Two dimensional features of the electronic structure of the layered diboride dicarbide YB_2C_2 superconductor.

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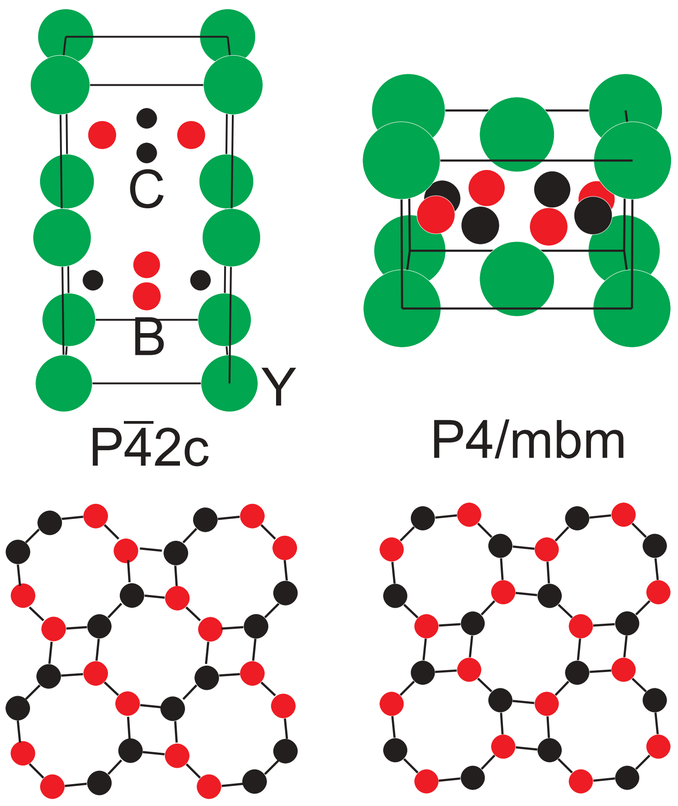
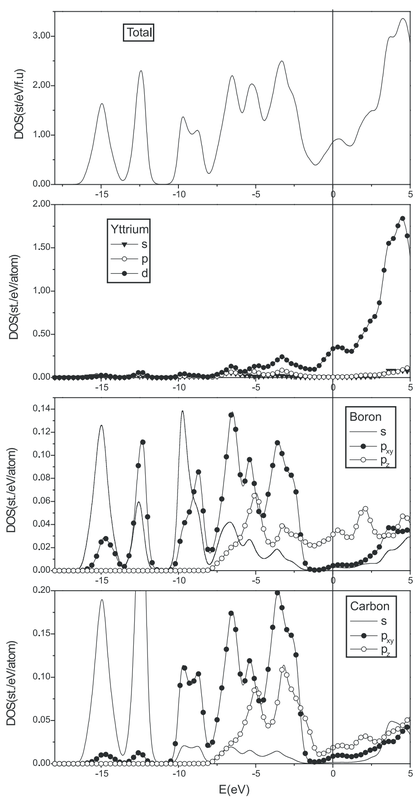
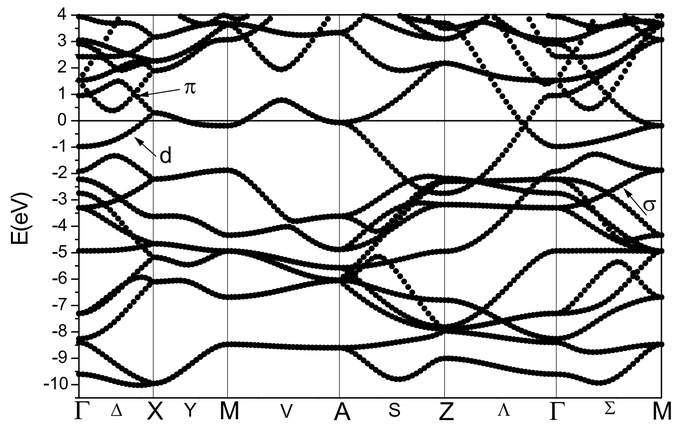
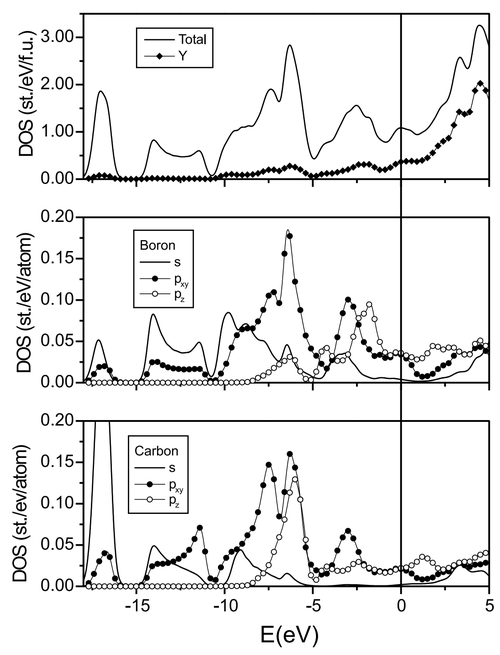
The electronic structure of the layered diboride dicarbide superconductor YB2C2 is calculated using the full potential LAPW method within the framework of ab initio density functional theory. Our results confirm that the crystal structure with P4/mbm symmetry is more stable than the originally claimed P42c structure, which is in accordance with recent interpretations of the diffraction patterns of other related compounds of LaB2C2-type. It is found that the metallic conductivity in the stable P4/mbm structure is due to Y d-bands partially hybridized with pz-states from the B-C planes. Thus the structure of the conduction bands differs from those found in MgB2. However, a large portion of the Fermi surface of YB2C2 exhibits distinctive two-dimensional features, which can make this compound interesting for experimental studies on superconductivity connected to effects of strong electronic structure anisotropy The interesting finding is also that unstable P42c structure have in contrast open conduction sigma-band similar to those in MgB2.

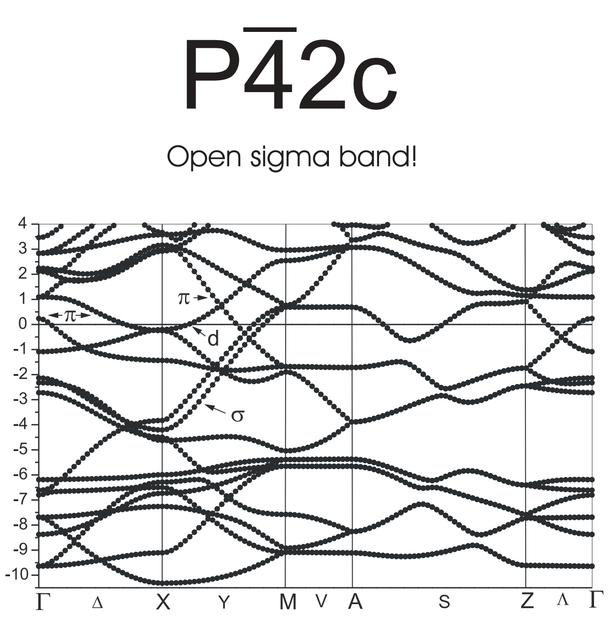


The mesh of 1728 *k*-points in the full Brillouin zone was used followed by an additional iteration with 8000 *k*-points to produce the DOS, band structure and Fermi surface plots. Potential and charge density where expanded up to $l = 8$ 1400 APW basis functions for each *k*-point. For the valence states scalar relativistic corrections are included, while core states are treated fully relativistically.

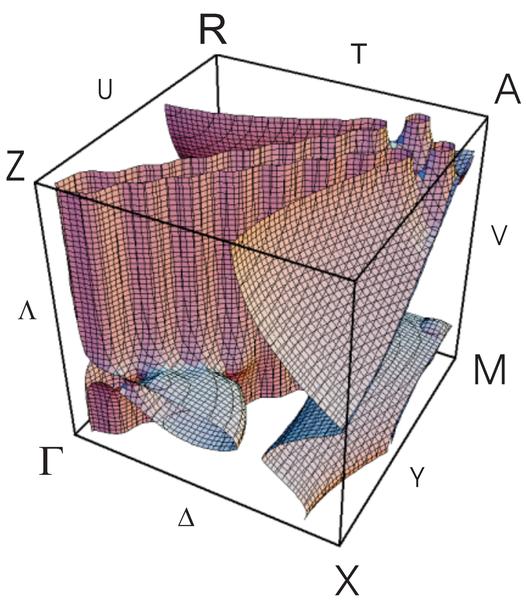


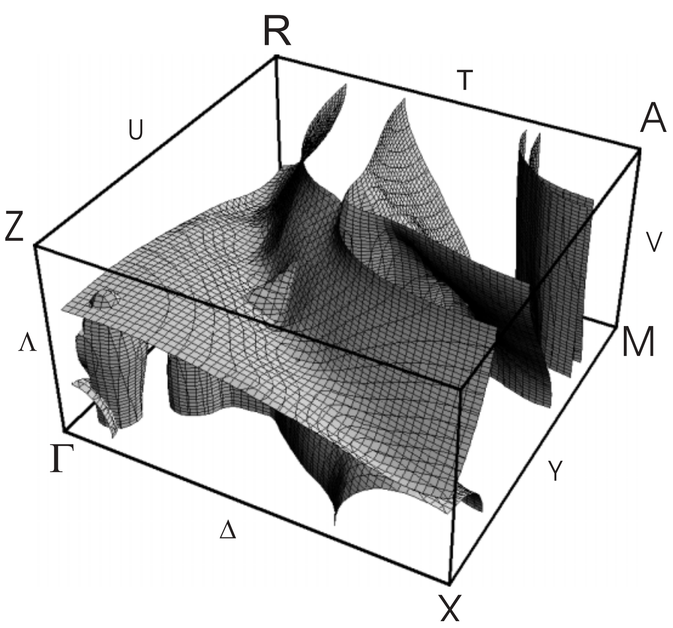






Some sheets of the Fermi surface have pronounce 2D features combined with 3D behaviour in another parts.





The Fermi surface of the p42c structure has two cilindrical sheets around MA direction similar to those of MgB2.

Calculated charge density distribution in BC plane:
π–electrons delocalization in 4-member rings.