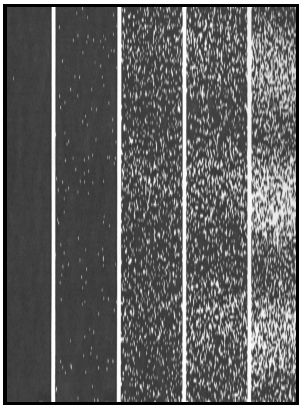
Augmented plane wave method - a guide to performing electronic structure calculations

W.A. Benjamin - Formats and Editions of Augmented plane wave method : a guide to performing electronic structure calculations [ne-x.uni.rf.gd]



Description: -
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Atomic theory.Augmented plane wave method - a guide to performing electronic structure calculations
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Frontiers in physicsAugmented plane wave method - a guide to performing electronic structure calculations
Notes: Includes bibliographies.
This edition was published in 1967

Tags: #Phys. #Rev. #B #82, #155121 #(2010)

A Projector Augmented Wave (PAW) code for electronic structure calculations, Part II: pwpaw for periodic solids in a plane wave basis

We have studied the physical properties first by carrying out optimization using different methods.

A Projector Augmented Wave (PAW) code for electronic structure calculations, Part II: pwpaw for periodic solids in a plane wave basis

Moreover, spin polarized density of states for Cu doped composites has also been calculated to confirm the large exchange splitting of Cu-3d states.

First principles study on electronic structure of β

The calculation performed by the LDA with mBJ exchange-correlation potential confirms the indirect electronic transition located in the Γ-Z direction and gives a bandgap energy closer to the experimental value compared with GGA and GGA-mBJ results.

Augmented plane wave method; a guide to performing electronic structure calculations (Book, 1967) [ne-x.uni.rf.gd]

Magnetic field orientation dependence of transverse and longitudinal flux line lattice form factors are theoretically studied in uniaxial superconductors with extremely large anisotropy ratio 60 for some field magnitudes. Due to the monochromation of the electron beam and to a spectrometer with an energy resolution of 20 meV, a direct measurement of the narrow bandgap energy, E 0, of about 0.

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The temperature is measured down to 160 mK in the dilution refrigerator. Both heterostructures are indirect band gap semiconductors with gap

values of 0. Besides, the critical temperature T c is about 470 K for the strain-free Zr 2N MXene, indicating that the antiferromagnetic ordering can be robust and maintained at room temperature.

First principles study on electronic structure of β

The hydrostatic pressure effects on the superconductivity were also investigated.

First principles study on electronic structure of β

Besides, the Hall effect, high pressure effect and the band structure were also investigated, which consistently support a phonon-mediated BCS pairing scenario for La 7Ir 3. From the λ ω curves in Fig.

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