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FIRST-PRINCIPLES INVESTIGATION OF THE ELECTRONIC PROPERTIES OF MONOLAYER MoS_2 USING DFT-BASED QuantumATK SIMULATIONS

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In this work, the electronic properties of monolayer molybdenum disulfide (MoS_2) were investigated using density functional theory (DFT) within the QuantumATK simulation environment. The band structure and density of states (DOS) calculations reveal that MoS_2 possesses a direct band gap of 1.74 eV and an indirect band gap of 1.27 eV. Further analysis including partial DOS and charge density distribution was performed to examine the orbital contributions and bonding characteristics. The influence of biaxial strain (±3%) on the electronic structure was also studied, showing a tunable band gap behavior. These results provide valuable insight into the electronic characteristics of MoS_2 and support its potential applications in nanoelectronic and flexible device technologies.

Keywords: *Density Functional Theory; QuantumATK; Band Structure; Density of States; 2D Materials*

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1. INTRODUCTION

Two-dimensional (2D) transition metal dichalcogenide monolayers, particularly molybdenum disulfide (MoS_2), have emerged as promising semiconducting materials due to their unique electronic properties and potential applications in nanoelectronics and optoelectronic devices [1]. Unlike bulk MoS_2, which exhibits an indirect band gap of approximately 1.2 eV [2], monolayer MoS_2 transitions to a direct band gap semiconductor with typical values around 1.8–1.9 eV at the K point of the Brillouin zone [3]. This direct gap offers significant advantages in optoelectronics, such as efficient light emission and detection [4].

Several first-principles DFT studies have focused on the electronic structure of monolayer MoS_2. Most report a direct band gap in the range of 1.8–1.9 eV within the PBE-GGA approximation, whereas many-body GW or hybrid functional calculations predict higher values (up to ~ 2.3 eV) [5]. Moreover, the effects of biaxial strain on the band gap have been widely explored; in particular, a tensile strain typically reduces the gap by 60–90 meV per percent [6].

In addition to band gap modulation, orbital-resolved analyses such as partial density of states (PDOS) and electron density distribution have been used to understand bonding characteristics in MoS_2 [7, 8]. These tools offer insight into the contribution of Mo-d and S-p orbitals, and into the spatial distribution of electron localization, which are important for understanding electronic transport and material interactions.

While previous works have provided valuable data on the electronic properties of MoS_2, many are limited to band structure and DOS analyses, lacking complementary studies on charge density or strain-dependent electronic descriptors.

In this context, our study presents a comprehensive first-principles analysis of pristine monolayer MoS_2. Using DFT-based QuantumATK simulations, we investigate the band structure, total and partial DOS, electron density distribution, and the effect of ±3% biaxial strain on the band gap. Our findings aim to deepen the understanding of how structural deformation influences the electronic behavior of MoS_2, thus supporting future applications in flexible nanoelectronic devices.

2. COMPUTATIONAL METHOD

The structural and electronic properties of monolayer molybdenum disulfide (MoS_2) were investigated using first-principles calculations within the framework of density functional theory (DFT), as implemented in the QuantumATK simulation package. The Localized Atomic Orbital (LCAO) method was employed with the Medium basis set and norm-conserving pseudopotentials. Exchange-correlation interactions were treated using the Generalized Gradient Approximation (GGA) in the form of the Perdew–Burke–Ernzerhof (PBE) functional [9].

The initial structure of monolayer MoS_2 was constructed based on experimental lattice constants and relaxed by geometry optimization using the Quasi-Newton minimization algorithm until the maximum force on atoms was less than 0.01 eV/Å. A vacuum spacing of 20 Å was introduced along the z-direction to eliminate interlayer interactions due to periodic boundary conditions. The final optimized structure is shown in Fig. 1.

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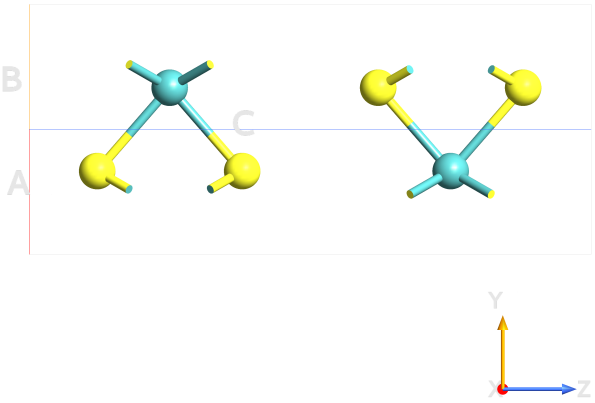

Figure 1. Relaxed atomic structure of monolayer MoS_2

The self-consistent field (SCF) procedure was enabled with a maximum of 100 iterations and energy tolerance of 10^{-5} eV. The Poisson equation for electrostatic potential was solved using the Fast Fourier Transform (FFT) solver. The k-point sampling of the Brillouin zone was performed using the Monkhorst–Pack scheme with a grid of 15×15×1 for the 2D periodic system. The mesh cutoff energy was set to 150 Hartree to ensure high numerical accuracy.

3. RESULTS AND DISCUSSION

3.1. Band Structure Analysis

The calculated electronic band structure of monolayer MoS_2 is presented in Fig. 2, where both direct and indirect band gap transitions are indicated with arrows. The results show that monolayer MoS_2 exhibits a direct band gap of 1.74 eV at the K-point, which aligns with many DFT-based predictions using the GGA-PBE approximation [9, 10]. Additionally, an indirect band gap of 1.27 eV was observed between the Γ-point (valence band maximum) and the K-point (conduction band minimum). These results demonstrate the quasi-direct nature of the band structure of monolayer MoS_2, and are in good agreement with previously reported theoretical values ranging from 1.7 to 1.9 eV [11, 12].

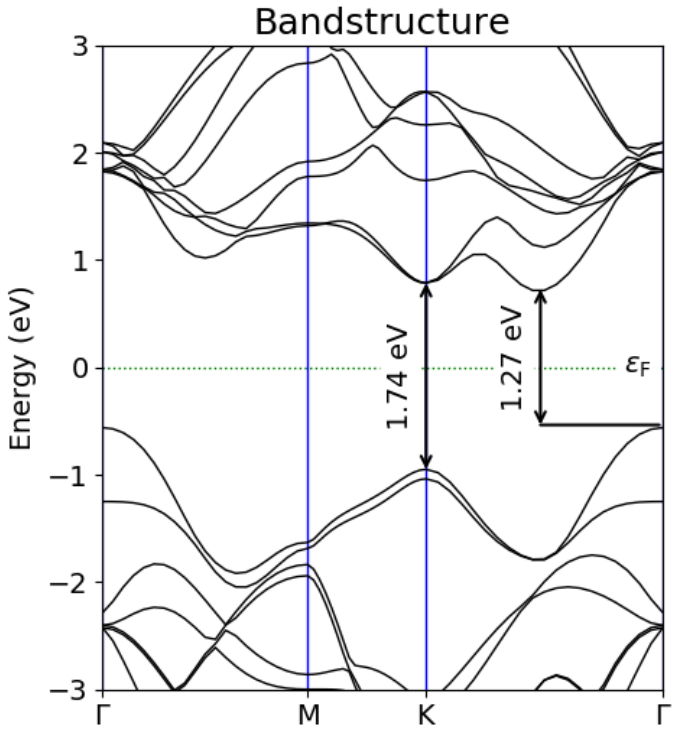

Figure 2. Calculated band structure of monolayer MoS_2 showing both direct (1.74 eV) and indirect (1.27 eV) band gaps

To support these values, the valence band maximum (VBM) and conduction band minimum (CBM) were extracted

from the band structure. The VBM is located at –0.56045 eV, and the CBM is at +0.71831 eV relative to the Fermi level, yielding a calculated gap of 1.2787 eV, which corresponds to the indirect transition. This supports the existence of a strong direct transition while also revealing possible indirect behavior, depending on external factors like strain or substrate effects.

Fig. 2. Electronic band structure of monolayer MoS_2. Both direct (1.74 eV) and indirect (1.27 eV) band gaps are marked with arrows.

3.2. Total Density of States (DOS)

The total density of states (DOS) of monolayer MoS_2 is shown in Fig. 3, where the Fermi level is aligned at 0 eV. The DOS plot clearly confirms the presence of a band gap around the Fermi level, with no electronic states in the energy range between the valence and conduction bands. The band gap value inferred from the DOS plot is approximately 1.27 eV, which is consistent with the band structure analysis discussed above.

Both spin-up and spin-down components were calculated within a spin-polarized framework. The two spin channels fully overlap, indicating the absence of exchange-induced spin polarization and confirming a non-magnetic ground state. Spin–orbit coupling (SOC) effects were not included in the present calculations; therefore, possible SOC-induced band splittings, known to occur in monolayer MoS_2, are beyond the scope of this work.

Although only the total DOS is discussed here, future analysis of the partial DOS (PDOS) will help identify the orbital contributions of the Mo (d-orbitals) and S (p-orbitals) atoms. Preliminary expectations suggest dominant Mo-4d and S-3p contributions near the band edges [13, 14].

Fig. 3. Total density of states (DOS) of monolayer MoS_2. The band gap of ~ 1.27 eV is indicated with an arrow. Fermi level is set at 0 eV.

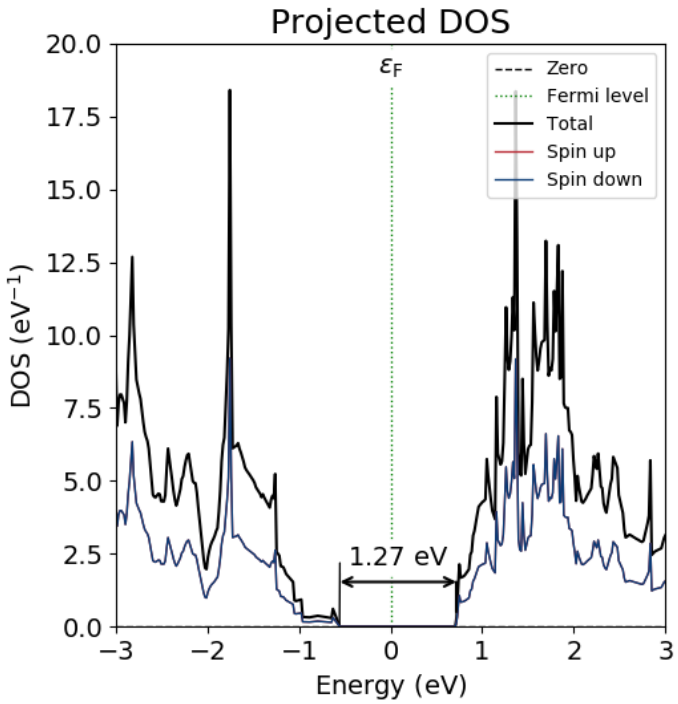

Figure 3. Total density of states (DOS) of monolayer MoS_2. The band gap of 1.27 eV is indicated

3.3. Partial Density of States (PDOS) Analysis

To gain deeper insight into the electronic structure of monolayer MoS_2, the projected density of states (PDOS) was computed and is shown in Fig. 4. The graph highlights the orbital contributions from Mo d-orbitals and S s+p orbitals. The Fermi level (ε_F) is set to 0 eV, and the calculated band gap (Eg) is clearly visible, measuring approximately 1.27 eV, consistent with previous band structure and total DOS results.

As evident from Fig. 4, the valence band maximum (VBM) is primarily composed of S 3p states, while the conduction band minimum (CBM) is dominated by Mo 4d states. This is in agreement with earlier theoretical findings, where Mo-d orbitals govern the conduction characteristics and S-p orbitals contribute to valence behavior [15, 16].

The strong contribution of Mo d-states near the conduction band edge suggests that the conduction mechanism in MoS_2 is primarily controlled by the transition metal atom. Conversely, the sulfur atoms influence the valence characteristics, which is vital for tuning optical and electronic transitions in device applications.

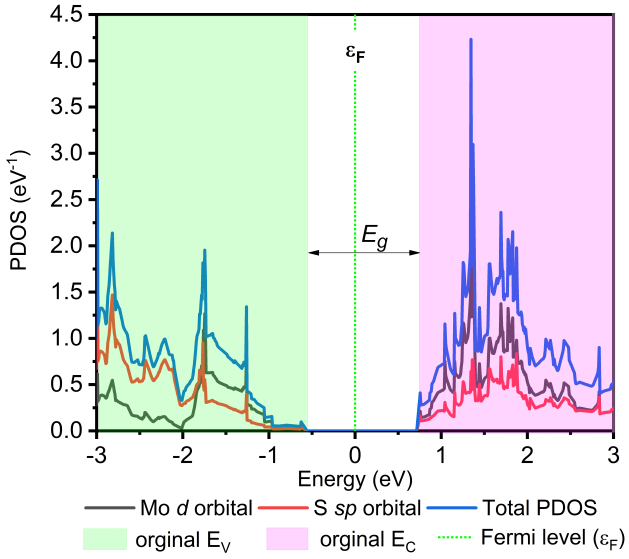

Figure 4. PDOS of monolayer MoS_2 showing total DOS, Mo d- and S s+p orbital contributions. The Fermi level ($\varepsilon_F = 0$ eV) and band gap ($E_g \approx 1.27$ eV) are indicated.

These orbital insights provide important guidelines for future work involving doping, strain engineering, or heterostructure design, where band alignment and charge transfer are sensitive to atomic orbitals.

Fig. 4. Partial density of states (PDOS) of monolayer MoS_2 showing contributions from Mo-d, S-sp orbitals. The band gap ($E_g \approx 1.27$ eV) and Fermi level (ε_F) are indicated. Color shading marks valence (E_V) and conduction (E_C) regions.

3.4. Electron Charge Density Distribution

To analyze the spatial distribution of electrons in the MoS_2 monolayer, the total electron charge density was calculated based on the self-consistent field (SCF) results. The charge density map is visualized in Fig. 5, showing a cross-sectional view along the XZ plane of the relaxed atomic structure. As observed in Fig. 5, the electron density is strongly localized around the Mo–S bonds, indicating a high degree of covalent bonding between molybdenum and sulfur atoms. The central regions of high density (colored red and green) represent the bonding areas, while the outer blue regions correspond to low-density vacuum or interlayer spacing.

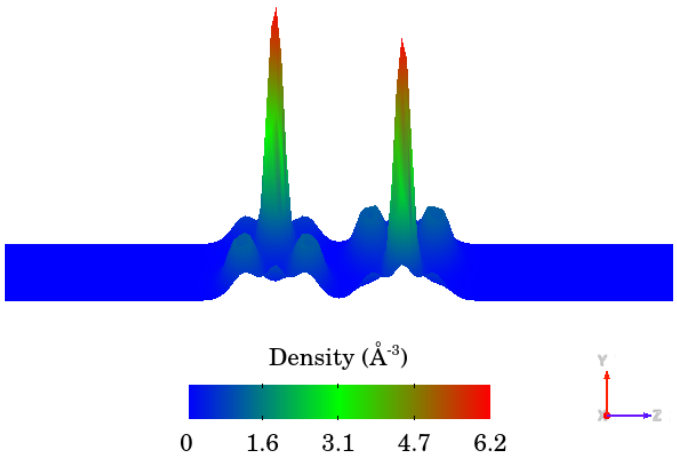

Figure 5. Electron charge density distribution of monolayer MoS_2 plotted along the XZ plane. The red and green regions indicate high electron accumulation, particularly around the Mo–S bonds, while blue areas correspond to low electron density. The color scale represents the charge density in A^{-3}

This distribution aligns well with the partial density of states (PDOS) results, where Mo-d and S-p orbitals are the

dominant contributors near the valence and conduction band edges. The symmetry and uniformity of the electron cloud also indicate structural relaxation and convergence of the optimized geometry.

Understanding the electron density map is crucial for identifying chemical reactivity zones, adsorption behavior, and defect sensitivity, which are significant in the design of optoelectronic and sensing devices based on MoS_2 and other 2D materials.

3.5. Strain Effect on the Electronic Properties

To understand the influence of biaxial mechanical deformation on the electronic properties of monolayer MoS_2, a series of calculations were performed by applying strain in the range of –3% to +3%. At each strain level, the lattice constant a was adjusted according to the equation (1):

$$a = a_0 \times (1 + \varepsilon) \tag{1}$$

where a_0=3.1604 Å and ε is the applied strain in percentage.

For each applied biaxial strain value, the in-plane lattice parameters were modified according to Eq. (1), while all internal atomic coordinates were fully relaxed under fixed strained lattice constants until the force convergence criterion (0.01 eV/Å) was satisfied. The vacuum spacing (20 Å), k-point mesh (15×15×1), mesh cutoff energy (150 Hartree), and SCF convergence parameters were kept unchanged for all strain configurations to ensure methodological consistency and reliable comparison of the calculated electronic properties.

The computed direct and indirect band gap values under various strain conditions are presented in Fig. 6 and summarized in Table 1. The results indicate that the band gap decreases almost linearly with increasing tensile strain, while compressive strain slightly enhances the band gap.

Table 1. Calculated direct and indirect band gaps of monolayer MoS_2 under various biaxial strain levels.

Strain (%)	Direct Band Gap (eV)	Indirect Band Gap (eV)
–3	2.1169	1.4879
–2	1.9853	1.5209
–1	1.8476	1.3042
0	1.7364	1.2787
+1	1.6286	1.1425
+2	1.5289	0.9527
+3	1.4366	0.7747

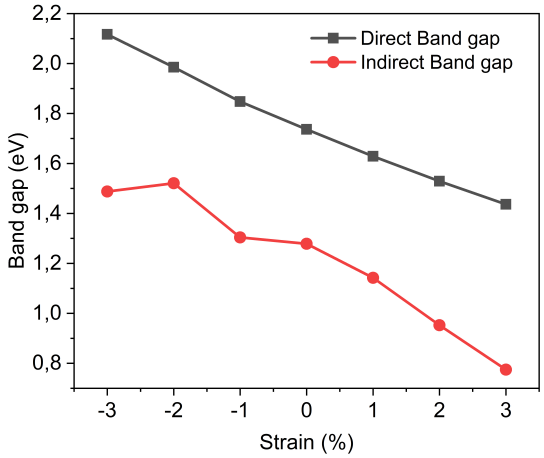

Figure 6. Variation of direct and indirect band gaps of monolayer MoS_2 under biaxial strain from –3% to +3%. The band gaps were extracted from calculated band structures at each strain level.

Specifically, the direct band gap decreased from 2.12 eV (–3%) to 1.44 eV (+3%), and the indirect band gap reduced from 1.49 eV to 0.77 eV. At 0% strain, the direct gap is 1.7364 eV and the indirect gap is 1.2787 eV, consistent with the earlier band structure results. This trend agrees with previous theoretical studies [1, 2], which report that tensile strain weakens interatomic interactions, narrowing the band gap. Furthermore, the transition from indirect to more pronounced

indirect band gap under large tensile strain suggests strain-induced electronic phase tunability, making MoS_2 a promising material for flexible electronics and strain-engineered devices.

4. CONCLUSIONS

In this study, the electronic properties of monolayer MoS_2 were systematically investigated using the density functional theory (DFT) approach implemented in QuantumATK with the LCAO basis set. The structural optimization was followed by calculations of the band structure, density of states (DOS), projected density of states (PDOS), charge density, and the effects of biaxial strain on the band gap.

The calculated band structure revealed that monolayer MoS_2 possesses a direct band gap of 1.74 eV and an indirect band gap of 1.27 eV, which is in good agreement with previously reported theoretical values. The total and partial DOS analysis showed that the Mo-d and S-p orbitals are the dominant contributors near the Fermi level, confirming the strong covalent interaction between the atoms. The charge density distribution further illustrated the bonding characteristics and electron localization along the Mo–S bonds.

The influence of biaxial strain on the electronic structure was also explored. It was found that increasing tensile strain led to a gradual decrease in both direct and indirect band gaps, with values ranging from 2.12 eV to 1.44 eV (direct) and 1.49 eV to 0.77 eV (indirect) over a strain range of –3% to +3%. These findings demonstrate the potential of strain engineering for tuning the electronic properties of 2D materials such as MoS_2.

Overall, the results confirm that monolayer MoS_2 exhibits tunable electronic behavior, making it a promising candidate for future applications in nanoelectronics, optoelectronics, and flexible device technologies.

Acknowledgments

The authors declare that there is no conflict of interest regarding the publication of this paper.

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REFERENCES

[1] K. F. Mak, C. Lee, J. Hone, J. Shan, and T. F. Heinz, "Atomically Thin MoS_2: A New Direct-Gap Semiconductor," Phys. Rev. Lett. **105**, 136805 (2010). https://doi.org/10.1103/PhysRevLett.105.136805

[2] A. Ramasubramaniam, "Large excitonic effects in monolayers of molybdenum and tungsten dichalcogenides," Phys. Rev. B, **86**, 115409 (2012). https://doi.org/10.1103/PhysRevB.86.115409

[3] J. Shi, T. Yu, M. Yang, *et al.*, "First-principles study of MoS_2 under strain," Superlattices Microstruct. **185**, 107912 (2023). https://doi.org/10.1016/j.spmi.2023.107912

[4] J. Kang, S. Tongay, J. Zhou, J. Li, and J. Wu, "Band offsets and heterostructures of two-dimensional semiconductors," Appl. Phys. Lett. **102**, 012111 (2013). https://doi.org/10.1063/1.4774090

[5] S. I. Sim, D. K. Lim, Y. M. Kim, *et al.*, "Photoluminescence of monolayer MoS_2 fabricated by chemical vapor deposition method," J. Korean Phys. Soc. **66**, 1789–1794 (2015). https://doi.org/10.3938/jkps.66.1789

[6] H. Fang, S. Chuang, T. C. Chang, K. Takei, T. Takahashi, and A. Javey, "High-performance single layered WSe_2 p-FETs with chemically doped contacts," Nano Lett. **12**, 3788–3792 (2012). https://doi.org/10.1021/nl301702r.

[7] L. Yu, Y. Chen, W. Zhang, P. Yang, and X. Feng, "Spin-Orbit-Coupling-Governed Optical Absorption in Bilayer MoS_2 via Strain, Twist, and Electric Field Engineering," Nanomaterials, **15**(14), 1100 (2025)/ https://doi.org/10.3390/nano15141100

[8] H. Rezania, M. Abdi, and B. Astinchap, "The effects of spin-orbit coupling on optical properties of monolayer MoS_2 due to mechanical strains," Sci. Rep. **13**, 1159 (2023). https://doi.org/10.1038/s41598-023-28258-z

[9] L. Yu, Y. Chen, W. Zhang, P. Yang, and X. Feng, "Spin-Orbit-Coupling-Governed Optical Absorption in Bilayer MoS_2 via Strain, Twist, and Electric Field Engineering," Nanomaterials, **15**(14), 1100 (2025). https://doi.org/10.3390/nano15141100

[10] W.-J. Lan, H.-X. Li, T. Du, X. Lin, and F. Pan, "Strain modulation on electronic structures and magnetic properties of Fe-doped monolayer 2H-MoS_2: A first-principles study," Eur. Phys. J. B, **98**, 24 (2025). https://doi.org/10.1140/epjb/s10051-025-00872-y

[11] H. Gan, G. Zhou, H. Zhang, and X. Hua, "Strain engineering of electronic and thermoelectric properties in MoS_2/WSe_2 bilayer heterostructure," Chem. Phys. **599**, 112859 (2025). https://doi.org/10.1016/j.chemphys.2025.112859

[12] A. Samy, S. Zeng, M. D. Birowosuto, and A. El Moutaouakil, "A review on MoS_2 properties, synthesis, sensing applications and challenges," Crystals, **11**(4), 355 (2021). https://doi.org/10.3390/cryst11040355

[13] B. Radisavljevic, A. Radenovic, J. Brivio, V. Giacometti, and A. Kis, "Single-layer MoS_2 transistors," Nat. Nanotechnol. **6**, 147–150 (2011). https://doi.org/10.1038/nnano.2010.279

[14] Q. Yue, S. Chang, J. Kang, X. Zhang, and S. Qin, "Mechanical and electronic properties of monolayer MoS_2 under elastic strain," Phys. Lett. A, **376**, 1166–1170 (2012). https://doi.org/10.1016/j.physleta.2012.02.021

[15] B. K. Ismaylov, K. A. Ismailov, N. F. Zikrillaev, A. E. Atamuratov, S. V. Koveshnikov, Z. T. Kenzhaev, M. M. Khalilloev, and P. K. Dilimbetov, "Investigation of the behavior of nickel impurity atoms in the silicon lattice based on first principles," East European Journal of Physics, (3), 48 (2025). https://doi.org/10.26565/2312-4334-2025-3-48

[16] T. Li, and G. Galli, "Electronic properties of MoS_2 nanoparticles," J. Phys. Chem. C, **111**, 16192–16196 (2007). https://doi.org/10.1021/jp0743773.

ДОСЛІДЖЕННЯ ЕЛЕКТРОННИХ ВЛАСТИВОСТЕЙ МОНОШАРУ MoS_2 З ПЕРШИХ ПРИНЦИПІВ ЗА ДОПОМОГОЮ DFT-МОДЕЛЮВАННЯ В QuantumATK

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У цій роботі електронні властивості моношару дисульфіду молібдену (MoS_2) досліджувалися з використанням теорії функціоналу густини (DFT) у середовищі моделювання QuantumATK. Розрахунки зонної структури та густини станів (DOS) показали, що MoS_2 має прямий заборонений зонний проміжок шириною 1,75 еВ та непрямий — 1,44 еВ. Додатково було проведено аналіз часткової густини станів (PDOS) та розподілу густини заряду з метою вивчення внеску орбіталей та характеристик хімічного зв'язування. Також було досліджено вплив біаксіального механічного напруження (±3%) на електронну структуру, що продемонструвало можливість керування шириною забороненої зони. Отримані результати надають цінну інформацію про електронні властивості MoS_2 та підтверджують його перспективність для застосування в наноелектроніці та гнучких електронних пристроях.

Ключові слова: *теорія функціонала густини; QuantumATK; зонна структура; густина станів; двовимірні матеріали*