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CPA approach: On Heavy Carbon
Doping of MgB₂



UC Davis

Deepa Kasinathan

Kwan-Woo Lee

Warren E. Pickett

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and D.J. Singh**

Outline

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

Experimental data

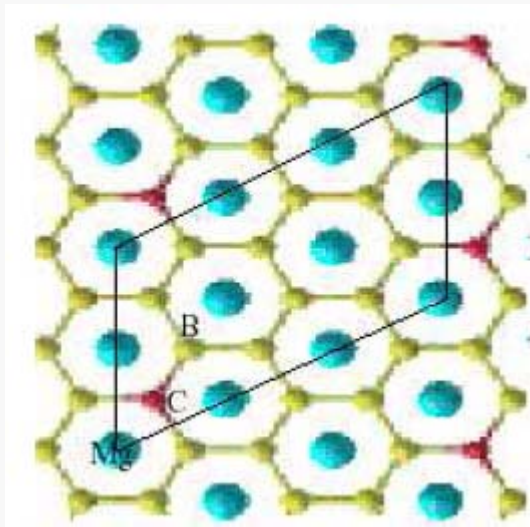
- ◇ **MgB₂**: a real possibility for a high field conductor, due to high parallel and perpendicular critical fields
- ◇ **Mg_{1-y}Al_yB₂**:
 1. up to $y=0.10$, T_c decreases smoothly
 2. $0.10 < y < 0.25$, two phase behavior (two c parameters)
 3. $y=0.25$, back to single phase with vanishing T_c
- ◇ **Mg(B_{1-x}C_x)₂**:
 1. $dT_c / dx = 1K / \% C$
 2. H_{c2} increases strongly with C content. ($\sim 33-35$ T)
 3. It remains the 2-band gap superconductor for $10 \pm 2\%$ C substitution for B.

Computational Method

LAPW (Wien2K)

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

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



FPLO

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

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

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

K. Koepnik, 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: $\text{Mg}(\text{B}_{1-x}\text{C}_x)_2$

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)

Smearred band structure (Bloch spectral density)

- ◇ For ordered single particle spectra,

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

$\left(\begin{array}{l} \text{if } \omega = \varepsilon_{kn}, \text{ black dot} \\ \text{otherwise, white} \end{array} \right) \Rightarrow \text{usual band structure}$

- ◇ In disorder case,

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

where $S(k)$: overlap matrix

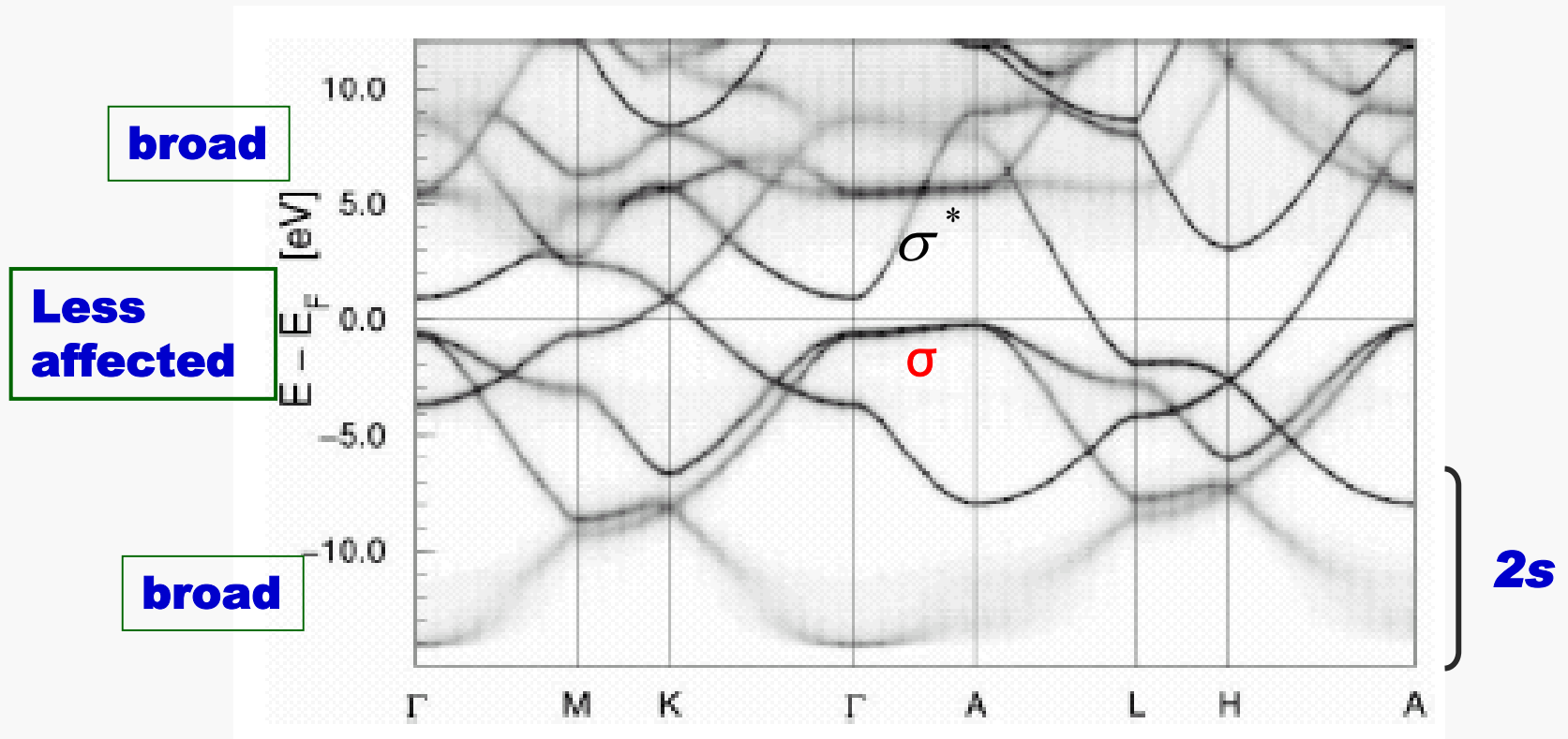
$\Gamma(k, \omega)$: nonstochastic nonlocal coherent Green function

∴ large A : dense darkness

small A: light

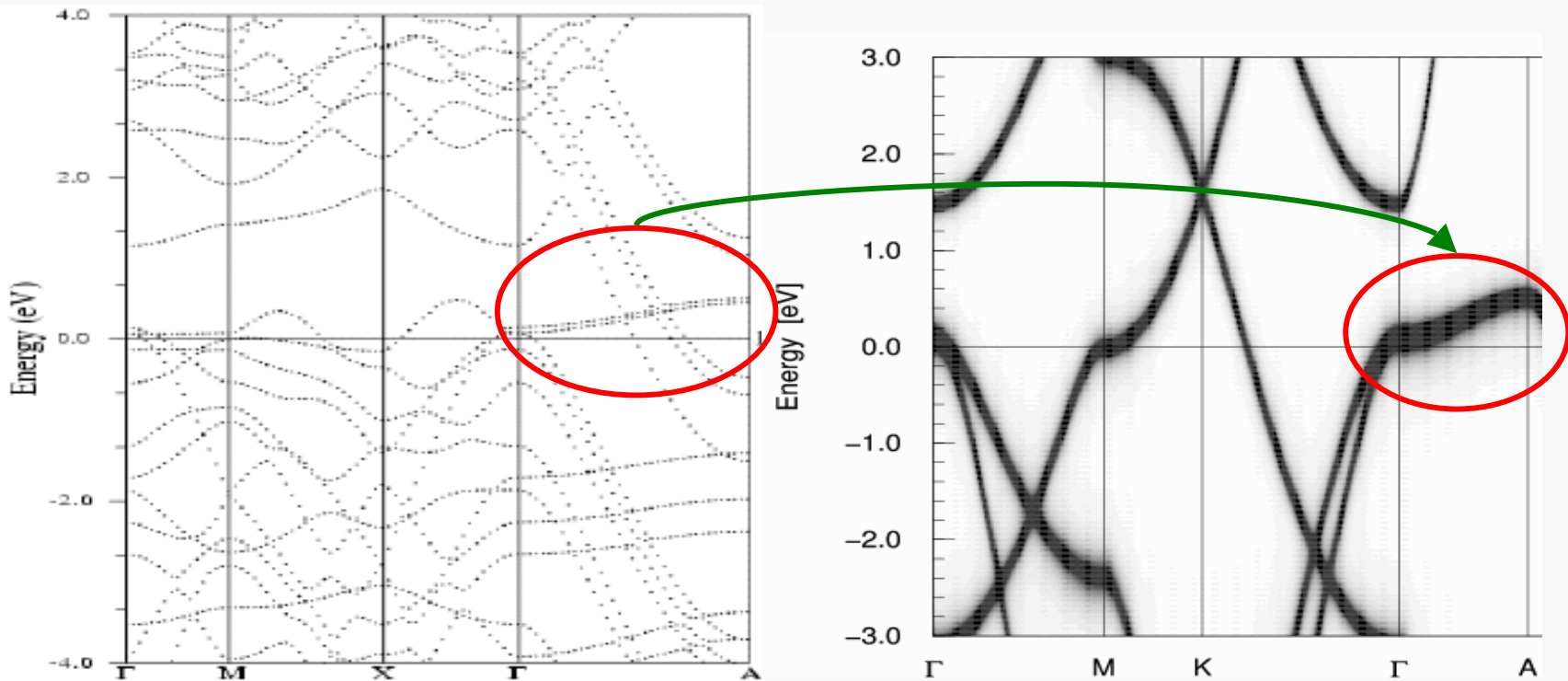
intermediate region: continuous gray gradients

CPA I ($x = 0.20$)



- ◇ 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 ($x=1/12$)

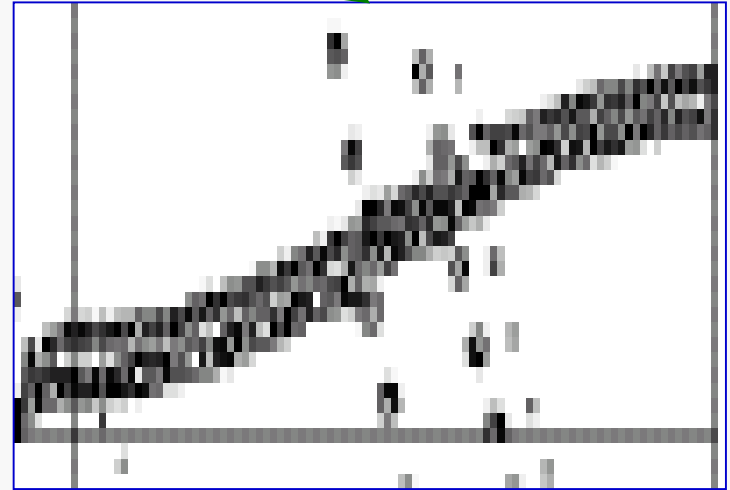
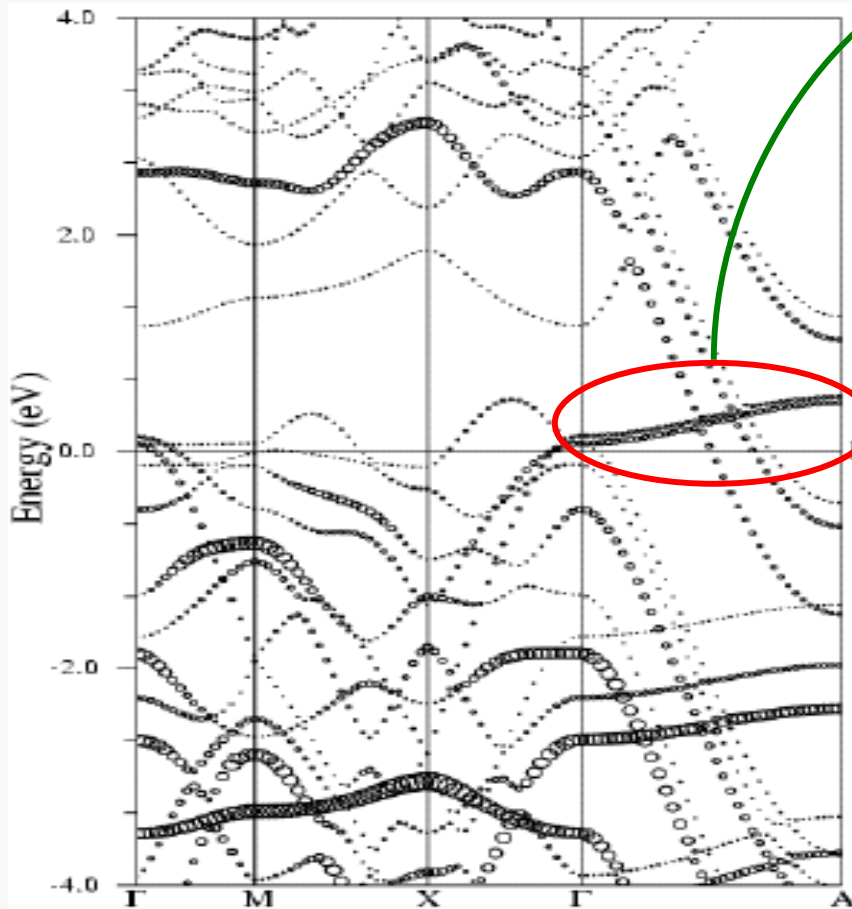


- **C substitution**

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**

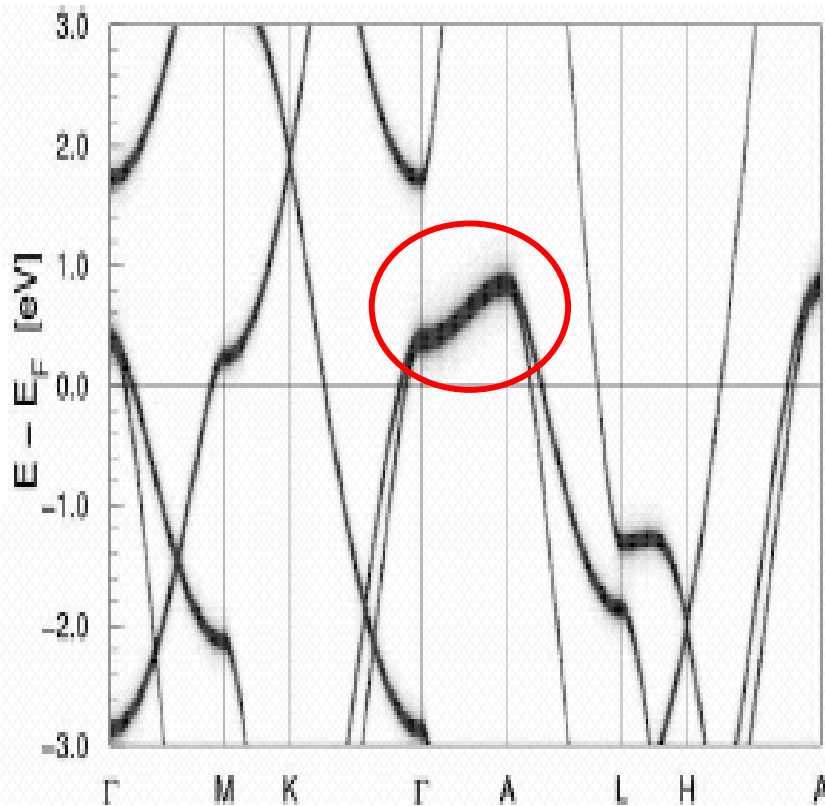
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Fatband of the C $2p$ character

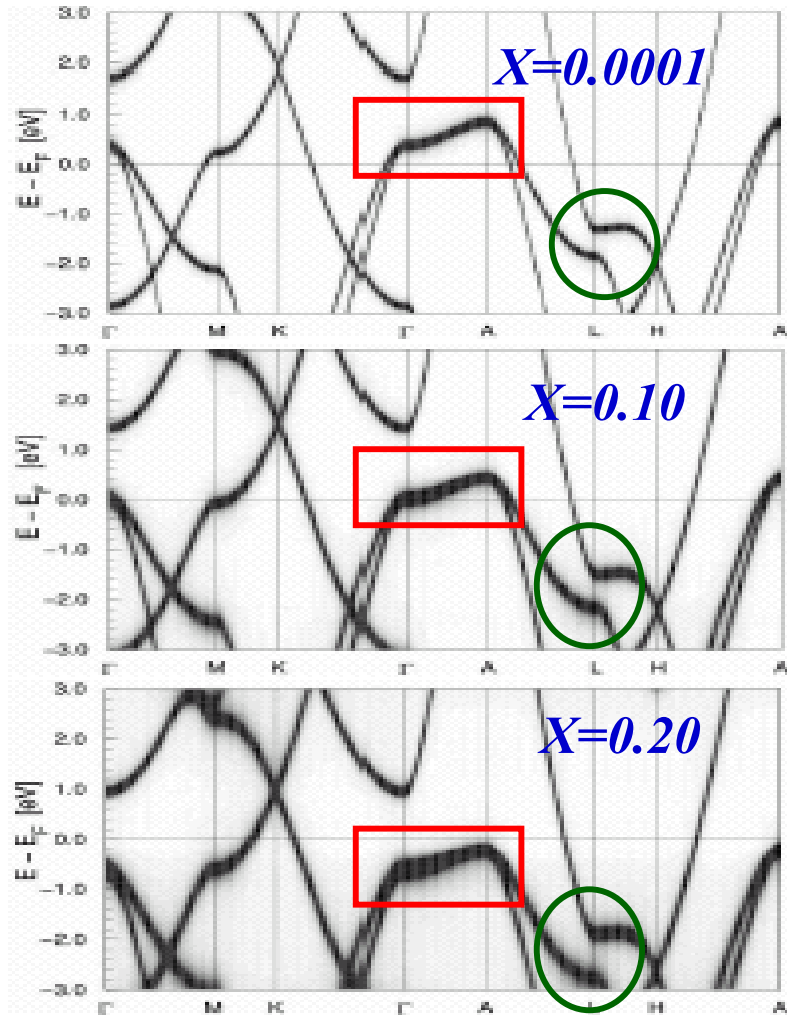
- Lower band is pulled down due to the stronger potential of the C atom than that of the B atom.
- The splitting provides an energy scale for σ -band broadening $\gamma_0 \approx 7 \text{ meV}/\%C$.

CPAlI ($x=0.0001$)



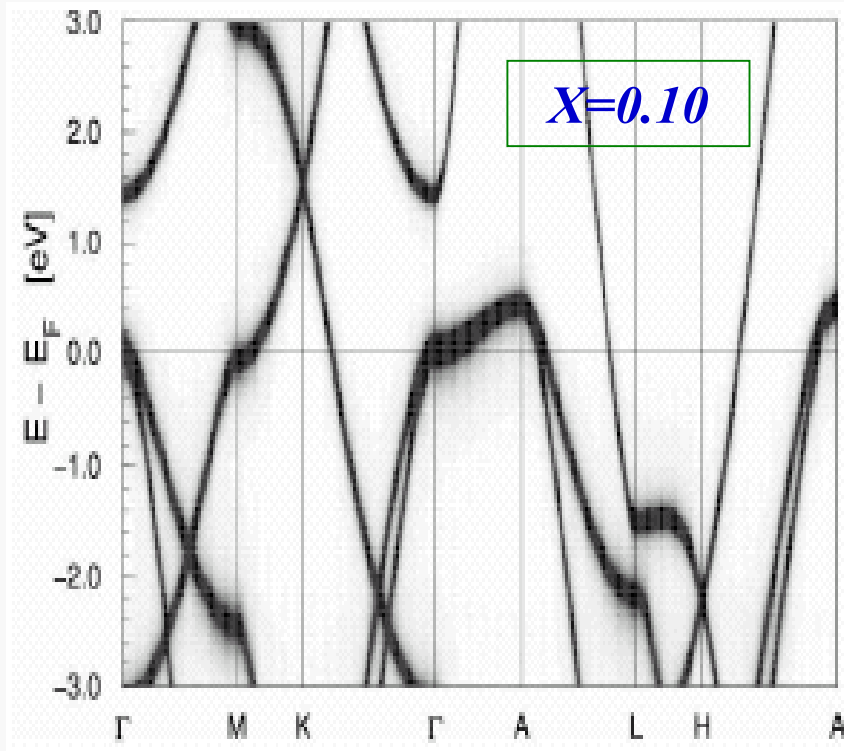
- ◇ Since the numerical algorithms cannot reproduce the δ -function bands for $x \rightarrow 0$, it is included as a reference for the algorithmic contribution to the width.
- ◇ **Width:**
 - algorithmic contribution
 - + disorder effect
 - + (order effect)

CPA III (Width of σ band)



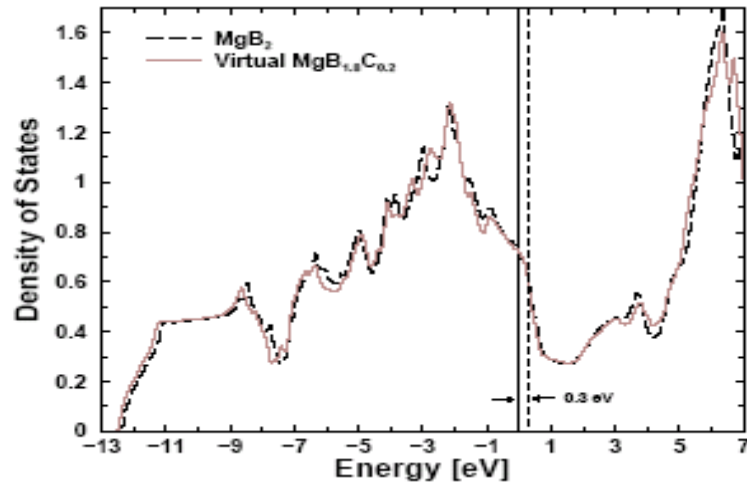
- ◇ $\delta E_F = -0.4$ eV for $x=0.10$
-1.0 eV for $x=0.20$
- ◇ The band shift is not entirely rigid.
 - ← The two valence bands at the L point split apart and broaden with increasing C.
- ◇ averaged $\gamma \approx 0.21$ eV
 - 0.06 eV from the B/C on-site energy difference
 - 0.15 eV from disorder 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 .
 \Rightarrow a very small l_F in the z-direction of the order of the layer spacing c .

VCA ($x=0.10$)

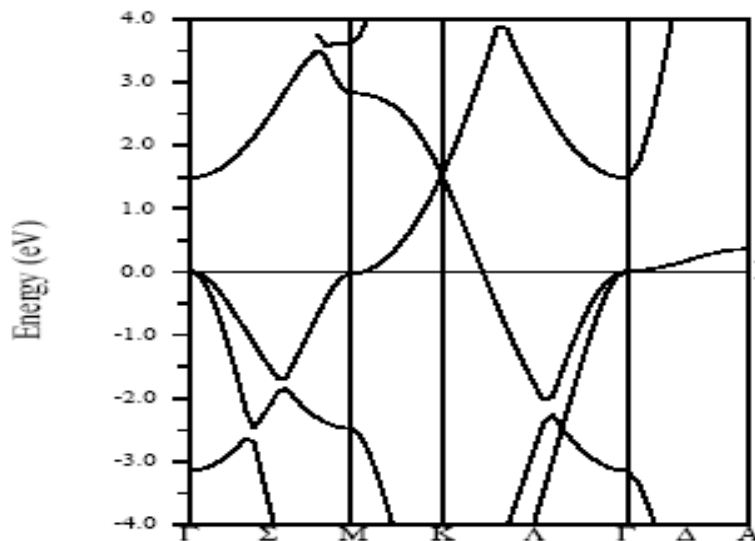


◇ 1% increase in the occupied bandwidth

◇ 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 $\text{Mg}_6\text{B}_{11}\text{C}$ supercell	0.070
10% doping $\text{MgB}_{1.8}\text{C}_{0.2}$ Virtual crystal	0.0463
8.33% doping $\text{MgB}_{1.833}\text{C}_{0.167}$ 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.)
- ◇ $\text{Mg}(\text{B}_{1-x}\text{C}_x)_2$ as well as $\text{Mg}_{1-x}\text{Al}_x\text{B}_2$ is a good system to study the evolution of the unusual el.-ph. Coupling character.