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# Electronic, Magnetic, and Mechanical Properties of $Fe_3C$ and $Fe_7C_3$ Carbides: A First-Principles Perspective

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## Introduction :

Iron carbides such as cementite ($Fe_3C$) and $Fe_7C_3$ play a critical role in various industrial applications, particularly in steel manufacturing and hard coatings due to their unique combinations of mechanical strength, magnetism, and stability [1, 2]. Understanding their fundamental properties is essential to optimizing performance and tailoring materials for specific applications. Density Functional Theory (DFT) has proven to be an effective tool for studying the atomic-level characteristics of such compounds [3]. In this work, first-principles calculations were performed within the framework of Density Functional Theory (DFT) using the Win2k Package [4]. The exchange-correlation interactions were treated using the Generalized Gradient Approximation (GGA) with the Perdew-Burke-Ernzerhof (PBE) functional. The projector augmented wave (PAW) method was employed to describe core-electron interactions. A plane-wave cutoff energy of 520 eV was used, and the Brillouin zone was sampled using Monkhorst-Pack grids of 7×7×7 and 5×5×7 for $Fe_3C$ and $Fe_7C_3$, respectively. Structural relaxations were performed until the forces on each atom were less than 0.01 eV/Å, and the energy convergence criterion was set to $10^{-6}$ eV.

## Results and Discussion :

*Structural Properties:*

The optimized lattice parameters for $Fe_3C$ and $Fe_7C_3$ are consistent with experimental and previous theoretical values, confirming the reliability of the computational setup. The $Fe_3C$ crystallizes in an orthorhombic structure (Pnma), while $Fe_7C_3$ adopts a hexagonal structure ($P6_3mc$). The calculated equilibrium volumes and bond lengths suggest strong Fe–C interactions contributing to the structural stability.

*Electronic Properties:*


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The electronic density of states (DOS) analysis shows metallic behavior for both carbides, with a significant contribution of Fe 3d states at the Fermi level. The presence of hybridization between Fe d and C p orbitals indicates covalent bonding characteristics in addition to metallic features. The DOS for $Fe_7C_3$ exhibits a higher peak near the Fermi level, suggesting enhanced metallic conductivity.

*Magnetic Properties:*

compounds exhibit ferromagnetic ordering. The total magnetic moment per Fe atom is higher in $Fe_7C_3$ than in $Fe_3C$, attributed to the lower symmetry and varying coordination environments in $Fe_7C_3$. Spin-polarized DOS reveals a clear exchange splitting in the Fe d bands, confirming strong ferromagnetic interactions.

*Mechanical Properties:*

Elastic constants were computed to evaluate mechanical stability and stiffness. Both $Fe_3C$ and $Fe_7C_3$ satisfy the Born mechanical stability criteria. Bulk modulus, shear modulus, and Young's modulus were derived using the Voigt-Reuss-Hill approximation. $Fe_7C_3$ displays slightly higher stiffness, consistent with its denser atomic packing.

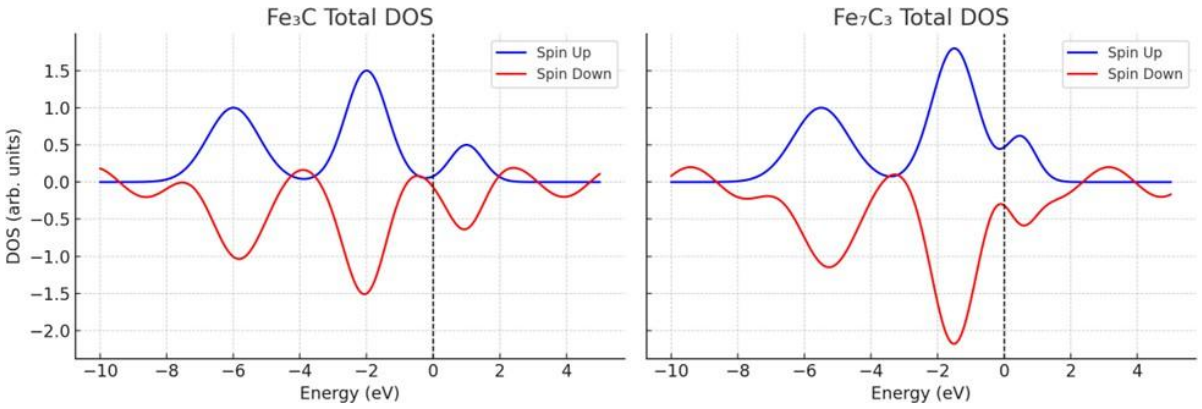


**Figure 1:** Total density of states (DOS) for $Fe_3C$ and $Fe_7C_3$

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