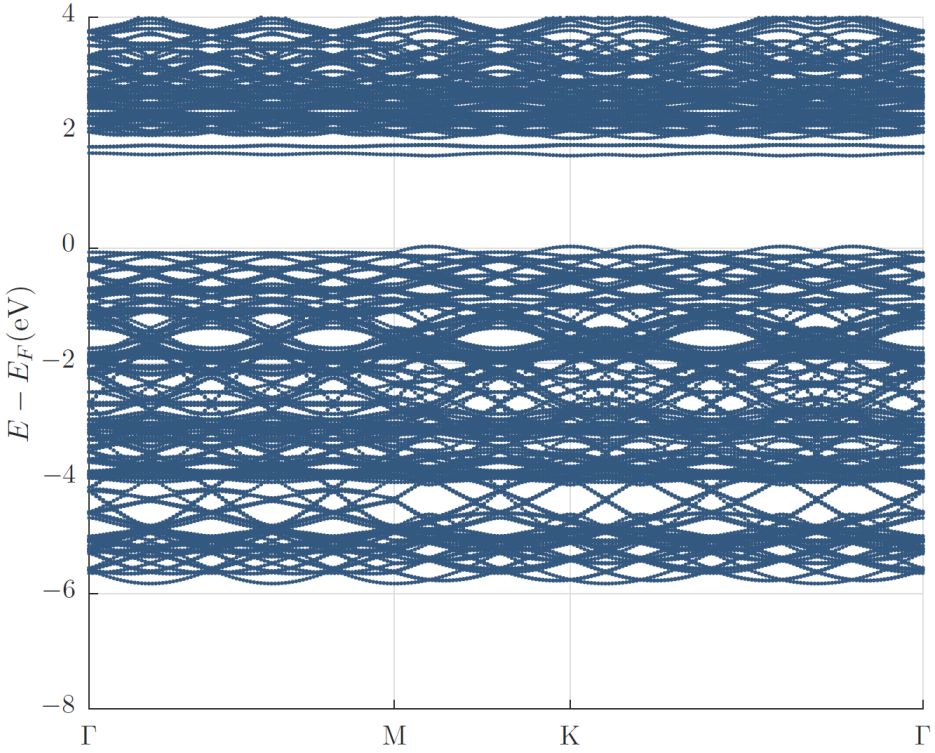
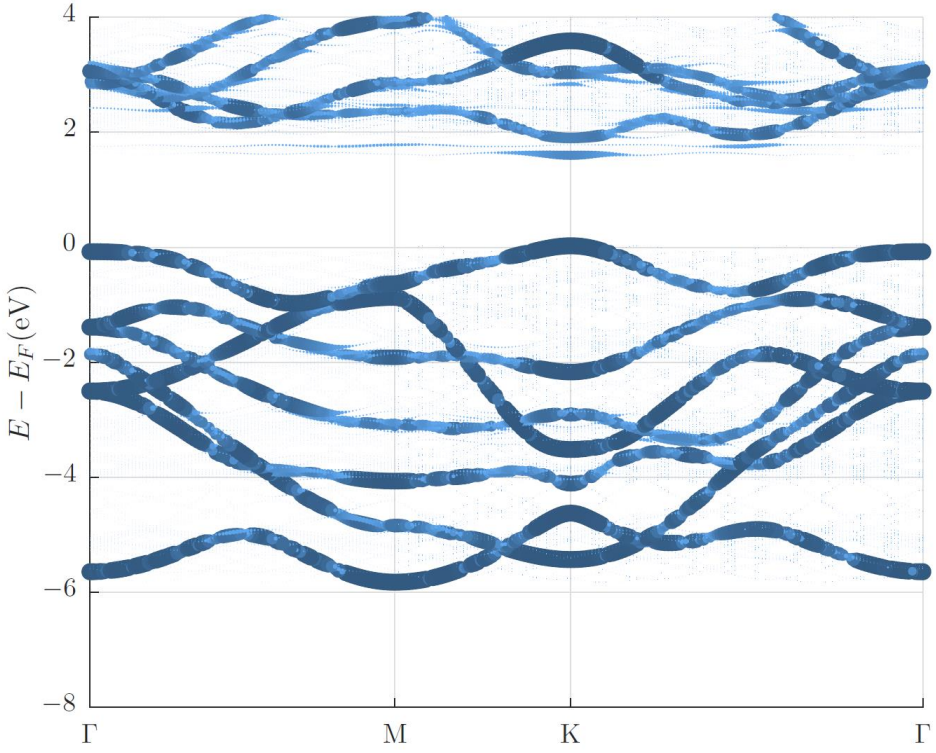
      <specialOutput form66="F" eonly="F" bmt="F"/>
   </output>
```

		Orbital.
unfoldingBand		
	unfoldBand	A boolean switch that defines if unfolding is used and additional weights are written.
	supercellX	The size of the supercell (in units of simple unit cells) (iteger value) in X direction.
	supercellY	The size of the supercell (in units of simple unit cells) (iteger value) in Y direction.
	supercellZ	The size of the supercell (in units of simple unit cells) (iteger value) in Z direction.

SUMMARY

- Unfolding of supercell band structures helps to understand the material properties
- Unfolded band structures represent the defect as a perturbation to the pristine system (like in ARPES experiments)