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CPA approach: On Heavy Carbon Doping of MgB_2

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Outline

- Experimental data
- Calculational methods
- Smeared band structure
- CPA & Supercell calculation results
- VCA results
- σ hole concentration
- Conclusion

Experimental data

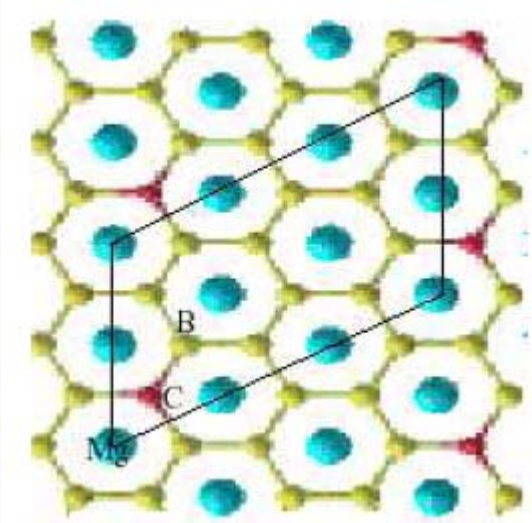
- MgB_2: a real possibility for a high field conductor, due to high parallel and perpendicular critical fields
- $Mg_{1-y}Al_yB_2$:
  1. up to $y=0.10$, T_c decreases smoothly
  2. $0.10<y<0.25$, two phase behavior (two c parameters)
  3. $y=0.25$, back to single phase with vanishing T_c
- $Mg(B_{1-x}C_x)_2$:
  1. $dT_c / dx = 1K / \%C$
  2. H_{c2} increases strongly with C content. (~33-35 T)
  3. It remains the 2-band gap superconductor for 10±2% C substitution for B.

Calculational Method

LAPW (Wien2K)

P.Blaha et al., Comput. Phys. Commun. 59, 399 (1990)

- VCA (10% C doping)
- 2x3 Supercell method: ordered impurity calculation



$$6\times[Mg(B_{1-x}C_x)_2], x=1/12$$

FPLO

K. Koepernik and H. Eschrig, PRB 59, 1743 (1999)

http://www.ifw-dresden.de/agtheo/FPLO/

- Coherent Potential Approximation (CPA): disordered (randomly substituted) alloy calculations

K. Koepernik, B. Velicky, R. Hayn, and H. Eschrig, PRB 55, 5717 (1997)

CPA detail

- Goal

1) determine the filling of the σ band hole states
2) obtain the broadening (and potentially splitting) of bands

- Doping level: $\mathrm{Mg}\left(\mathrm{B}_{1-x}\mathrm{C}_{x}\right)_2$

x	Goal
0.0001	"perfect crystal" reference for evaluation of the numerical algorithms in CPA
0.0833	to compare with x=1/12 supercell calculation
0.10 & 0.20	Representative of the system toward the achievable upper range

- k-mesh: 45x45x10 (1152 irreducible k-point)
- Valence orbitals: 2s2p3s3p3d (Mg), 2s2p3d (B&C)

Smeared band structure (Bloch spectral density)

- For ordered single particle spectra,

$$A_k^{bl}(\omega) = \sum_n \delta(\omega - \varepsilon_{kn})$$

$$\begin{pmatrix} if\ \omega = \varepsilon_{kn}, & \text{black dot} \\ otherwise, & \text{white} \end{pmatrix} \Rightarrow \text{usual band struture}$$

- In disorder case,

$$A_k^{bl}(\omega) = Tr\left(S(k)\Gamma(k,\omega)\right)$$

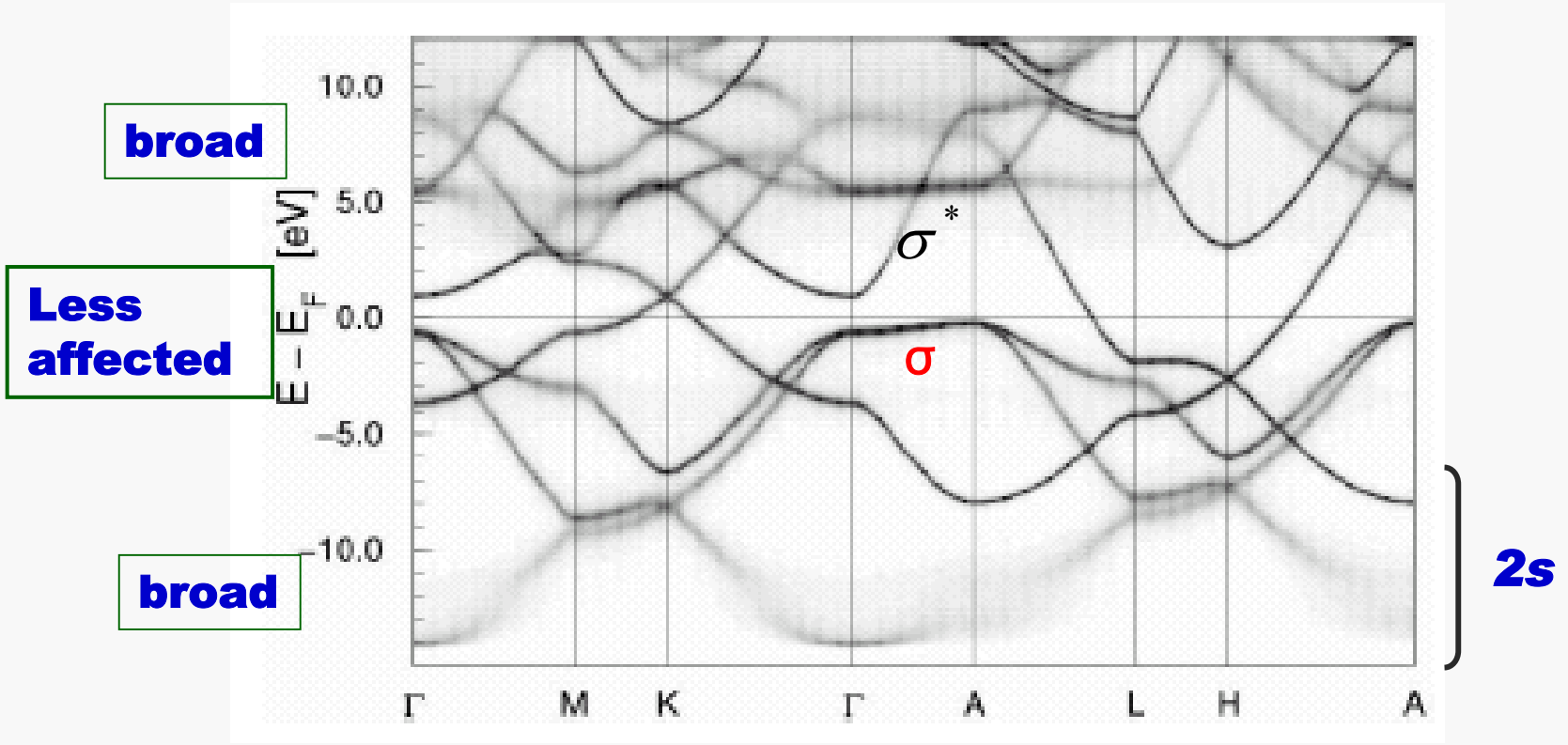
where S(k): overlap matrix

Γ(k,ω): nonstochastic nonlocal coherent Green function

∴ large A : dense darkness
small A: light
intermediate region: continuous gray gradients

http://biela.ifw-dresden.de/pipermail/fplo-users/

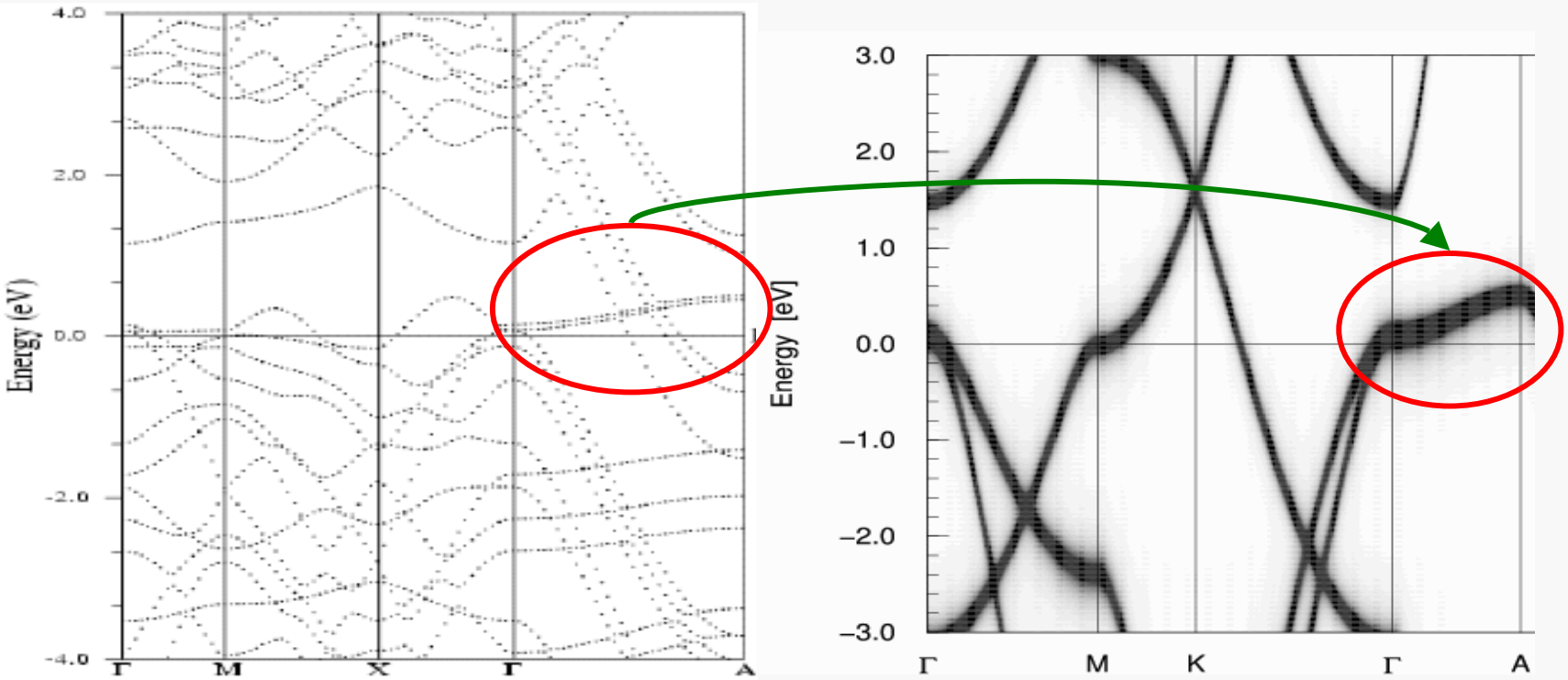
CPA | (x =0.20)



- Largest broadening (*2s*): C *2s* state is noticeably lower in energy leading to increased smearing.
- Near E_F, less affected by the chemical disorder.
- The σ band holes are completely filled.

  ⇒ The two-gap superconductivity disappears.

2x3 Supercell & CPA (*x=1/12*)

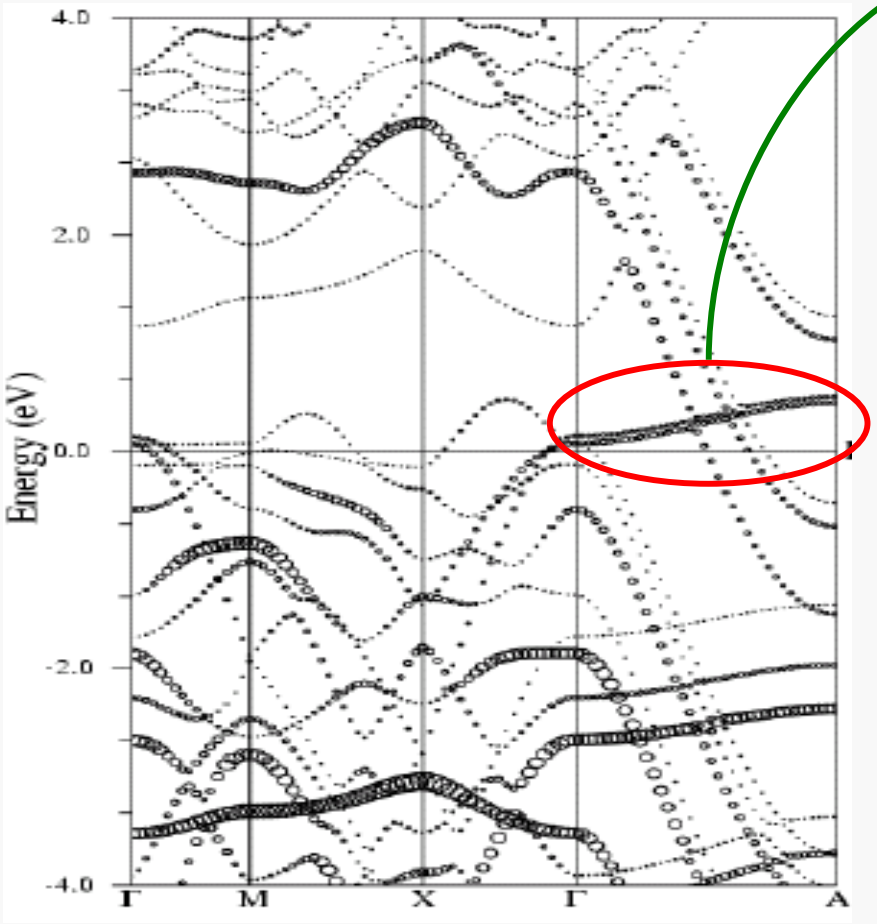


- C substitution

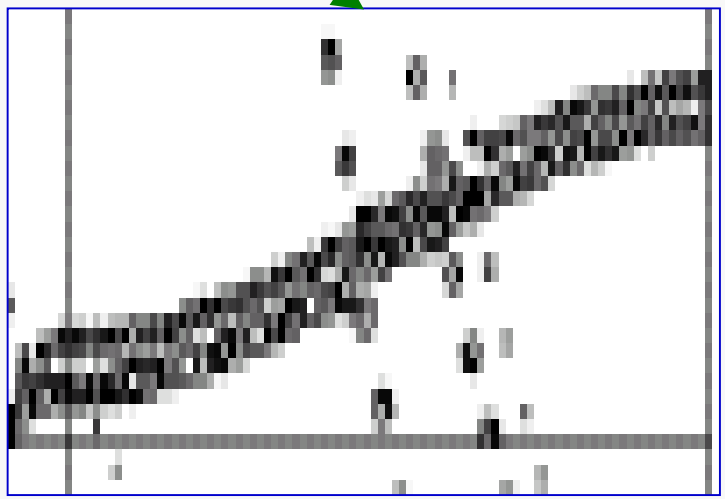
1. a change in the average potential in the B-C layer
2. the breaking of symmetry by C replacement of B in the supercell

- the splitting of the σ bands along Γ-A by 60 meV

continued

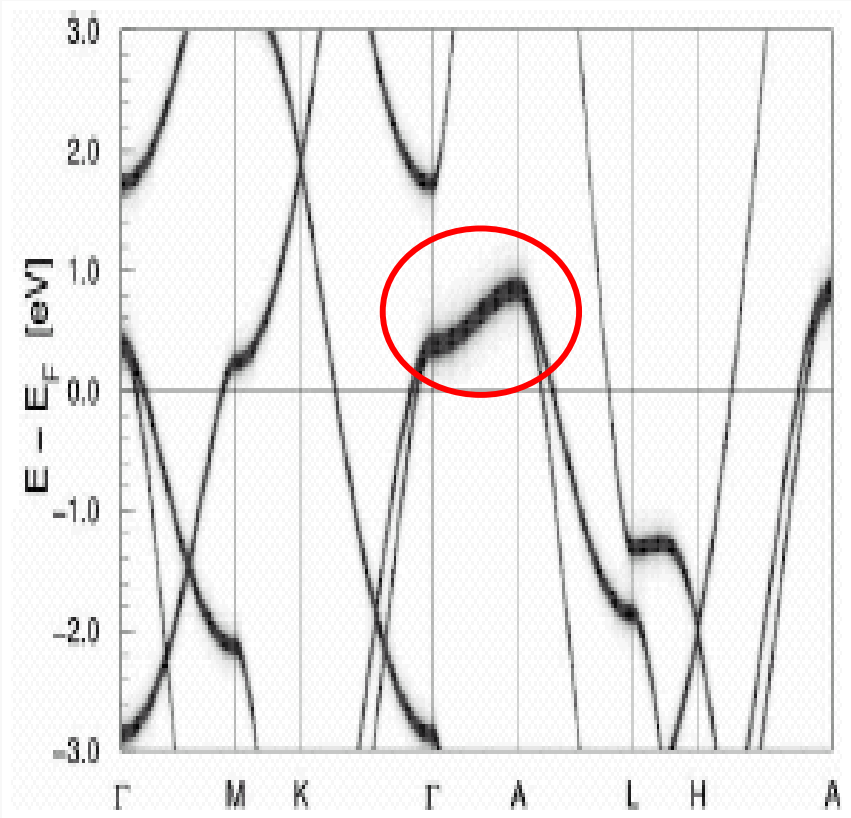


Fatband of the C *2p* character



- Lower band is pulled down due to the stronger potential of the C atom than that of the B atom.
- The splitting provides an energy scale for σ-band broadening $\gamma_0 \approx 7$ meV/%C.

CPAll (x=*0.0001*)



- Since the numerical algorithms cannot reproduce the δ-function bands for $x \to 0$, it is included as a reference for the algorithmic contribution to the width.

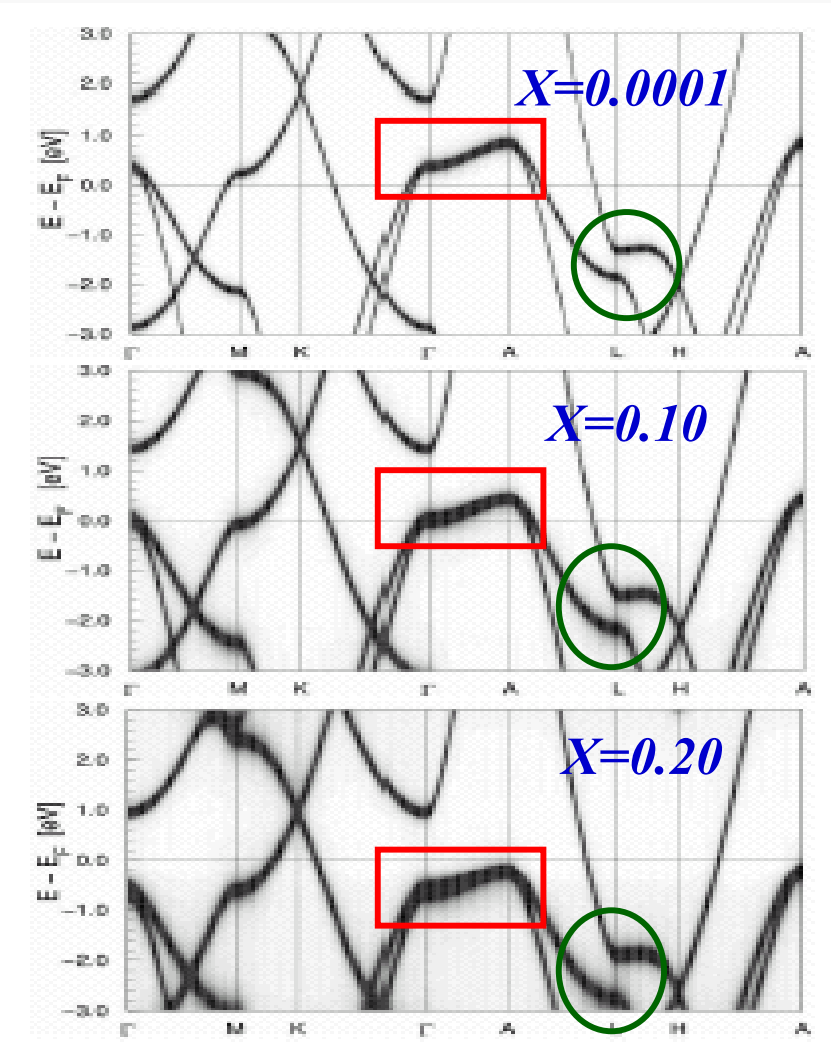
- Width:

  algorithmic contribution

  + disorder effect

  + (order effect)

CPA III (Width of σ band)



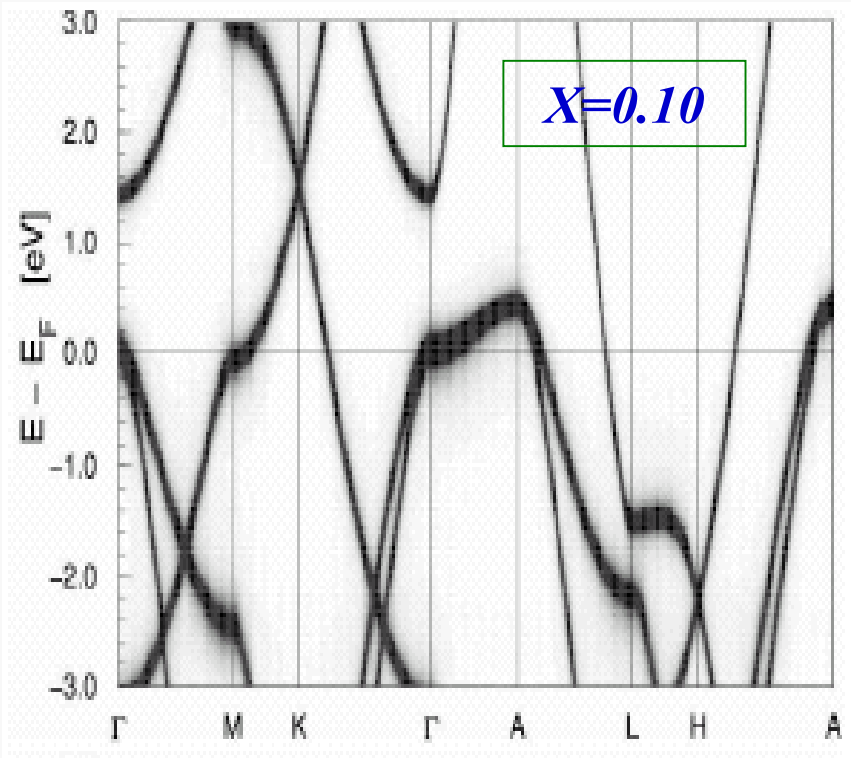
- δE_F = -0.4 eV for $x=0.10$
  -1.0 eV for $x=0.20$

- The band shift is not entirely rigid.

← The two valence bands at the L point split apart and broaden with increasing C.

- averaged γ ≈ 0.21 eV
  - 0.06 eV from the B/C on-site energy difference
  - 0.15 eV from disorder itself

CPA IV (mean free path)

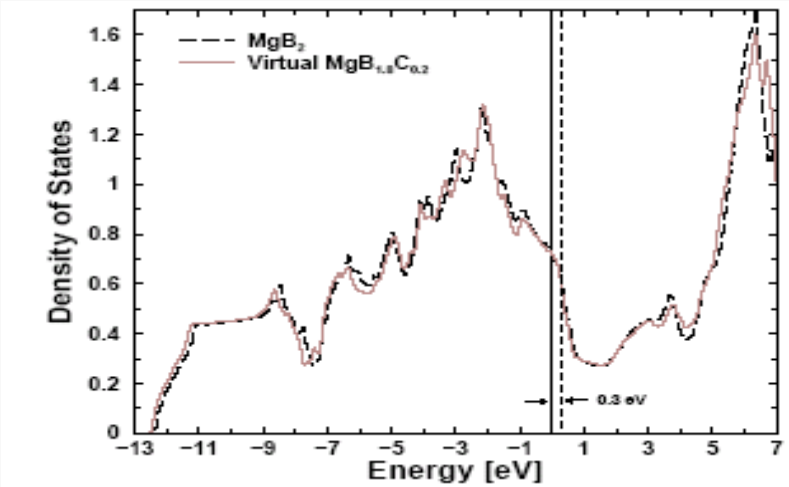


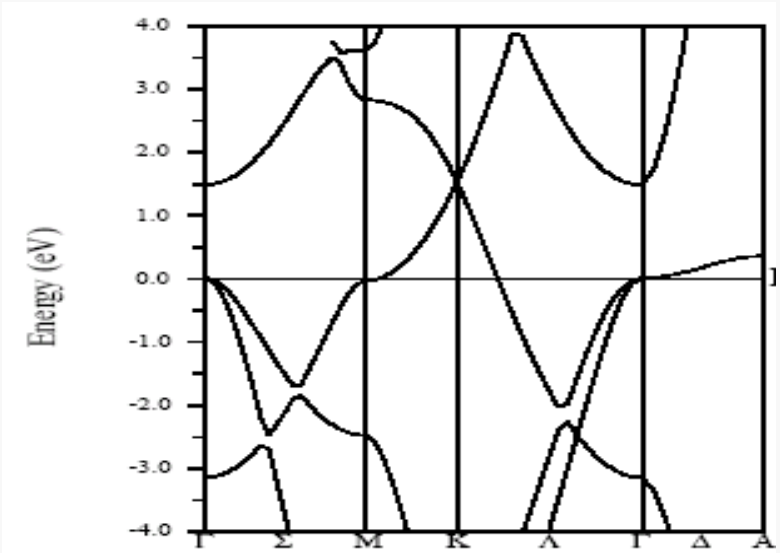
- The width corresponds to a width in wavevector given by $\gamma = v_F \delta k$.

  $\therefore\ l_F = 2\pi v_F / \gamma$
- At *x=0.10*, l_F may vary considerably over the FS due to the anisotropy of the v_F.
- At Γ, the cylinder radius shrunk to a point and the very small z-component of v_F.

⇒ a very small l_F in the z-direction of the order of the layer spacing c.

VCA (*x=0.10*)





- 1% increase in the occupied bandwidth
- The raising of E_F by 0.3 eV
- The cylindrical FS radii of the σ bands at Γ vanish.

⇒ corresponding to a topological transition

σ hole concentration

	No. of holes (holes/cell)
MgB_2	0.11
8.33% doping $Mg_6B_{11}C$ supercell	0.070
10% doping $MgB_{1.8}C_{0.2}$ Virtual crystal	0.0463
8.33% doping $MgB_{1.833}C_{0.167}$ extrapolation	0.057

- Both the σ band FS are still intact, consistent with the 2-band superconductivity with substantial T_c as seen in experiments.
- VCA is not reliable for substitutional C.

⇒ C cannot be thought simply as "B + e^-".

Conclusion

- The σ band holes begin to disappear rapidly for $x > 0.10$.
- CPA reproduces the σ filling well, while VCA overestimates it.
- The largest disorder occurs in the *2s* region in the lower valence band.
- As the σ band fills, there will be very strong deviation from "business as usual" in the coupled el.-ph. system.

  (The strength of coupling of bond-stretching modes with $Q < 2k_F$ continues to increase.)
- $Mg(B_{1-x}C_x)_2$ as well as $Mg_{1-x}Al_xB_2$ is a good system to study the evolution of the unusual el.-ph. Coupling character.