Report on calculation of Band structure of Magnesium

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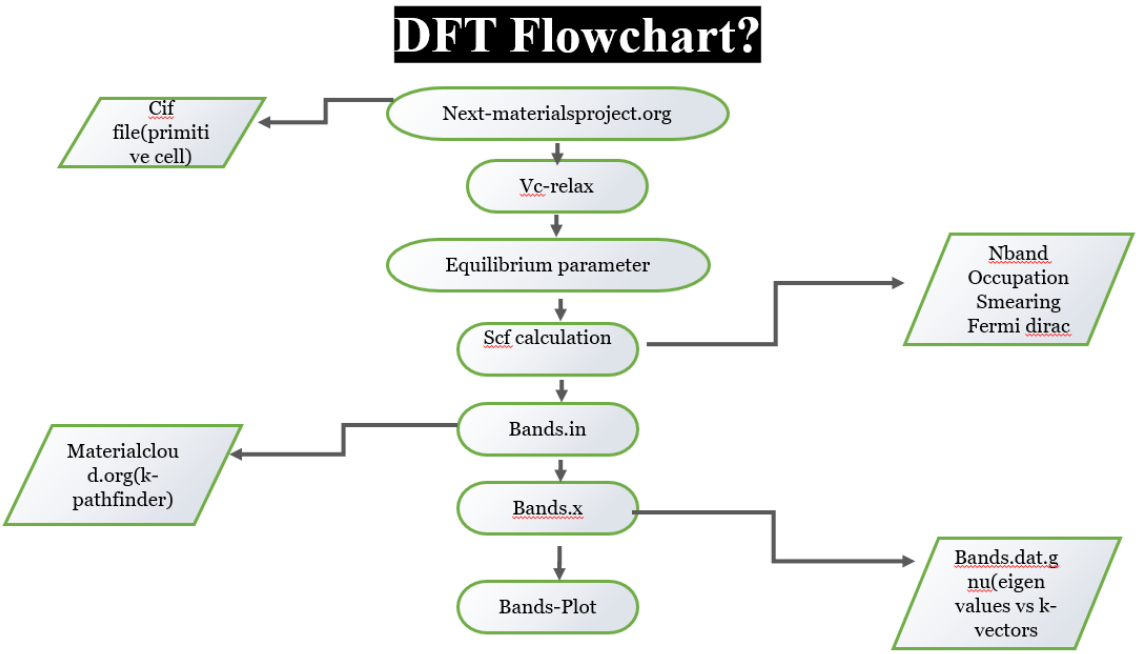
Objective:

The objective of calculating the band structure is to understand the electronic properties of materials, specifically how electrons occupy energy levels in a crystalline lattice. It provides crucial insights into a material's conductivity, optical behavior, and fundamental electronic characteristics, enabling tailored design for diverse technological applications.

Introduction:

Exploring the digital shape of materials is fundamental for comprehending their properties. This observe centers on magnesium, making use of Density Functional Theory (DFT) to compute its band shape. Magnesium, a key metal, holds importance in numerous programs. Investigating its band shape goals to unveil treasured insights into its electronic homes, contributing to the knowledge of its conduct in one of a kind contexts.

Methodology:



In our approach, we use Quantum Espresso and Python algorithms to conduct Density Functional Theory (DFT) calculations. We create a model of silicon's crystal structure and employ KohnSham equations to compute electronic properties. This helps us find crucial details like the band structure, lattice parameter, Fermi Energy, and density of states. To ensure accuracy, we select suitable exchangecorrelation functionals, and careful parameter tuning guarantees convergence in our calculations.

Ultrasoft pseudopotentials enhance accuracy and efficiency in DFT band structure calculations for conductive materials like magnesium, ensuring reliable predictions.

Reason for chossing USPPpbekjpaw pseudopotential because Handling Electron Localization, Accurate Description of Wave Functions , Improved Convergence etc.

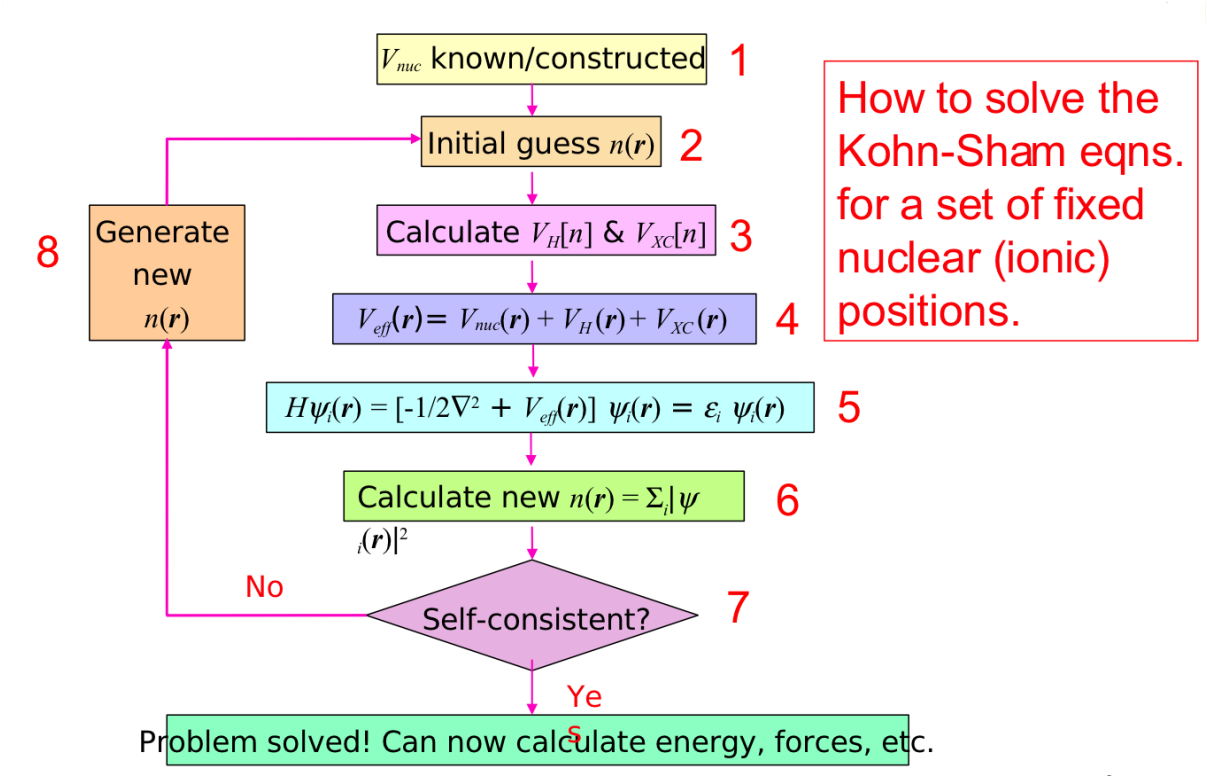


Figure: DFT computational SCF cycle → Total Energy and Force Minimization

Explaination

Execute VCRelax script using pw.x to determine relaxed parameters with minimized forces/pressure (e.g., 0.1 atmP).

SCF.out script yields Fermi energy and minimum energy for converged lattice parameters and kpoints.

Bands.out script provides high symmetry points and corresponding energy values, matching the Band diagram.

DOS.out script generates energy values and corresponding Density of State.

Run Bands.x script to produce Cartesian coordinates in dat.gnu file (Energy vs Kpoints).

Run DOS.x script to generate Cartesian coordinates in dat.gnu file (Energy vs Density).

Utilize Plot Band/Dos script to generate Cartesian coordinates for plotting with external software.

Results + discussion:

Band structure calculations for magnesium reveal electronic behavior.

Determine approximate band gap, crucial for semiconductor applications.

Results depict energy level distribution and electronic states nature.

Indirect band gap nature elucidated, offering optoelectronic insights.

Comparison with experimental data validates DFT's reliability for magnesium.

DOS graph informs semiconductor type (ntype or ptype) for magnesium.

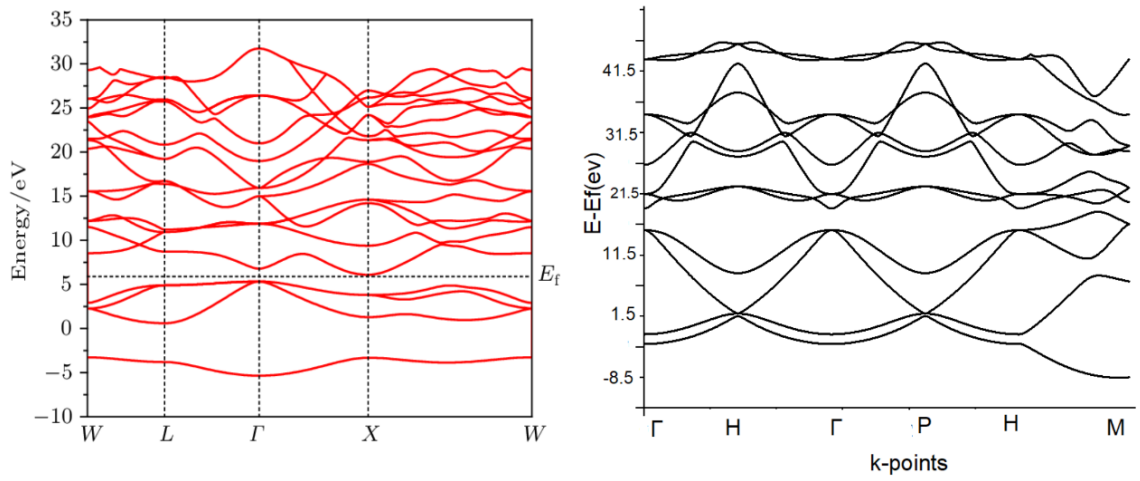
Fermi level position and characteristics inferred from DOS.

Higher DOS near Fermi level indicates higher carrier concentration.

Peaks in DOS at specific energy levels correlate with optical spectrum peaks.

DOS provides insights into magnesium's electronic nature (metallic, insulating, or semiconducting).

Material	K_POINTS {crystal_b}	Space group	No. of atoms	Lattice parameter (vc-relax)	Pseudopotential
Conductor (Magnesium)	! Γ—H—N—Γ—P—H|P—N K_POINTS {crystal_b} 4 0.0000000000 0.0000000000 0.5000000000 100 0.5000000000 -0.5000000000 0.5000000000 100 0.0000000000 0.0000000000 0.5000000000 100 0.2500000000 0.2500000000 0.2500000000 100	Im$\bar{3}$m	1(primitive)	6.7085280015	Mg.pbe-spnl-rrkjus_psl.1.0.0.UPF



Magnesium

Figure: Band Diagram → clearly shows it has 0 band gap(Metal).

Conclusion

Lattice Parameter:

Experimental: 6.7085 nm

DFT Theoretical (vcrelax): 6.580 nm

Band Gap:

Experimental: 0 eV

DFT Theoretical: 0 eV (No Band gap metallic nature)

Density of State (DOS):

Experimental: No Band gap (metal)

DFT Theoretical: No Band gap (metal)

Fermi Level:

Experimental: 7.06 eV

DFT Theoretical: 7.085 eV

Band Diagram:

Experimental: Overlap

DFT Theoretical: Overlap

The comparison between experimental and DFT theoretical values indicates some discrepancies, particularly in the lattice parameter and Fermi level. The band gap and the nature of the material in terms of the DOS and Band Diagram are consistent with both experimental and theoretical values, showing a metallic nature for magnesium. Further refinement in theoretical calculations may be considered for better alignment with experimental data.

References

Quantumexpresso.in

Nextmaterial.org

Researchgate.in