Ordered Supercell & Virtual Crystal approximation : On Heavy Carbon Doping of MgB_2

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Experimental Facts :

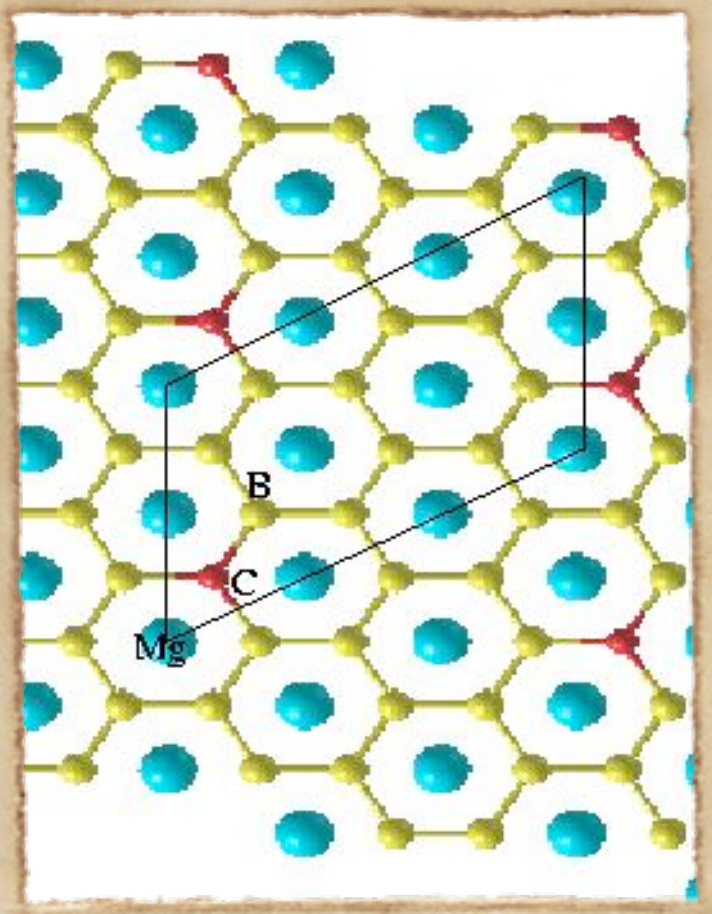
- MgB_2 - a real possibility for a high field conductor, due to high parallel and perpendicular critical fields
- $Mg_{1-y}Al_yB_2$ ---> upto $y = 0.10$ T_c decreases smoothly ; $0.10 < y < 0.25$ - two phase behavior; $y = 0.25$ - back to single phase with vanishing T
- Carbon doped MgB_2 - highly mixed phase; miscibilty of C really small; $dT_c/dx = 1$ K/%C
- Substituional C doping upto 10% still retains the two-band superconductivity

Calculational Method :

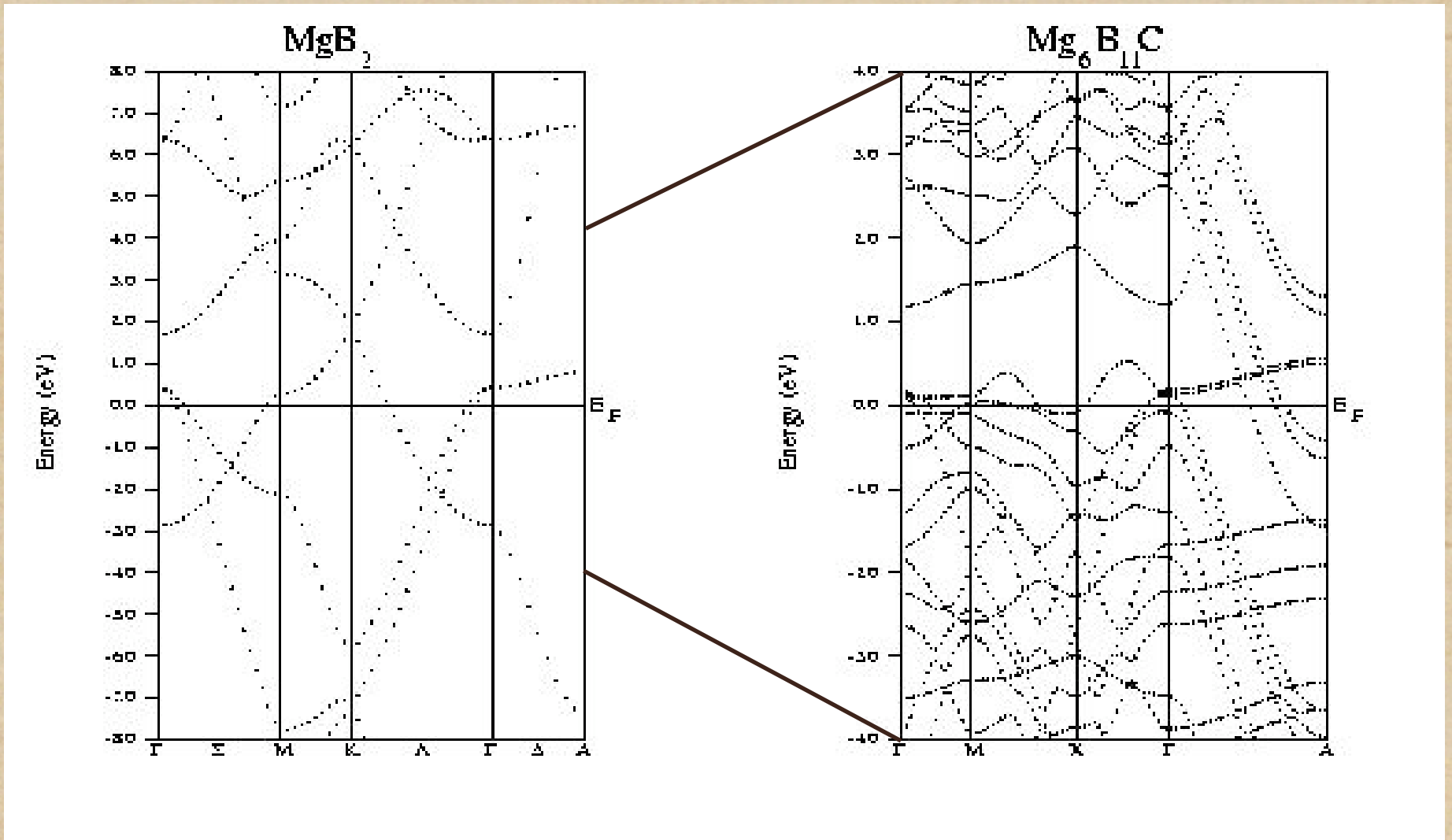
- Full-potential LAPW code WIEN2K
  P.Blaha, K.Schwarz, G.K.H.Madsen, D.Kvasnicka, J.Luitz, J.Phys. Chem. Sol. 63, 2201 (2002)
- Exchange-correlation potential approximated using GGA
- RK_{max} = 7.00 (good for s-p electron systems)
- k-mesh : 432 irreducible k points
- Lattice parameters - Avdeev et al. (both supercell and virtual crystal)

Ordered $Mg(B_{1-x}C_x)_2$, $x = 0.0833$

- Maximum separation of C atoms - supercell $Mg_6B_{11}C$
- $B_{11}C$ layer is 2 x3 times that of MgB_2
- a = 9.16 A^0 , b = 6.11A^0 c = 3.525 A^0
- Carbon has 3 first, 5 second & 3 third N.N B atoms

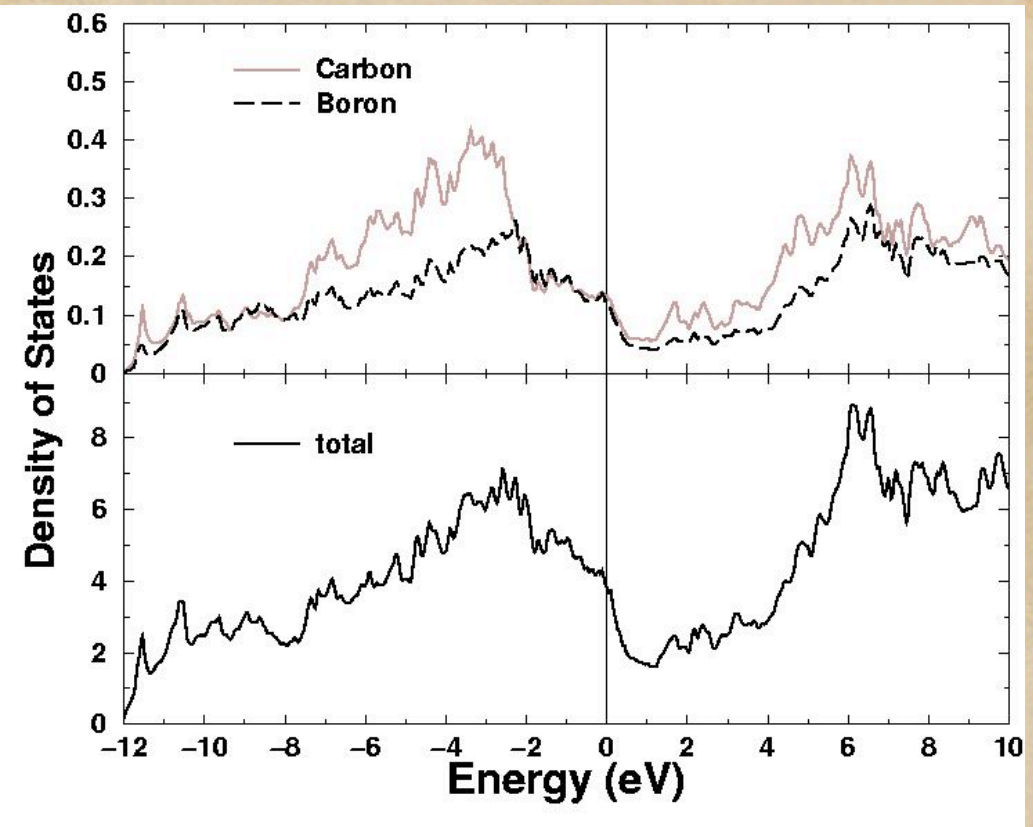


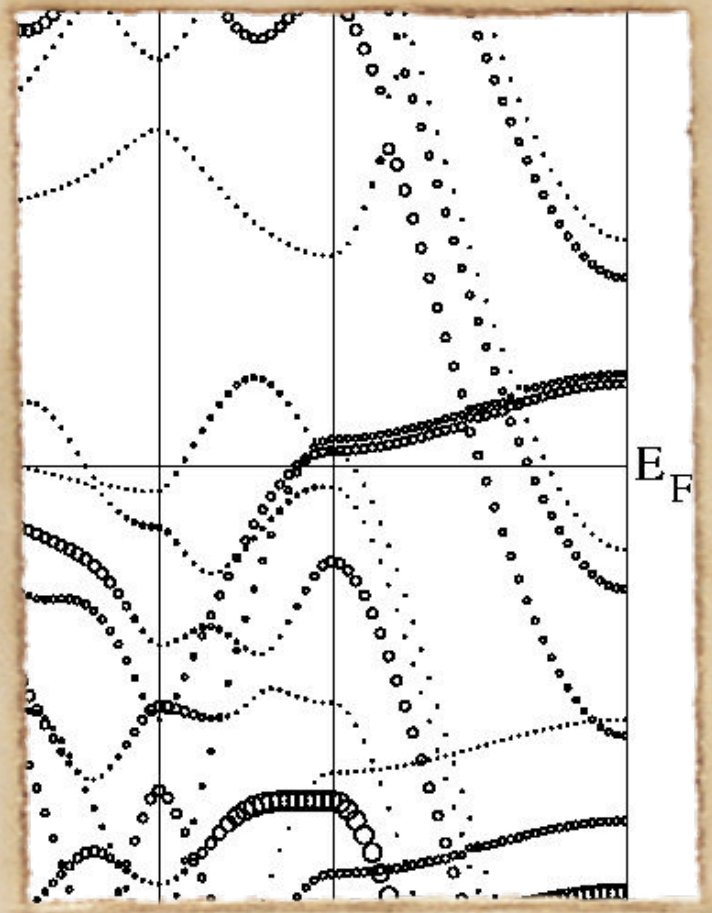
Bandstructure



C doping - Degenerate σ bands split by 60 meV along Γ - A

Projected DOS & Bandstructure



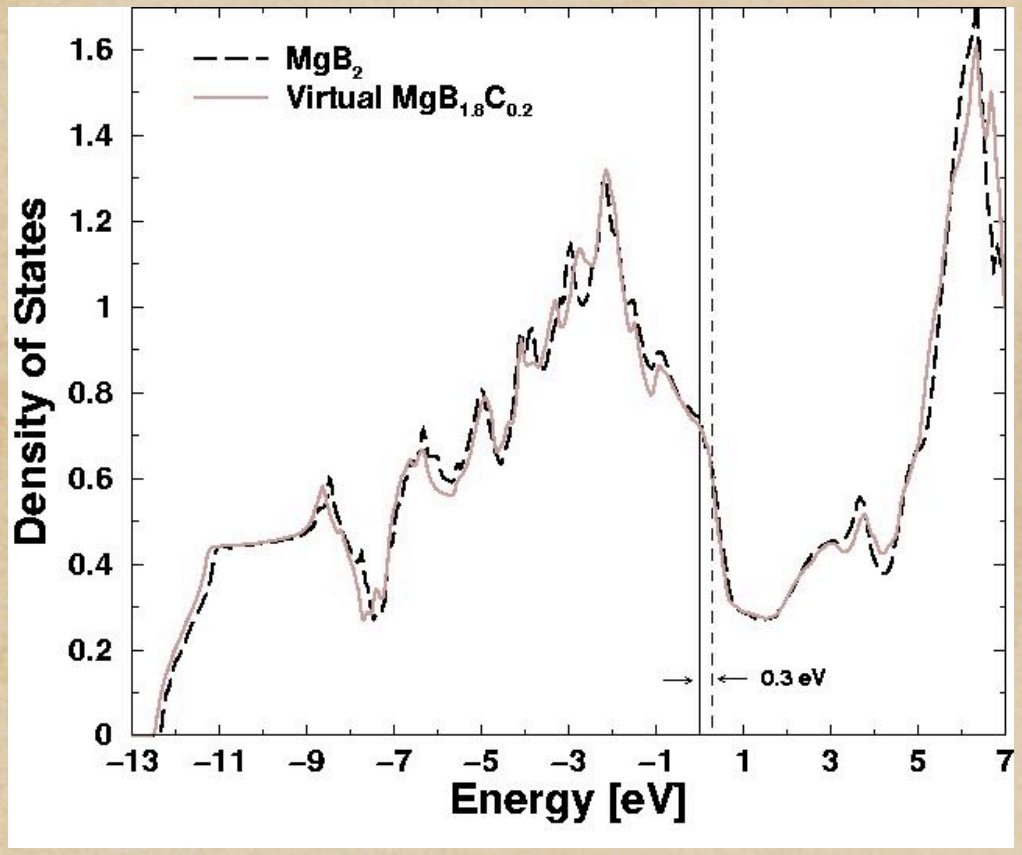


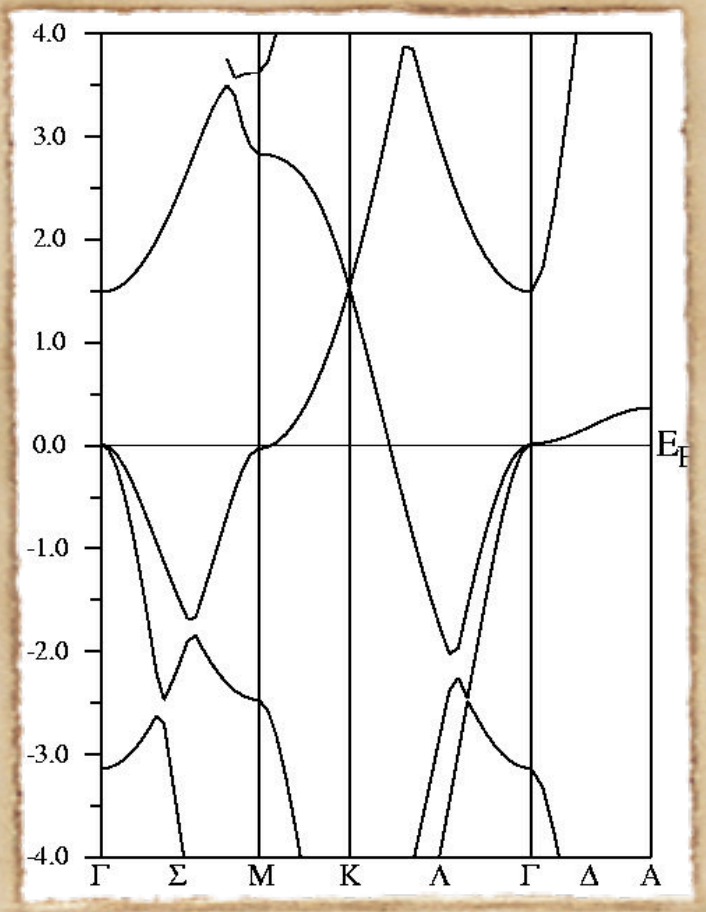
C potential - pulls down the lower split band

Energy scale for σ-band broadening $\Upsilon_o \approx 7$ meV /% C

Charge transfer for $0.095e^-$ to C from the 3 first N.N B's

$Mg(B_{0.9}C_{0.1})_2$ - 10% doping - VCA





1% increase in occupied bandwidth; Fermi level raised by 0.3eV.
Both cylindrical Fermi surfaces have shrunk to a point at Γ.

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

Fermi surfaces are still intact - consistent with two-band superconductivity and substantial T_c observed in expts.

Virtual Crystal : Carbon = Boron + e^- ! Not very reliable.