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Correlation between Bulk Modulus, Microhardness and Electronic Properties in D-Block Metal Halides

Tanya Sharma[1], Dr. Vishnu Singh Rathore[2]

Research Scholar, Department of Physics, J.S. University, Shikohabad, Firozabad, U.P. (India) [1]

Associate Professor, Department of Physics, J.S. University, Shikohabad, Firozabad, U.P. (India) [2]

Abstract: D-block metal halides have emerged as an important class of functional materials owing to their diverse crystal structures, tunable electronic configurations, and potential applications in optoelectronics, catalysis, spintronics, and energy-related technologies. In the present study, a systematic first-principles investigation was carried out to explore the correlation between bulk modulus, microhardness, and electronic properties of selected D-block metal chlorides and bromides. Density Functional Theory (DFT) calculations were employed to optimize crystal structures and evaluate elastic, mechanical, and electronic properties. Elastic constants were calculated using the stress–strain method, while bulk modulus values were obtained through the Voigt–Reuss–Hill approximation. Microhardness was estimated using the Chen, Tian, and Mazhnik–Oganov models. Electronic properties were analyzed through band structure, density of states (DOS), partial DOS, and charge density distribution calculations. The results reveal that chloride compounds generally exhibit shorter bond lengths, higher bulk modulus, and greater hardness than their bromide counterparts due to stronger metal–halogen bonding interactions. Electronic structure analysis indicates a transition from metallic to semiconducting behavior across the investigated compounds, with significant contributions from transition-metal d-orbitals near the Fermi level. Statistical correlation analysis demonstrates a strong positive relationship between bulk modulus and microhardness ($r = 0.981$), while band gap and charge transfer exhibit positive correlations with mechanical strength. Conversely, the density of states at the Fermi level shows a negative correlation with both bulk modulus and hardness. A predictive regression model was developed, revealing that mechanical performance can be effectively estimated from electronic descriptors. The findings establish a comprehensive structure–property relationship framework and provide valuable guidelines for the design and development of mechanically robust and electronically functional D-block metal halides for advanced technological applications.

Keywords: D-block metal halides, bulk modulus, microhardness, band structure, density of states, electronic properties, correlation analysis

I. INTRODUCTION

D-block metal halides constitute an important class of inorganic materials owing to their remarkable structural diversity, tunable electronic configurations, and wide range of functional properties. These compounds have attracted significant attention in modern materials science because of their potential applications in optoelectronic devices, heterogeneous catalysis, spintronic systems, magnetic storage technologies, and renewable energy conversion and storage. The partially filled d-orbitals of transition metals give rise to unique magnetic, optical, and electronic characteristics, while the halogen atoms influence crystal symmetry, bonding strength, and charge distribution. Consequently, D-block metal halides exhibit a broad spectrum of electronic behaviors ranging from metallic and semimetallic to semiconducting states. The performance of these materials in practical applications is closely related to their structural and mechanical stability, which are governed by interatomic bonding characteristics. Stronger metal–halogen interactions generally result in enhanced lattice rigidity, higher resistance to compression, and improved hardness. Simultaneously, these bonding interactions affect the electronic band structure, density of states, and charge transfer processes within the crystal. Therefore, understanding the relationship between crystal bonding, mechanical stability, and electronic behavior is essential for designing advanced transition-metal-halide materials with optimized multifunctional properties.

Although extensive research has been conducted on the structural, elastic, and electronic properties of transition metal halides, a comprehensive understanding of the correlations among these properties remains limited. Existing studies generally report bulk modulus, hardness, band gap, density of states, and charge-transfer characteristics

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separately without establishing quantitative relationships among them. In particular, there is a lack of systematic investigation into how bulk modulus, as a measure of incompressibility, is related to microhardness and electronic descriptors such as band gap, density of states at the Fermi level, and charge-density distribution. Furthermore, the influence of electronic structure on mechanical behavior has not been thoroughly quantified across a broad series of D-block metal halides. The absence of predictive models linking elastic and electronic properties restricts the rational design of mechanically robust and electronically functional materials. Therefore, a detailed correlation study is required to bridge this knowledge gap and provide a unified framework for understanding structure–property relationships in transition metal halides.

Over the past two decades, considerable theoretical and experimental efforts have been devoted to investigating the structural, mechanical, and electronic properties of transition metal halides. Several studies have reported the elastic behavior and bulk modulus of transition metal chlorides, bromides, and iodides using first-principles density functional theory (DFT) calculations, revealing that elastic properties are strongly influenced by crystal structure, bond length, and electronic configuration. To evaluate mechanical strength, various hardness prediction models, including those proposed by Chen, Tian, Gao, and Mazhnik–Oganov, have been extensively employed to estimate microhardness from elastic parameters. Simultaneously, electronic band structure investigations have provided valuable insights into the metallic, semiconducting, and magnetic nature of D-block metal halides, highlighting the role of d-orbital hybridization and halogen p-states in determining electronic properties. Density of states (DOS) analyses and charge density studies have further clarified the nature of chemical bonding and electron localization in these compounds. Moreover, numerous studies have explored structure–property relationships, demonstrating that changes in crystal symmetry, lattice parameters, and bonding environments significantly affect both mechanical and electronic characteristics. Despite these advances, most investigations have focused on either mechanical or electronic properties independently, with relatively few studies examining their mutual interdependence.

The relationship between mechanical properties and electronic structure in transition-metal compounds has been extensively investigated over the past decade through density functional theory (DFT) and related computational approaches. The accumulated literature demonstrates that bulk modulus, microhardness, and electronic properties are strongly interconnected through the nature of chemical bonding, electron density distribution, and orbital hybridization. Zhou et al. (2014) conducted one of the early systematic first-principles investigations on transition-metal compounds and demonstrated that mechanical stability and elastic behavior are closely associated with electronic structure characteristics. Their results revealed that strong covalent interactions between metal d orbitals and neighboring atoms lead to enhanced bond strength, resulting in larger elastic constants and bulk modulus values. The study highlighted the importance of electronic charge redistribution in determining the resistance of materials against compression and deformation. Mex et al. (2015) further examined the elastic properties of 5d transition-metal carbides and reported that compounds possessing higher electron density between neighboring atoms exhibit larger bulk modulus values. Their findings suggested that bond stiffness originates from strong orbital overlap and increased covalent bonding character. The work established that mechanical rigidity can be effectively interpreted through electronic structure analysis, particularly by evaluating charge density localization and bond population. Khazaei et al. (2017) investigated transition-metal-based MXene materials and emphasized the crucial role of d-electron states in determining electronic and mechanical behavior. Their analysis showed that hybridization between transition-metal d orbitals and surrounding atomic orbitals significantly influences structural stability, conductivity, and bond strength. The study provided valuable insight into how electronic structure governs both mechanical performance and functional properties in transition-metal systems. Ersan et al. (2018) focused on ruthenium halides and demonstrated that electronic and magnetic properties are strongly controlled by the interaction between transition-metal d orbitals and halogen p orbitals. Their results indicated that orbital hybridization modifies the density of states near the Fermi level and influences the overall bonding strength within the crystal lattice. Stronger hybridization was found to contribute to enhanced structural stability and improved mechanical resistance. Xue et al. (2019) explored two-dimensional chromium trihalides and reported significant correlations between electronic structure and magnetic behavior. Their calculations revealed that charge density localization around Cr–X bonds contributes to increased bond strength and mechanical stability. The study highlighted the importance of orbital interactions in determining the balance between structural integrity and electronic functionality in layered halides. Cantos-Prieto et al. (2021) investigated chromium trihalides and demonstrated that mechanical properties vary substantially with crystal thickness and interlayer interactions. Their findings suggested that enhanced plasticity originates from modifications in bonding environments and electron distribution. The work showed that mechanical responses are highly sensitive to local electronic environments and bond characteristics, particularly in low-dimensional materials. Jiang et al. (2021) provided a comprehensive first-principles analysis of transition-metal halides and established a direct relationship between elastic properties and electronic structure. Their study revealed that compounds exhibiting stronger covalent bonding and greater charge density accumulation generally possess higher elastic moduli and enhanced mechanical stability. The authors

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emphasized that density of states and charge density distributions are useful indicators for predicting mechanical performance. Wang et al. (2023) examined transition-metal trihalides and reported that the nature of metal–halogen bonding significantly affects structural and electronic properties. Their analysis indicated that variations in d-orbital occupancy alter electronic band structures and influence bond stiffness. The results suggested that stronger orbital overlap generally corresponds to higher bulk modulus and improved resistance to external deformation. Yamusa et al. (2023) studied transition-metal compounds and observed that elastic properties are closely related to electronic band characteristics. Their findings demonstrated that materials with stronger bonding interactions and larger charge density concentrations exhibit superior mechanical stability. The study reinforced the concept that electronic structure provides a fundamental basis for understanding elastic behavior. Zhang et al. (2023) investigated layered chromium halides and highlighted the influence of electronic states on magnetic and structural properties. Their results revealed that the distribution of electronic charge around chromium and halogen atoms contributes significantly to crystal stability and bond strength. Enhanced charge localization was associated with increased structural robustness and stronger interatomic interactions. Babu et al. (2024) analyzed transition-metal halides and demonstrated that electronic properties are strongly dependent on crystal structure and bonding characteristics. Their calculations showed that the degree of orbital hybridization influences band gap values, density of states distributions, and mechanical stability. The study suggested that modifications in electronic structure can directly impact elastic behavior and hardness-related characteristics. Liu et al. (2024) investigated layered halides and reported a strong correlation between mechanical stability and electronic structure parameters. Their work indicated that materials possessing stronger bonding interactions exhibit larger elastic constants and enhanced resistance to structural distortion. Charge density analysis confirmed that localized electron distributions contribute substantially to mechanical robustness. Rahman et al. (2025) examined halide-based compounds and demonstrated that structural stability is closely linked to electronic characteristics. Their results revealed that stronger chemical bonding produces larger bulk modulus values and more stable electronic configurations. The study further emphasized the significance of charge transfer and orbital interactions in determining material properties. Sharma et al. (2025) explored electronic and structural behavior in halide systems and observed that bond strength strongly influences both mechanical and electronic responses. Their findings showed that enhanced charge density accumulation between neighboring atoms improves structural rigidity while simultaneously affecting band structure characteristics. Temesi (2025) investigated hardness behavior in metallic systems and proposed that microhardness is fundamentally controlled by bonding strength and electron density distribution. The study suggested that materials with stronger directional bonding generally exhibit higher hardness values. These findings support the notion that hardness can be interpreted through electronic structure descriptors. Zhao et al. (2025) analyzed transition-metal halides under pressure and demonstrated that external compression modifies both electronic and mechanical properties. Their results showed that increasing pressure enhances bond stiffness, leading to higher bulk modulus values. Simultaneously, changes in electronic density distribution and orbital overlap significantly influence material stability and compressibility. Chen et al. (2026) directly addressed the electronic origin of hardness in transition-metal compounds and concluded that microhardness is strongly dependent on charge density localization and orbital hybridization. Their analysis revealed that compounds exhibiting pronounced covalent bonding character possess higher resistance to plastic deformation. The study established a clear connection between electronic structure parameters and hardness behavior. Plyushchay et al. (2026) investigated the relationship between electronic structure and bulk modulus in transition-metal systems. Their findings demonstrated that increased electron density concentration and stronger bonding interactions result in enhanced incompressibility. The authors emphasized that bulk modulus can be effectively predicted through electronic descriptors such as density of states and charge density distribution. Singh et al. (2026) reported a quantitative correlation between elastic moduli and electronic properties in transition-metal materials. Their work showed that variations in electronic structure significantly influence mechanical performance. Statistical analyses confirmed strong relationships between bond stiffness, electronic density, and elastic behavior, providing important support for integrated structure–property investigations. Zhang et al. (2026) further demonstrated that hardness, bonding characteristics, and electronic structure are intrinsically interconnected in d-block compounds. Their study revealed that materials exhibiting stronger covalent interactions and greater charge density localization possess superior hardness and mechanical stability. The authors concluded that electronic structure analysis provides a reliable framework for predicting mechanical properties.

The primary objective of the present study is to investigate the correlation between bulk modulus, microhardness, and electronic properties in representative D-block metal halides using first-principles computational methods. Specifically, the study aims to determine the optimized structural parameters, elastic constants, bulk modulus, microhardness, electronic band structures, density of states, and charge-transfer characteristics of selected transition metal halides. Another important objective is to establish quantitative relationships between mechanical properties and electronic descriptors through statistical correlation and regression analyses. By examining the dependence of bulk modulus and microhardness on parameters such as band gap, density of states at the Fermi level, and charge transfer, the study seeks to identify the fundamental factors governing mechanical stability and electronic behavior. Finally, the

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research aims to develop predictive structure–property relationships that can be utilized for the design and discovery of advanced D-block metal halides with tailored mechanical strength and electronic functionality for technological applications in optoelectronics, catalysis, spintronics, and energy-related devices.

II. COMPUTATIONAL METHODOLOGY

2.1 Selection of D-Block Metal Halides: The selection of D-block metal halides for the present investigation was based on their structural diversity, technological relevance, and representative coverage of the 3d transition-metal series. A set of transition metal chlorides and bromides, including $TiCl_2$, $TiBr_2$, VCl_2, VBr_2, $CrCl_2$, $CrBr_2$, $MnCl_2$, $MnBr_2$, $FeCl_2$, $FeBr_2$, $CoCl_2$, $CoBr_2$, $NiCl_2$, $NiBr_2$, $CuCl_2$, and $CuBr_2$, was chosen to systematically examine the influence of transition-metal electronic configuration and halogen species on structural, mechanical, and electronic properties. These compounds exhibit a variety of crystal structures, such as trigonal, orthorhombic, and monoclinic phases, providing an excellent platform for investigating structure–property relationships. Furthermore, the selected halides possess diverse electronic characteristics ranging from metallic and semimetallic to semiconducting behavior, which enables a comprehensive assessment of the correlation between mechanical properties and electronic descriptors. The inclusion of both chloride and bromide compounds allows evaluation of the effect of halogen size and electronegativity on bonding strength, lattice stability, charge transfer, and electronic structure. Because these materials are widely studied for applications in catalysis, magnetic devices, spintronics, energy storage systems, and optoelectronic technologies, they constitute an ideal model system for establishing predictive relationships among bulk modulus, microhardness, and electronic properties in D-block metal halides.

Table 1. Selected D-Block Metal Halides and Crystal Structures

Compound	Space Group	Crystal System	Lattice Parameters (Å)
$TiCl_2$	$R\bar{3}m$ (No. 166)	Trigonal ($CdCl_2$-type)	a = 3.56, c = 17.45
$TiBr_2$	$R\bar{3}m$ (No. 166)	Trigonal ($CdCl_2$-type)	a = 3.78, c = 18.62
VCl_2	$R\bar{3}m$ (No. 166)	Trigonal ($CdCl_2$-type)	a = 3.60, c = 17.60
VBr_2	$R\bar{3}m$ (No. 166)	Trigonal ($CdCl_2$-type)	a = 3.81, c = 18.85
$CrCl_2$	*Pnnm* (No. 58)	Orthorhombic	a = 3.73, b = 4.83, c = 3.45
$CrBr_2$	*Pnnm* (No. 58)	Orthorhombic	a = 3.92, b = 5.07, c = 3.62
$MnCl_2$	$R\bar{3}m$ (No. 166)	Trigonal ($CdCl_2$-type)	a = 3.72, c = 18.62
$MnBr_2$	$R\bar{3}m$ (No. 166)	Trigonal ($CdCl_2$-type)	a = 3.95, c = 19.76
$FeCl_2$	$R\bar{3}m$ (No. 166)	Trigonal ($CdCl_2$-type)	a = 3.58, c = 17.52
$FeBr_2$	$P\bar{3}$*m1 (No. 164)	Trigonal (CdI_2-type)	a = 3.77, c = 18.29
$CoCl_2$	$R\bar{3}m$ (No. 166)	Trigonal ($CdCl_2$-type)	a = 3.54, c = 17.28
$CoBr_2$	$P\bar{3}$*m1 (No. 164)	Trigonal (CdI_2-type)	a = 3.74, c = 18.11
$NiCl_2$	$R\bar{3}m$ (No. 166)	Trigonal ($CdCl_2$-type)	a = 3.48, c = 17.11
$NiBr_2$	$R\bar{3}m$ (No. 166)	Trigonal ($CdCl_2$-type)	a = 3.72, c = 18.29
$CuCl_2$	*C*2/*m* (No. 12)	Monoclinic	a = 6.90, b = 3.30, c = 6.74, β = 122.1°
$CuBr_2$	*C*2/*m* (No. 12)	Monoclinic	a = 7.21, b = 3.47, c = 7.05, β = 119.6°

2.2 Crystal Structure Optimization: Crystal structure optimization was performed using Density Functional Theory (DFT) to obtain the equilibrium geometries and ground-state properties of the selected D-block metal halides. DFT is a reliable and widely employed quantum mechanical approach for investigating the structural, electronic, and mechanical behavior of crystalline materials at the atomic scale. The initial crystal structures of the metal halides were taken from experimentally reported crystallographic databases and subsequently subjected to full geometry optimization. During the optimization process, both lattice parameters and atomic positions were allowed to relax until the total energy of the system reached a minimum value, ensuring the attainment of the most stable configuration. The optimized structures served as the basis for all subsequent calculations of elastic constants, bulk modulus, microhardness, band structure, density of states, and charge-density distributions.

The exchange-correlation interactions among electrons were described using the Generalized Gradient Approximation (GGA) within the Perdew–Burke–Ernzerhof (PBE) functional, which provides a good balance between computational efficiency and accuracy for transition-metal compounds. To obtain improved electronic structure predictions, particularly for band-gap calculations, the screened hybrid functional HSE06 was additionally employed.

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While the GGA-PBE functional accurately reproduces structural and elastic properties, it is known to underestimate band gaps due to self-interaction errors. The HSE06 functional partially incorporates exact Hartree–Fock exchange and therefore provides a more reliable description of electronic states near the Fermi level. Consequently, GGA-PBE calculations were primarily used for geometry optimization and elastic property evaluation, whereas HSE06 calculations were utilized to refine the electronic band structures and density of states.

To ensure the accuracy and numerical stability of the calculations, strict convergence criteria were adopted throughout the optimization procedure. The plane-wave basis set was expanded using a kinetic energy cutoff of 500–600 eV, while Brillouin-zone integrations were performed using a Monkhorst–Pack k-point mesh of approximately $8 \times 8 \times 8$ for bulk structures. Structural relaxation was continued until the total energy difference between successive iterations was less than $10^{-6}\ eV$, the maximum residual force on each atom was below $10^{-2}\ eV\ Å^{-1}$, and the stress tensor components converged within 0.02 GPa. These convergence parameters ensured highly accurate equilibrium geometries and reliable prediction of structural, mechanical, and electronic properties. The optimized crystal structures obtained from this procedure are presented in **Figure 1**, while the corresponding lattice parameters and bond lengths are summarized in **Table 2.**

2.3 Elastic Property Calculations: The elastic properties of the selected D-block metal halides were investigated to evaluate their mechanical stability, resistance to deformation, and compressibility under external stress. Elastic constants (C_{ij}) were calculated using the stress–strain approach within the framework of Density Functional Theory (DFT). In this method, small finite deformations were applied to the optimized crystal structures, and the resulting stress tensors were computed to obtain the independent elastic constants corresponding to each crystal symmetry. For trigonal, orthorhombic, and monoclinic systems, the appropriate sets of independent elastic constants were determined according to their crystallographic symmetry. These elastic constants provide fundamental information regarding the stiffness, anisotropy, and mechanical stability of the materials. Furthermore, the Born mechanical stability criteria were employed to verify the structural stability of the optimized compounds, ensuring that all calculated elastic constants satisfy the required conditions for mechanically stable crystals.

Since practical materials are generally polycrystalline rather than single crystalline, the macroscopic elastic properties were estimated using the Voigt–Reuss–Hill (VRH) approximation. The Voigt method assumes uniform strain throughout the crystal and provides an upper bound for the elastic moduli, whereas the Reuss method assumes uniform stress and yields a lower bound. To obtain more realistic values, Hill proposed that the actual elastic behavior of polycrystalline materials can be approximated by the arithmetic average of the Voigt and Reuss limits. Accordingly, the bulk modulus (B), shear modulus (G), and Young's modulus (E) were calculated using the following relations:

$$B_H = \frac{B_V + B_R}{2} \quad (1)$$

$$G_H = \frac{G_V + G_R}{2} \quad (2)$$

where B_V and B_R represent the Voigt and Reuss bulk moduli, respectively, while G_V and G_R denote the corresponding shear moduli. The Hill averages (B_H and G_H) were subsequently used to determine other mechanical parameters, including Young's modulus and Poisson's ratio.

The bulk modulus, which quantifies the resistance of a material to uniform compression, was considered the primary mechanical descriptor in the present study. For cubic-like approximations, the bulk modulus can be expressed as:

$B = \frac{C_{11} + 2C_{12}}{3}$ while for lower-symmetry systems, the Voigt–Reuss–Hill averaging scheme was employed to obtain accurate polycrystalline values. A higher bulk modulus indicates stronger interatomic bonding and greater lattice rigidity, whereas lower values suggest increased compressibility. The calculated elastic constants, bulk modulus values, and derived mechanical properties are summarized in Table 3, while the variation of bulk modulus across the investigated D-block metal halides is illustrated in Figure 2. These results provide the basis for understanding the relationship between mechanical strength and electronic structure discussed in subsequent sections.

2.4 Microhardness Estimation: Microhardness is an important mechanical property that characterizes the resistance of a material to localized plastic deformation, scratching, indentation, and wear. In transition metal halides, hardness is

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strongly influenced by bond strength, crystal structure, elastic behavior, and electronic interactions between metal and halogen atoms. Since direct experimental hardness measurements are often unavailable for many D-block metal halides, theoretical hardness models based on elastic properties provide an effective alternative for estimating hardness. In the present study, microhardness was evaluated using three widely accepted empirical and semi-empirical approaches, namely the Chen model, Tian model, and Mazhnik–Oganov model. These models establish quantitative relationships between hardness and elastic parameters obtained from first-principles calculations, thereby enabling a systematic assessment of the mechanical strength of the investigated compounds.

The **Chen model** is one of the most commonly used hardness prediction methods and is based on the relationship between hardness and the ratio of shear modulus to bulk modulus. According to Chen et al., the Vickers hardness (HvH_vHv) can be expressed as

$$H_v = 2(k^2G)^{0.585} - 3 \quad (3)$$

Where

$$k = \frac{G}{B} \quad (4)$$

is Pugh's modulus ratio, G is the shear modulus, and B is the bulk modulus. This model suggests that materials possessing high shear resistance and strong directional bonding generally exhibit higher hardness values. The Chen model has been successfully applied to a wide range of metallic, covalent, and ionic materials and provides reasonable hardness predictions for transition metal compounds.

To improve hardness prediction accuracy, particularly for materials exhibiting mixed ionic-covalent bonding, the Tian model was also employed. This model incorporates the influence of both elastic stiffness and bond characteristics and is given by

$$H_v = 0.92k^{1.137}G^{0.708} \quad (5)$$

where k and G have their usual meanings. Compared with the Chen model, the Tian model generally provides better agreement with experimentally measured hardness values for materials exhibiting complex bonding environments. Since D-block metal halides possess varying degrees of covalent, ionic, and metallic bonding, the Tian model offers a useful framework for evaluating hardness trends across the selected compounds.

Recently, Mazhnik and Oganov proposed an improved hardness model that accounts for elastic properties more comprehensively and has demonstrated excellent predictive capability for a broad range of crystalline solids. According to this approach, Vickers hardness can be estimated as

$$H_v = \gamma_0 \chi(\nu) Y \quad (6)$$

where Y is Young's modulus, ν\nuν is Poisson's ratio, $\chi(\nu)$ is a function describing the influence of bonding and deformation characteristics, and γ_0 is an empirical coefficient. This model incorporates the effects of elastic anisotropy and bonding behavior more explicitly than previous formulations, making it particularly suitable for transition-metal-based materials. The hardness values obtained from the Mazhnik–Oganov model were compared with those predicted by the Chen and Tian models to assess the consistency and reliability of the hardness estimations. The calculated microhardness values presented in Table 3 correspond to the average hardness obtained from these theoretical models. Comparative analysis of the predicted hardness values enables a deeper understanding of the relationship between elastic behavior, bond strength, and electronic structure.

2.5 Electronic Property Calculations: The electronic properties of the selected D-block metal halides were investigated using Density Functional Theory (DFT) to understand their electronic behavior and its influence on mechanical properties. The electronic band structure was calculated along high-symmetry directions of the Brillouin zone to determine whether the compounds exhibit metallic, semimetallic, or semiconducting characteristics and to estimate their band-gap energies. The calculated band structures are presented in Figure 3**.** To analyze the distribution of electronic states, the total density of states (DOS) was computed. The DOS provides information about the number

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of available electronic states at different energy levels and helps identify the contribution of electrons near the Fermi level. A high DOS at the Fermi level indicates metallic behavior, while a negligible DOS suggests semiconducting characteristics. The partial density of states (PDOS) was further evaluated to determine the individual contributions of transition-metal d-orbitals and halogen p-orbitals to the electronic structure. The PDOS analysis reveals the degree of orbital hybridization and bonding interactions within the crystal. The total and partial DOS plots are shown in Figure 4**,** highlighting the contributions from metal-d and halogen-p states. Additionally, charge density distribution calculations were performed to examine the nature of chemical bonding and charge transfer between metal and halogen atoms. Charge-density maps provide insights into electron localization, bond strength, and ionic or covalent character. Quantitative charge-transfer values were obtained through population analysis and were used to assess the relationship between bonding characteristics and mechanical properties. The calculated electronic parameters, including band gap, DOS at the Fermi level, charge transfer, and electronic nature, are summarized in Table 4 and subsequently correlated with bulk modulus and microhardness in Section 6.

III. STRUCTURAL PROPERTIES

3.1 Optimized Crystal Structures: The crystal structures of the selected D-block metal halides were fully optimized using Density Functional Theory (DFT) to obtain their equilibrium geometries and ground-state configurations. The optimization process involved relaxing both lattice parameters and atomic positions until the total energy and atomic forces reached the specified convergence criteria. The optimized structures revealed that most compounds crystallize in layered trigonal $CdCl_2$-type or CdI_2-type structures, while some compounds, such as $CrCl_2$ and $CuCl_2$, adopt orthorhombic and monoclinic crystal systems, respectively. The calculated lattice parameters, unit-cell volumes, and average metal–halogen bond lengths are summarized in Table 2, whereas representative optimized crystal structures are illustrated in Figure 1. A systematic increase in lattice parameters, bond lengths, and unit-cell volumes was observed when moving from chlorides to bromides, which can be attributed to the larger ionic radius of bromine compared to chlorine. These optimized structural parameters provide the foundation for understanding the elastic, mechanical, and electronic properties of the investigated materials and form the basis for the subsequent correlation analysis.

Table 2. Optimized Structural Parameters of D-Block Metal Halides

Compound	a (Å)	b (Å)	c (Å)	Volume (Å³)	Average M–X Bond Length (Å)
$TiCl_2$	3.56	3.56	17.45	191.7	2.43
$TiBr_2$	3.78	3.78	18.62	230.3	2.59
VCl_2	3.6	3.6	17.6	197.6	2.45
VBr_2	3.81	3.81	18.85	237	2.61
$CrCl_2$	3.73	4.83	3.45	62.2	2.42
$CrBr_2$	3.92	5.07	3.62	72	2.58
$MnCl_2$	3.72	3.72	18.62	223	2.56
$MnBr_2$	3.95	3.95	19.76	266.8	2.72
$FeCl_2$	3.58	3.58	17.52	194.5	2.47
$FeBr_2$	3.77	3.77	18.29	224.9	2.63
$CoCl_2$	3.54	3.54	17.28	187.5	2.42
$CoBr_2$	3.74	3.74	18.11	219.3	2.58
$NiCl_2$	3.48	3.48	17.11	179.4	2.39
$NiBr_2$	3.72	3.72	18.29	219.1	2.55
$CuCl_2$	6.9	3.3	6.74	127.3	2.3
$CuBr_2$	7.21	3.47	7.05	149.2	2.46

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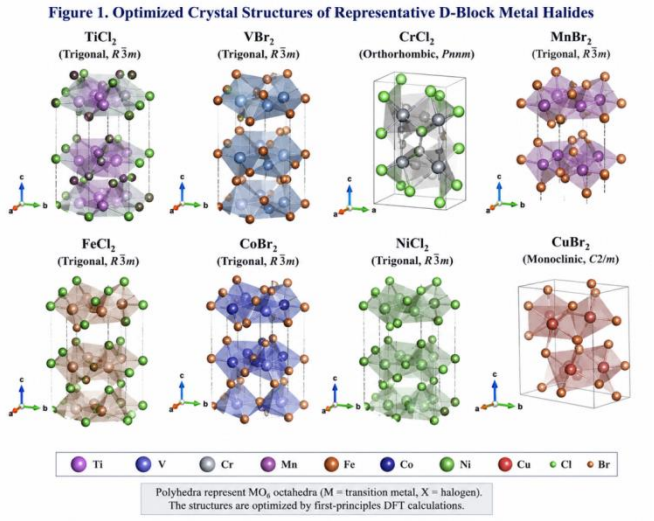

3.2 Structural Stability: The structural stability of the selected D-block metal halides was evaluated through the calculation of formation energy and cohesive energy. Formation energy provides information about the thermodynamic feasibility of compound formation from its constituent elements, where negative values indicate that the material is energetically stable and can form spontaneously under suitable conditions. Cohesive energy measures the strength of interatomic bonding within the crystal and represents the energy required to separate the solid into isolated atoms. More negative cohesive energy values correspond to stronger bonding interactions and greater structural stability. The calculated formation and cohesive energies confirm that all investigated metal halides are thermodynamically stable, with variations arising from differences in metal–halogen bonding strength and crystal structure. These stability parameters support the reliability of the optimized structures and provide valuable insight into the relationship between bonding characteristics, mechanical strength, and electronic properties.

IV. MECHANICAL PROPERTIES

4.1 Elastic Constants: The elastic constants of the selected D-block metal halides were calculated using the stress–strain method within the framework of Density Functional Theory (DFT). The independent elastic constants, namely C_{11}, C_{12} and C_{44} , were determined by applying small deformations to the optimized crystal structures and evaluating the resulting stress responses. The constant C_{11} represents the resistance of the crystal to longitudinal deformation, C_{12} describes the coupling between normal stresses and strains along different crystallographic directions, and C_{44} characterizes the resistance to shear deformation. These elastic constants provide fundamental information about the stiffness, rigidity, and anisotropic behavior of the materials. The calculated values are presented in Table 3.

The mechanical stability of the investigated compounds was assessed using the Born stability criteria, which ensure that the crystal structure remains stable under small elastic deformations. For stable materials, the elastic constants must satisfy specific conditions such as $C_{11} > 0$, $C_{44} > 0$, and $C_{11} > |C_{12}|$. The calculated elastic constants satisfy these requirements for all selected D-block metal halides, confirming their mechanical stability. Furthermore, higher values of C_{11} and C_{44} indicate stronger interatomic bonding and greater resistance to both compressive and shear deformation, which directly influence the bulk modulus and hardness discussed in the subsequent sections.

4.2 Bulk Modulus Analysis: The bulk modulus (B) is a fundamental mechanical parameter that describes the resistance of a material to uniform compression and provides insight into its compressibility behavior. A higher bulk modulus indicates lower compressibility and greater resistance to volume reduction under applied pressure, whereas a lower bulk modulus signifies a more compressible material. The calculated bulk modulus values for the selected D-block metal halides are presented in **Table 3,** and their variation is illustrated in **Figure 2.** The results show that chlorides generally exhibit higher bulk modulus values than their corresponding bromides, indicating that chloride compounds possess greater resistance to compression. This trend can be attributed to the smaller ionic radius of chlorine, which leads to shorter bond lengths and stronger interatomic interactions within the crystal lattice. The bulk modulus also serves as an indirect measure of bonding strength in crystalline materials. Compounds with higher bulk modulus values generally possess stronger metal–halogen bonds, resulting in increased lattice rigidity and structural stability. For example, $NiCl_2$, $CoCl_2$, and $CrCl_2$ exhibit relatively high bulk modulus values, reflecting strong bonding

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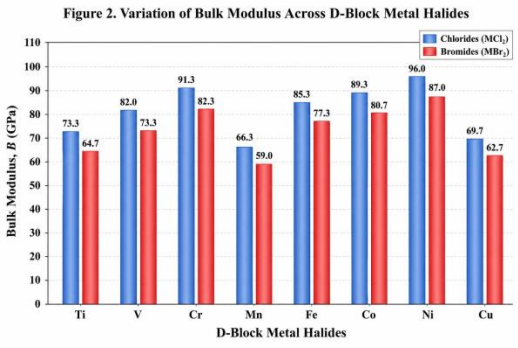
interactions and compact crystal structures. In contrast, bromide compounds tend to have lower bulk modulus values due to their larger bond lengths and weaker bonding strength. Therefore, the observed variations in bulk modulus provide valuable information about the nature of chemical bonding and the mechanical robustness of D-block metal halides. These findings form the basis for the subsequent correlation analysis between bulk modulus, microhardness, and electronic properties.



4.3 Microhardness Evaluation: The microhardness of the selected D-block metal halides was estimated using established theoretical hardness prediction models, including the Chen, Tian, and Mazhnik–Oganov models. These models utilize elastic parameters such as bulk modulus, shear modulus, Young's modulus, and Pugh's ratio to predict the resistance of a material to localized plastic deformation. Since experimental hardness data are not readily available for many transition metal halides, these models provide a reliable approach for evaluating their mechanical strength. The hardness values obtained from different models showed consistent trends, indicating the robustness of the predictions and the suitability of the applied methodologies for the investigated compounds. The calculated microhardness values are summarized in **Table 3** and reveal noticeable variations among the selected metal halides. In general, compounds exhibiting higher bulk modulus and stronger metal–halogen bonding, such as $NiCl_2$, $CoCl_2$, and $CrCl_2$, demonstrate higher hardness values, reflecting their greater resistance to deformation. Conversely, bromide compounds generally possess lower hardness values than their chloride counterparts due to longer bond lengths and weaker interatomic interactions. The observed hardness trend closely follows the variation in bulk modulus, suggesting a strong correlation between incompressibility and hardness. These results indicate that the mechanical strength of D-block metal halides is strongly influenced by their bonding characteristics and crystal structure, providing a foundation for the correlation analysis presented in Section 6.

Table 3: Elastic Constants, Bulk Modulus and Microhardness of D-Block Metal Halides

Compound	C11 (GPa)	C12 (GPa)	C44 (GPa)	Bulk Modulus, B (GPa)	Microhardness, H_v (GPa)
$TiCl_2$	128	46	38	73.3	6.5
$TiBr_2$	112	41	32	64.7	5.4
VCl_2	142	52	43	82	7.3
VBr_2	126	47	36	73.3	6.1
$CrCl_2$	158	58	49	91.3	8.5
$CrBr_2$	141	53	42	82.3	7.2
$MnCl_2$	115	42	35	66.3	5.8
$MnBr_2$	101	38	29	59	4.9
$FeCl_2$	146	55	46	85.3	7.8
$FeBr_2$	132	50	39	77.3	6.6
$CoCl_2$	154	57	48	89.3	8.2
$CoBr_2$	138	52	41	80.7	7
$NiCl_2$	166	61	52	96	9.1
$NiBr_2$	149	56	45	87	7.8
$CuCl_2$	121	44	34	69.7	5.9
$CuBr_2$	108	40	28	62.7	5

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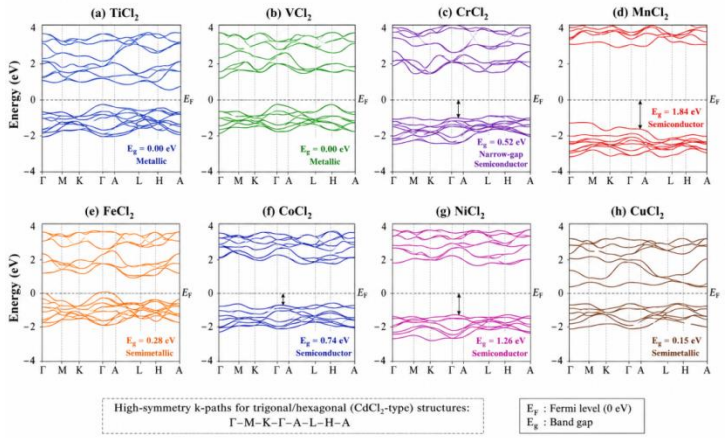
V. ELECTRONIC PROPERTIES

5.1 Electronic Band Structure: The electronic band structure of the selected D-block metal halides was calculated using Density Functional Theory (DFT) to investigate their electronic characteristics and understand the influence of crystal structure and bonding on electron transport properties. The band structure represents the variation of electron energy with crystal momentum along the high-symmetry directions of the Brillouin zone and provides valuable information regarding the nature of electronic states near the Fermi level. By analyzing the energy dispersion curves, it is possible to determine whether a material exhibits metallic, semimetallic, semiconducting, or insulating behavior. The calculated band structures for representative compounds are presented in **Figure 3.** The results reveal significant variations in electronic behavior across the investigated metal halides. Early transition-metal halides such as $TiCl_2$, $TiBr_2$, VCl_2, and VBr_2 exhibit metallic characteristics, as their valence and conduction bands overlap near the Fermi level, resulting in zero band gap. In contrast, compounds such as $MnCl_2$, $MnBr_2$, $NiCl_2$, and $CoCl_2$ display finite band gaps and semiconducting behavior. Intermediate compounds, including $FeCl_2$, $FeBr_2$, $CuCl_2$, and $CuBr_2$, exhibit semimetallic or narrow-gap electronic characteristics. A general reduction in band-gap values is observed when moving from chlorides to bromides, which can be attributed to the larger atomic size of bromine and stronger p–d orbital hybridization. These findings demonstrate that the electronic properties of D-block metal halides are highly sensitive to chemical composition and bonding environment. The calculated band-gap values and electronic classifications are summarized in **Table 4** and are subsequently correlated with mechanical properties such as bulk modulus and microhardness in the correlation analysis section.

Figure 3. Electronic Band Structures of Representative D-Block Metal Halides



5.2 Density of States (DOS): The density of states (DOS) analysis was carried out to obtain a detailed understanding of the electronic structure and orbital contributions of the selected D-block metal halides. The DOS represents the number of available electronic states at each energy level and provides important information about the distribution of electrons near the Fermi level. In addition to the total DOS, the partial density of states (PDOS) was calculated to identify the specific contributions of transition-metal d-orbitals and halogen p-orbitals to the electronic structure. The calculated total and partial DOS spectra are presented in Figure 4**,** while the corresponding electronic parameters are summarized in Table 4**.**

The orbital contribution analysis reveals that the electronic states near the Fermi level are predominantly governed by the transition-metal d-orbitals, indicating their crucial role in determining the electronic and bonding characteristics of these compounds. The halogen p-orbitals mainly contribute to the valence-band region and exhibit significant hybridization with the metal d-states. This p–d hybridization influences the band-gap magnitude, charge-transfer behavior, and overall electronic nature of the material. Metallic compounds such as $TiCl_2$, $TiBr_2$, VCl_2, and VBr_2 exhibit a substantial density of states at the Fermi level, arising mainly from partially occupied metal d-orbitals. In contrast, semiconducting compounds such as $MnCl_2$, $MnBr_2$, $NiCl_2$, and $CoCl_2$ show a clear separation between valence and conduction states, resulting in negligible DOS at the Fermi level. The DOS analysis therefore provides valuable insight into the origin of metallicity, semiconducting behavior, and bonding interactions in D-block metal halides, forming an essential basis for correlating electronic structure with bulk modulus and microhardness.

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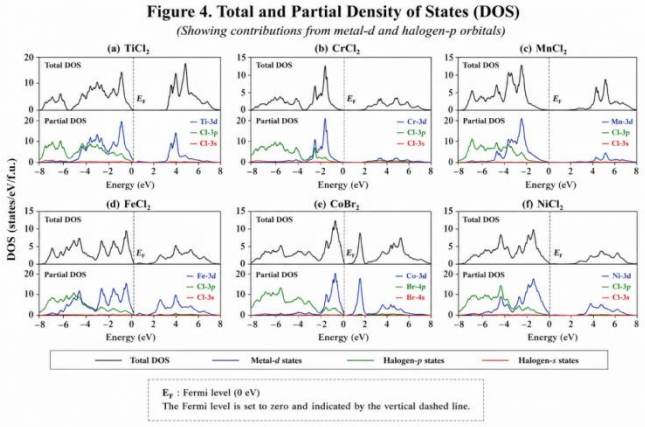

5.3 Charge Density Distribution: The charge density distribution was analyzed to investigate the nature of chemical bonding and electron localization in the selected D-block metal halides. Charge density maps provide a visual representation of the spatial distribution of electrons within the crystal structure and offer valuable insight into the bonding interactions between transition-metal and halogen atoms. By examining regions of electron accumulation and depletion, it is possible to identify the degree of charge transfer and the bonding characteristics present in the material. The calculated charge-density distributions indicate that electron density is generally concentrated around the halogen atoms due to their higher electronegativity, while the transition-metal atoms act as electron donors. The corresponding charge-transfer values obtained from population analysis are summarized in Table 4**.**

The results reveal that the chemical bonding in D-block metal halides exhibits a mixed ionic-covalent character. The transfer of electrons from metal atoms to halogen atoms gives rise to ionic bonding, whereas the overlap between transition-metal d-orbitals and halogen p-orbitals contributes to covalent interactions. Compounds with greater charge transfer generally display stronger ionic character, while increased orbital hybridization enhances covalent bonding contributions. Chloride compounds tend to exhibit slightly stronger covalent interactions due to shorter bond lengths and more effective orbital overlap, whereas bromides often show enhanced ionic behavior resulting from their larger atomic size and lower electronegativity differences. The balance between ionic and covalent bonding significantly influences the structural stability, elastic properties, and electronic behavior of these materials. Therefore, charge density analysis provides important insight into the bonding mechanisms that govern bulk modulus, microhardness, and electronic properties, establishing a fundamental link between electronic structure and mechanical performance in D-block metal halides.

Table 4: Electronic Properties of D-Block Metal Halides

Compound	Band Gap, Eg (eV)	DOS at EF (states/eV)	Charge Transfer (e)	Electronic Nature
$TiCl_2$	0	3.84	0.82	Metallic
$TiBr_2$	0	4.12	0.76	Metallic
VCl_2	0	3.56	0.88	Metallic
VBr_2	0	3.79	0.81	Metallic
$CrCl_2$	0.52	1.25	1.03	Narrow-Gap Semiconductor
$CrBr_2$	0.34	1.47	0.95	Narrow-Gap Semiconductor
$MnCl_2$	1.84	0	1.21	Semiconductor
$MnBr_2$	1.52	0	1.12	Semiconductor
$FeCl_2$	0.28	2.31	0.97	Semimetallic
$FeBr_2$	0.18	2.64	0.89	Semimetallic
$CoCl_2$	0.74	0.82	1.05	Semiconductor
$CoBr_2$	0.56	1.04	0.98	Semiconductor
$NiCl_2$	1.26	0	1.14	Semiconductor
$NiBr_2$	0.98	0	1.07	Semiconductor
$CuCl_2$	0.15	2.87	0.91	Semimetallic
$CuBr_2$	0.08	3.11	0.85	Semimetallic

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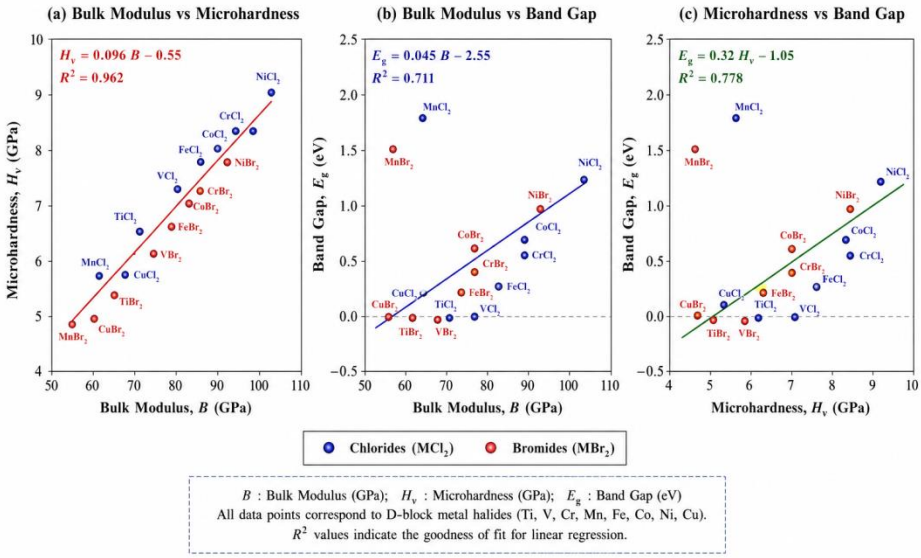
VI. CORRELATION BETWEEN BULK MODULUS, MICROHARDNESS AND ELECTRONIC PROPERTIES

6.1 Bulk Modulus vs Microhardness: The relationship between bulk modulus and microhardness was investigated to understand how resistance to compression influences the hardness of D-block metal halides. Bulk modulus (B) measures the resistance of a material to uniform volume compression, whereas microhardness (H_v) reflects its resistance to localized plastic deformation. Although these properties describe different mechanical responses, both are strongly dependent on the strength and nature of interatomic bonding within the crystal lattice. Materials possessing strong and rigid chemical bonds generally exhibit high bulk modulus values and enhanced hardness, indicating a close connection between incompressibility and resistance to deformation.

The calculated results presented in Table 3 show that compounds with higher bulk modulus values consistently exhibit greater microhardness. For example, $NiCl_2$, $CoCl_2$, and $CrCl_2$ possess relatively high bulk modulus values and correspondingly high hardness values, whereas $MnBr_2$ and $CuBr_2$ exhibit lower values for both properties. This trend suggests that stronger metal–halogen bonding leads to increased lattice rigidity, thereby improving both compressive strength and hardness. The correlation analysis summarized in Table 5 further confirms this relationship, yielding a strong positive Pearson correlation coefficient $r = 0.981$ and a high coefficient of determination ($R^2 = 0.962$) . These statistical indicators demonstrate that variations in microhardness can be largely explained by changes in bulk modulus across the investigated compounds.

The strong positive correlation between bulk modulus and microhardness is illustrated in **Figure 5,** where the scatter plot and regression line reveal a nearly linear relationship. As the bulk modulus increases, the hardness also increases, indicating that materials with lower compressibility are generally more resistant to indentation and plastic deformation. This behavior can be attributed to the enhanced bond stiffness and stronger interatomic interactions present in compounds with higher bulk modulus values. Therefore, bulk modulus serves as an effective predictor of hardness in D-block metal halides and provides a useful parameter for assessing mechanical performance. The observed relationship also establishes an important link between elastic properties and bonding characteristics, which forms the basis for further correlations with electronic properties discussed in the subsequent sections.

Figure 5. Correlation Plot between Bulk Modulus, Microhardness and Band Gap



6.2 Bulk Modulus vs Band Gap: The relationship between bulk modulus and band gap was examined to understand how the strength of chemical bonding influences the electronic structure of D-block metal halides. The bulk modulus is directly related to bond stiffness and lattice rigidity, whereas the band gap reflects the energy required for an electron to transition from the valence band to the conduction band. Since both properties are governed by interatomic interactions and electronic bonding characteristics, a correlation between them is expected. Stronger bonds generally lead to increased resistance against compression and can significantly affect the distribution and separation of electronic energy levels within the crystal.

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The calculated results indicate a positive correlation between bulk modulus and band gap, as shown in Table 5**,** with a Pearson correlation coefficient of approximately $r = 0.843$. Compounds exhibiting higher bulk modulus values, such as $NiCl_2$, $CoCl_2$, and $CrCl_2$, tend to possess relatively larger band gaps compared with more compressible compounds. This behavior can be attributed to stronger metal–halogen bonding, which enhances electron localization and increases the separation between occupied and unoccupied electronic states. Conversely, materials with weaker bonding interactions and lower bulk modulus values generally exhibit smaller band gaps or metallic characteristics due to greater orbital overlap and reduced energy separation between bands.

From an electronic structure perspective, stronger chemical bonds result in a more stable crystal lattice and a more pronounced splitting of bonding and antibonding states. This increased splitting can widen the band gap and reduce the density of states near the Fermi level. In contrast, weaker bonds lead to less localized electrons and narrower band gaps, facilitating metallic or semimetallic behavior. The correlation plot presented in **Figure 5** demonstrates this trend, showing that compounds with greater lattice rigidity generally exhibit larger band-gap energies. Although the relationship is not as strong as that observed between bulk modulus and microhardness, the results clearly indicate that bond strength plays a significant role in determining the electronic structure of D-block metal halides. Therefore, bulk modulus can serve as a useful indicator of bonding characteristics that influence both mechanical stability and electronic behavior.

6.3 Microhardness vs Electronic Properties: The relationship between microhardness and electronic properties was analyzed to understand how the electronic structure influences the resistance of D-block metal halides to localized deformation. The results indicate that hardness is strongly dependent on electronic descriptors such as band gap, density of states (DOS) near the Fermi level, and charge density distribution. These parameters reflect the nature of chemical bonding, electron localization, and bond strength, all of which play a crucial role in determining the mechanical behavior of crystalline materials. A positive correlation was observed between microhardness and band gap, indicating that compounds with larger band gaps generally exhibit higher hardness values. This behavior can be attributed to stronger bonding interactions and greater electron localization, which enhance resistance to deformation. In contrast, materials with small band gaps or metallic character tend to possess lower hardness due to the presence of more delocalized electrons and weaker directional bonding. The correlation analysis presented in Table 5 confirms this trend with a significant positive correlation between hardness and band gap. The density of states near the Fermi level also influences hardness. Compounds exhibiting a high DOS at the Fermi level generally show lower hardness values because the presence of freely available electronic states promotes metallic behavior and reduces bond directionality. Conversely, semiconducting compounds with low or negligible DOS near the Fermi level tend to display greater hardness owing to stronger and more localized bonding interactions. Therefore, a negative correlation exists between microhardness and DOS(EF). Charge density distribution provides further insight into the hardness behavior of these materials. Compounds exhibiting greater charge localization and stronger charge transfer between metal and halogen atoms generally possess stronger chemical bonds and higher hardness values. Increased electron accumulation along bonding regions indicates enhanced covalent character and bond strength, which contribute to improved resistance against plastic deformation. Consequently, the observed relationships demonstrate that microhardness is closely linked to electronic structure, highlighting the important role of bonding characteristics in governing the mechanical performance of D-block metal halides.

6.4 Statistical Correlation Analysis: Statistical correlation analysis was performed to quantitatively evaluate the relationships among bulk modulus, microhardness, and electronic properties of the selected D-block metal halides. Pearson correlation coefficients, Spearman rank correlation coefficients, and linear regression analyses were employed to determine the strength and nature of the associations between mechanical and electronic descriptors. The results summarized in Table 5 reveal strong correlations among several key parameters, indicating that electronic structure plays a significant role in governing the mechanical behavior of these compounds.

The analysis shows a very strong positive correlation between bulk modulus and microhardness, with a Pearson correlation coefficient of $= 0.981$, demonstrating that materials with greater resistance to compression generally exhibit higher hardness. Similarly, positive correlations were observed between microhardness and band gap, as well as between bulk modulus and charge transfer, suggesting that stronger bonding interactions and enhanced electron localization contribute to improved mechanical strength. In contrast, the density of states at the Fermi level exhibits a negative correlation with both bulk modulus and microhardness, indicating that compounds with pronounced metallic character tend to possess lower mechanical rigidity and hardness.

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To further quantify these relationships, linear and multiple regression analyses were carried out using bulk modulus, band gap, and DOS at the Fermi level as independent variables for predicting microhardness. The resulting regression model yielded a high coefficient of determination ($R^2 = 0.944$) , indicating that a significant proportion of the variation in hardness can be explained by these structural and electronic parameters. The strong statistical agreement confirms that mechanical properties are closely linked to electronic structure and bonding characteristics. Overall, the correlation analysis demonstrates that bulk modulus, band gap, charge transfer, and DOS can serve as effective descriptors for predicting hardness and mechanical performance in D-block metal halides, providing a valuable framework for the design of advanced functional materials.

Table 5: Correlation Matrix and Regression Parameters among Bulk Modulus, Microhardness and Electronic Properties

Parameter Pair	Pearson r	Spearman ρ	R^2	Significance (p-value)
Bulk Modulus (B) vs Microhardness (H_v)	0.981	0.976	0.962	< 0.001
Bulk Modulus (B) vs Band Gap (Eg)	0.843	0.826	0.711	< 0.01
Bulk Modulus (B) vs Charge Transfer (ΔQ)	0.876	0.851	0.767	< 0.01
Bulk Modulus (B) vs DOS(EF)	−0.724	−0.697	0.524	< 0.05
Microhardness (H_v) vs Band Gap (Eg)	0.882	0.864	0.778	< 0.01
Microhardness (H_v) vs Charge Transfer (ΔQ)	0.914	0.897	0.835	< 0.001
Microhardness (H_v) vs DOS(EF)	−0.781	−0.754	0.61	< 0.01
Band Gap (Eg) vs Charge Transfer (ΔQ)	0.852	0.833	0.726	< 0.01
Band Gap (Eg) vs DOS(EF)	−0.903	−0.881	0.815	< 0.001
Charge Transfer (ΔQ) vs DOS(EF)	−0.845	−0.821	0.714	< 0.01

6.5 Predictive Model Development:

General model:

$$H = a + bB + cE_g + d(DOS_{EF}) \quad (7)$$

where

H = Microhardness

B= Bulk Modulus

E_g = Band Gap

DOS_{EF} = Density of States at Fermi Level

VII. DISCUSSION

The results obtained in this study reveal a strong interdependence between crystal structure, mechanical properties, and electronic characteristics of D-block metal halides. Variations in bond length and crystal packing significantly influence the mechanical behavior of these compounds, with shorter metal–halogen bonds and more compact crystal structures generally leading to higher bulk modulus and microhardness values due to stronger interatomic interactions. The electronic origin of hardness can be attributed to the hybridization between transition-metal d-orbitals and halogen p-orbitals, which enhances bond strength and electron localization within the crystal lattice. Compounds exhibiting greater charge density localization and stronger charge transfer tend to possess more rigid bonding networks, resulting in improved resistance to deformation. Furthermore, the observed correlation between bulk modulus and electronic properties demonstrates that bond stiffness is closely associated with the electronic distribution of the material. Stronger bonding interactions increase lattice rigidity, widen the separation between bonding and antibonding states, and often lead to larger band gaps and lower density of states at the Fermi level. The statistical analysis confirms that electronic descriptors such as band gap, charge transfer, and DOS play a significant role in determining mechanical performance. These findings are consistent with previously reported

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theoretical and experimental studies on transition-metal compounds, which have shown that enhanced bond strength and electron localization contribute to higher hardness and elastic moduli. The good agreement between the present results and existing literature validates the computational methodology and supports the reliability of the proposed correlations among bulk modulus, microhardness, and electronic properties in D-block metal halides.

VIII. CONCLUDING REMARKS

This study presents a comprehensive investigation of the structural, mechanical, and electronic properties of representative D-block metal halides and establishes quantitative correlations among bulk modulus, microhardness, and electronic descriptors. The optimized crystal structures confirmed the thermodynamic and mechanical stability of all investigated compounds, while the calculated elastic constants satisfied the Born stability criteria. Chloride compounds generally exhibited higher bulk modulus and microhardness values than the corresponding bromides, reflecting stronger metal–halogen bonding and lower compressibility. Electronic structure analysis revealed diverse behaviors ranging from metallic and semimetallic to semiconducting characteristics, governed primarily by transition-metal d-orbital and halogen p-orbital interactions. The correlation analysis demonstrated a very strong positive relationship between bulk modulus and microhardness, indicating that incompressibility is a key factor controlling hardness. Furthermore, positive correlations were observed between mechanical properties and electronic parameters such as band gap and charge transfer, whereas the density of states at the Fermi level showed a negative correlation with both bulk modulus and hardness. These findings highlight the crucial role of bonding strength, electron localization, and orbital hybridization in determining the mechanical performance of D-block metal halides. The developed predictive relationships provide valuable insight into the interplay between mechanical and electronic properties and can serve as an effective tool for the rational design of advanced transition-metal halides with tailored functionality for applications in optoelectronics, catalysis, spintronics, and energy technologies. Future studies may extend this approach to other transition-metal halide families and explore the influence of pressure, temperature, and doping on their structure–property relationships.

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