FIRST-PRINCIPLES STUDY OF MONOLAYER CrS_2 AS ANODE MATERIAL FOR VEHICLE FUEL CELL

Yahui Qiao[1], Yiyang Liu[1], Fei Wang[2]*
[1]School of Intelligent Engineering, Zhengzhou College of Finance and Economics, Zhengzhou, 450000, China
[2]International Laboratory for Quantum Functional Materials of Henan, School of Physics, Zhengzhou University, Zhengzhou 450001, China

Abstract - Fuel cell vehicles have been widely regarded as a highly promising development direction in the new energy vehicle sector due to their significant low carbon emissions, outstanding environmental friendliness, and excellent energy conversion efficiency. However, the high manufacturing cost of negative electrode materials in fuel cells, has become one of the key bottlenecks restricting their large-scale commercial application. Therefore, exploring and screening new negative electrode materials with excellent performance and controllable costs has become a research focus and hotspot in this field. As an emerging two-dimensional (2D) layered material, single-layer chromium sulfide (CrS_2) demonstrates great potential for application as a negative electrode material in calcium-ion (Ca^{2+}) batteries due to its unique physicochemical properties. To deeply evaluate its performance, this paper systematically investigates the key electrochemical characteristics of monolayer CrS_2 as a negative electrode material for Ca^{2+} batteries using first-principles calculations based on density functional theory (DFT). The calculation results show that the migration and diffusion energy barrier of Ca^{2+} in monolayer CrS_2 is extremely low, with the calculated barrier being only 0.14 eV. Additionally, monolayer CrS_2 exhibits a very high theoretical specific capacity, reaching 1848.34 $mAh \cdot g^{-1}$. Monolayer CrS_2 demonstrates significant advantages in aspects such as Ca^{2+} adsorption stability, ion migration kinetics, theoretical calcium storage capacity, and operating voltage characteristics, confirming its great potential as a high-performance negative electrode material for calcium-ion batteries. This provides important theoretical support for the development of next-generation energy storage devices with high energy density and low cost.

Keywords: Anode material, Monolayer CrS_2, Fuell cell, First-principles, Density functional theory.

1.Introduction

With the development of economy and technology, the production and sales volume of automobiles in the world have continued to rise. In recent years, global vehicle ownership has ranked first in the world, making it the largest automotive consumer globally. However, with the continuous increase in oil prices, petroleum-based fuels face significant threats. Therefore, the development of new energy has become an inevitable choice for the automotive industry's growth. As an efficient and clean energy source, fuel cells can directly convert chemical energy into electrical energy [1]. Fuel cell vehicles, which utilize the electrical energy generated by fuel cells for power propulsion, represent one of the development directions for the new energy vehicle industry. Thus, the development of chemical energy holds great significance for addressing energy scarcity and environmental pollution issues. Common electrochemical energy storage devices include primary batteries, secondary batteries, and super capacitors, which enable the mutual conversion between chemical energy and electrical energy to facilitate people's lives [2].

Primary batteries, such as the dry batteries in daily life, can only convert chemical energy into electrical energy. Once discharged, they cannot be recharged to their original state and are not reusable. Secondary batteries, also known as rechargeable batteries or storage batteries, enable frequent conversion between chemical energy and electrical energy and can be reused. Electrochemical energy storage primarily relies on reusable secondary batteries. Currently, electrochemical energy storage systems represented by lithium-ion batteries meet

dx.doi.org/10.17683/ijomam/issue21.18

requirements such as low cost, long lifespan, and high safety, making them a vital component of the energy storage field [3]. However, lithium-ion batteries have strict requirements for electrode materials. Due to their high energy density, they are prone to severe consequences such as combustion and explosion caused by thermal runaway. Additionally, the scarcity of lithium resources inevitably restricts the long-term development of the lithium-ion industry. Statistics show that lithium accounts for only 0.0065% of the Earth's crust, with 70% of global lithium reserves concentrated in South America. As demand for lithium-ion batteries continues to grow, lithium resources may struggle to meet future needs. Against this backdrop, researching new non-lithium-ion batteries is crucial for the future development of electrochemical energy storage systems. Currently, ion batteries based on Na^+ [4], K^+ [5], Mg^{2+} [6], Ca^{2+} [7], and Al^{3+} [8] have garnered widespread attention. Among them, calcium-ion batteries have proven to be a viable alternative to lithium-ion batteries. Compared to lithium, calcium offers advantages such as safety, abundant crustal reserves, and low cost. Meanwhile, the divalent nature of calcium ions can provide higher energy density than monovalent lithium, giving calcium-ion batteries a theoretical capacity twice that of lithium-ion batteries. In the future, calcium-ion batteries are more likely to meet the demand for higher energy density energy storage.

In ion batteries, anode materials play a pivotal role in determining battery performance, making the search for high-performance anode materials to enhance ion battery capabilities an urgent priority. Currently, common anode materials for metal-ion batteries include carbon-based materials (mesophase carbon microspheres, artificial graphite, etc.), lithium titanate, silicon-carbon alloys, and so on. Recently, an increasing number of researchers have turned to novel two-dimensional (2D) materials as anode materials for ion batteries, such as graphene, silicene [9], phosphorene [10], arsenene, antimonene, and transition metal dichalcogenides (TMDs) [11]. The monolayer structure and large specific surface area of 2D materials endow them with fast ion diffusion capabilities and abundant ion insertion channels, imparting special properties to the base materials of ion batteries[12]. Among them, single-layer TMDs have shown broad application prospects in hydrogen evolution reaction catalysts, nanoelectronics, nanophotonics, solar cell absorber layers, anode materials, field-effect transistors, etc., becoming a hotspot in theoretical and experimental research. For example, Choi et al. reported that TMDs can be used as additive materials in Li-Se batteries to prevent the decomposition of LiPSe [13]. Additionally, TMDs can capture LiPSe more effectively than graphene. W. Shi et al. predicted that the ductile characteristics, intrinsic bandgap, and unique electro-optical properties of 2D TMDs make them applicable in multiple fields [14]. As representatives of TMDs, MoS_2 and WS_2 have received extensive attention [15-16]. In this context, Cr, as a element of Mo and W, makes monolayer CrS_2 equally worthy of study. Zhang, J. et al. found through research that doping various alkali metal atoms into monolayer CrS_2 can induce stable magnetism in the ground state of the doped system, demonstrating the possibility of monolayer CrS_2 as an anode material for ion batteries [17]. You, S., et al. pointed out that monolayer CrS_2 not only exhibits higher optical absorbance but also better piezoelectric properties than monolayer MoS_2, indicating that further research on monolayer CrS_2 is warranted [18]. Generally, 2D TMD materials are essentially non-magnetic, and regulating the electronic and magnetic properties of intrinsically non-magnetic materials through substitutional doping is an effective approach.

The high cost, durability issues, and scarcity of negative electrode materials for vehicle fuel cells have limited their application. Therefore, the development of inexpensive, stable, and efficient negative electrode materials has garnered widespread attention. In this paper, first-principles methods were employed to investigate the feasibility of calcium storage in CrS_2 monolayers. The study primarily focuses on the diffusion and adsorption of Ca atoms on CrS_2 monolayer materials, as well as the adsorption energies of Ca atoms at different sites. Additionally, performance metrics such as theoretical capacity, open-circuit voltage (OCV), diffusion characteristics, metal adsorption, electronic structure, and geometric structure were calculated.

2.Computational Method

This study employs first-principles calculations based on density functional theory (DFT), implemented using the Vienna Ab initio Simulation Package (VASP) [19-20]. The electronic exchange-correlation effects are described using the generalized gradient approximation (GGA) with the Perdew-Burke-Ernzerhof (PBE) function. The interactions between ionic cores and valence electrons are treated using the projector augmented wave (PAW) pseudopotential method. The computational parameters are set as follows: a plane-wave cutoff energy of 500 eV; convergence criteria for energy and force of 1×10^{-5} eV and 0.01 eV/Å, respectively; a vacuum layer thickness of over 15 Å perpendicular to the monolayer direction to eliminate interactions between periodic images; a 4 × 4 × 1 supercell model; and sampling of the Brillouin zone with a 5 × 5 × 1 k-point mesh using the Monkhorst-Pack method. All systems are corrected for van der Waals (vdW) interactions using the DFT-D3 method [21].

3.Results and Discussion

3.1 Structure and Electronic Properties of Monolayer CrS_2

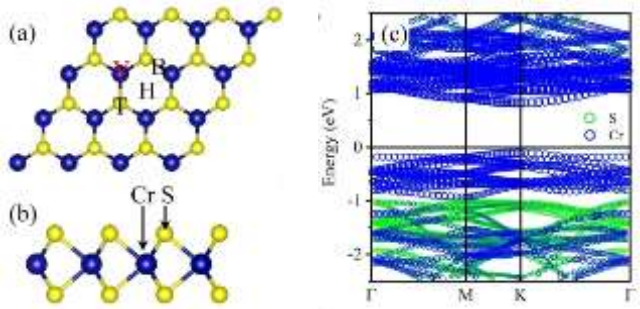
The geometric structure of the monolayer CrS_2 is shown in Figure 1 (a) and (b). The structure of monolayer CrS_2 is similar to that of graphene, exhibiting a typical hexagonal structure of two-dimensional materials. After optimization of the CrS_2 unit cell, the calculated lattice constant (a = b) is 3.05 Å, the corresponding Cr-S bond length in CrS_2 is 2.30 Å, and the interlayer distance between the upper and lower atomic layers is 2.97 Å. The bond angle of S-Cr-S in the single molecular layer is 80.31°. As shown in its energy band diagram in Figure 1(c), single-layer CrS_2 is a semiconductor with a bandgap of less than 1 eV.

To understand the interaction between the single-layer CrS_2 and Ca atoms, the most favorable adsorption positions of Ca atoms on the surface of the monolayer CrS_2 was first calculated.

Four different adsorption sites were selected on the monolayer CrS_2: the position above the Cr atom (Valley site), the position above the center of the hexagonal ring (Hollow site), the bridge position of the Cr-S bond (Bond site), and the position above the S atom (Top site), as shown in Figure 1(a). The calculation formula for the adsorption energy is:

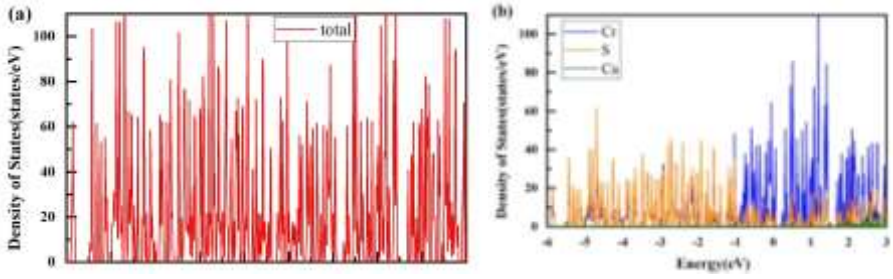
$$\Delta E = E_{CrS_2} + E_{Ca} - E_{CrS_2/Ca} \quad (1)$$

where E_{CrS2},E_{Ca}, and $E_{CrS2/Ca}$are the energies of the CrS_2 molecule, Ca ion, and CrS_2 molecule after Ca ion adsorption, respectively. The calculation results show that Ca ions placed at different positions tend to adsorb at the Valley site, with an adsorption energy of -2.55 eV. The negative adsorption energy indicates relatively stable adsorption. Additionally, the adsorption energy is greater than the cohesive energy, suggesting that Ca atoms can be stably dispersed on the material surface without forming metal clusters.



(a), (b) Structure of CrS_2 monolayer. (c) Band structure of CrS_2 monolayer
Figure 1: Schematic diagram of CrS_2 crystal structure

The results of the density of states (DOS) analysis are shown in Figure 2 (a) and (b). Significant DOS peaks near the Fermi level indicate that the two materials exhibit high carrier density, which is crucial for carrier replenishment during charge transfer processes. The partial density of states (PDOS) further reveals that the semiconducting properties primarily originate from the hybridization and overlap of the 3d orbitals of the metal element Cr and the 2p orbitals of the nonmetal element S—a feature analogous to that of other typical anode materials. In summary, the excellent metallic characteristics of these two functionalized materials ensure their outstanding electrical conductivity and high carrier density. The advantages of their semiconducting nature help reduce ohmic heat generated during battery operation and decrease the need for conductive additives. Additionally, higher carrier density generally implies higher electronic conductivity, which facilitates fast charging/discharging and reduces energy loss. These properties highlight the significant application potential of these materials as electrode materials for ion batteries.



(a) Total density of states (TDOS) of monolayer CrS_2.
(b) Partial density of states (PDOS) of monolayer CrS_2.
Figure 2: Schematic diagram of electronic structure of CrS_2

3.2 Differential Charge Density and Diffusion Barrier

To analyze the nature of bonding, differential charge density calculations were performed. The formula for the differential charge density $\Delta\rho$ between two-dimensional CrS_2 and Ca ions is:

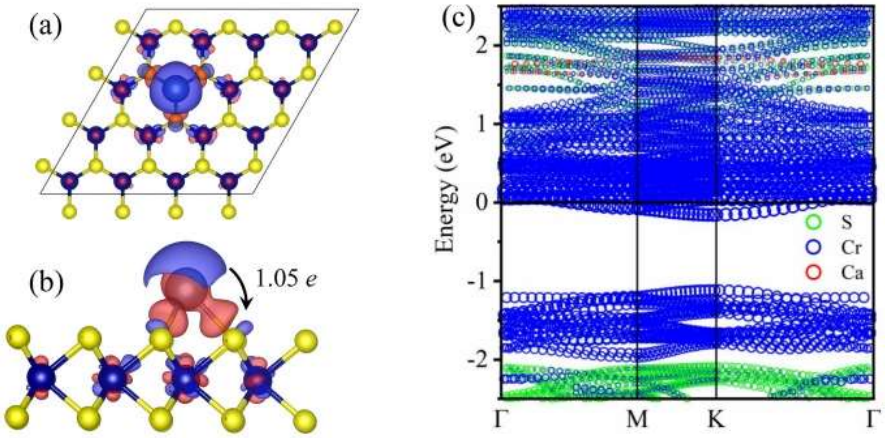
$$\Delta\rho = \rho_{CrS_2/Ca} - \rho_{CrS_2} - \rho_{Ca} \quad (2)$$

where $\rho(CaCrS_2)$, $\rho(CrS_2)$, and $\rho(Ca)$ represent the charge densities of Ca on CrS_2, pure CrS_2, and the Ca atom, respectively. As shown in Figure 3 (a) and (b), the charge distribution of Ca on the CrS_2 monolayer is visualized.

Electron accumulation and depletion are indicated by red and blue regions, respectively. In the CrS_2 monolayer, charge tends to accumulate around S atoms. Approximately 1.05 e of charge is transferred from the Ca atom to the CrS_2 surface, which facilitates chemical bond formation and prevents the aggregation of Ca into clusters.

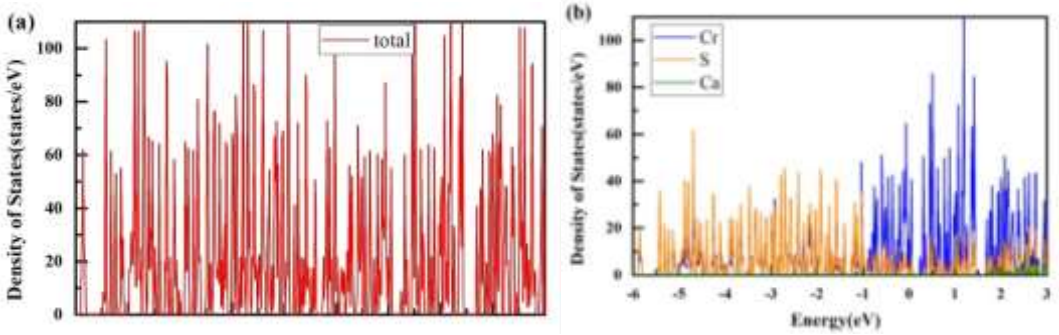
Figure 3 (c) shows that the energy bands of CrS_2 after Ca adsorption cross the Fermi level, exhibiting metallic behavior, which aligns with previous conclusions.

The metallic character of the Ca-adsorbed CrS_2 monolayer ensures good electrical conductivity during battery cycling.



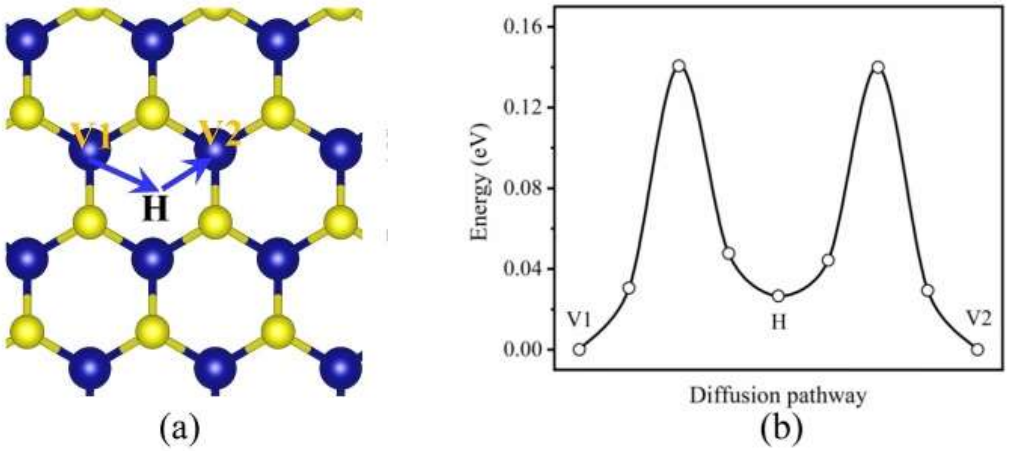
(a),(b) Differential charge density of CrS_2 monolayer adsorbed Ca ion
(c) Energy band of CrS_2 monolayer adsorbed Ca ion
Figure 3: Schematic diagram of differential charge density of CrS_2-Ca

Electron conductivity is a desirable factor in anode materials for rechargeable ion batteries. To verify the metallic properties illustrated in Figure 2, the electron density of states (DOS) of the calcified structure was calculated and displayed in Figure 4 (a) and (b). It can be clearly observed that there are electron states at the Fermi level of the monolayer CrS_2 after metallic calcium absorption, indicating that it has become a metallic system, which confirms the above-mentioned band diagram. This suggests that the monolayer CrS_2 has a sufficient concentration of free electrons during the charging and discharging process, ensuring ideal electrical conductivity. Obviously, throughout the calcification process, the conductivity of the system is enhanced, and the structure changes from semiconductor properties to metallic properties at the beginning. Therefore, the good electrical conductivity of calcification may improve its application prospects in the design of anode materials for ion batteries.



(a) Total density of states (DOS) diagram of monolayer CrS_2-Ca.
(b) Partial density of states (PDOS) diagram of monolayer CrS_2-Ca.
Figure 4: Schematic diagram of electronic structure of CrS_2-Ca

The charge/discharge rate performance of rechargeable batteries is closely related to the ionic migration kinetics of electrode materials. Therefore, CI-NEB method was employed to investigate the diffusion barrier of Ca ions on the surface of monolayer CrS_2. As shown in Figure 5 (a) and (b), the most stable adsorption site for Ca ions is the V site. The Ca atom diffuses from the V_1 site (top of the Cr atom) to the H site (hexagonal center) and then moves to the V_2 site (top of the adjacent Cr atom). The V_1–H–V_2 pathway represents the most favorable diffusion route for Ca ions, with a calculated diffusion barrier of 0.14 eV. This value is relatively low compared with other typical 2D materials (e.g., 0.25 eV for C_2N [22] and 0.29 eV for TiS_3 [23]). The low diffusion barrier facilitates Ca-ion diffusion on monolayer CrS_2, suggesting that monolayer CrS_2 is promising electrode material for Ca-ion batteries.



(a) Diffusion paths of Ca ions (b) Diffusion barriers

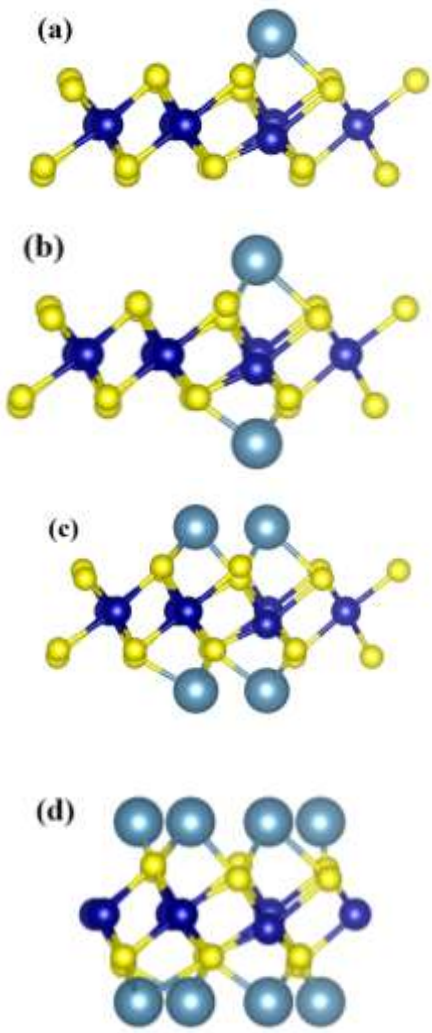
Figure 5: NEB diagram of Ca ions

3.3 Open Circuit Voltage and Theoretical Capacity

As a core parameter determining the energy density of batteries, the theoretical specific capacity requires that high-performance anode materials must exhibit significant electrochemical charge storage capabilities. In this study, a 4×4×1 supercell model was constructed, and a progressive calcification strategy was adopted to systematically investigate the calcium storage mechanism of monolayer CrS_2. As shown in Figure 6 (a), if the calcium loading is further increased, the second layer of Ca atoms will spontaneously migrate to the top sites of S atoms, after Ca atoms preferentially occupy the top sites of Cr atoms (V sites) and form symmetric saturated adsorption. It is worth noting that during the wide-range change of Ca concentration from $Ca_{0.25}CrS_2$ to Ca_4CrS_2 (with corresponding adsorption energies of -1.72, -1.95, -1.81, -1.12, and -2.10 eV), the average adsorption energy (-1.74 eV) remains stable and negative, significantly exceeding the bulk Ca binding energy (-1.69 eV). This confirms that the multi-layer adsorption process neither induces structural reconstruction nor maintains continuous strong interfacial interactions. As shown in Figure 5 (b), the ultra-low diffusion barrier (0.14 eV) of Ca ions indicates excellent rate performance, and the Ca_4CrS_2 configuration (as shown in Figure 7) exhibits the ultimate calcium storage capacity. Determine the theoretical specific capacity of the electrode material according to the following calculation formula:

$$C = xzF / M \tag{3}$$

where x represents the maximum adsorption concentration, z represents the valence electron number of Ca atoms, F represents the Faraday constant (26801 mAh/mol), and M represents the molar mass of the matrix structure. When the momolayer CrS_2 reaches the maximum saturated adsorption state, its corresponding chemical composition is Ca_4CrS_2, as shown in Figure (6). which means that each chemical formula unit (CrS_2) can stably adsorb up to 16 Ca atoms, as shown in Figure 6. Based on this high calcium loading, the calculated theoretical specific capacity is as high as 1848.34 mAh·g^{-1}. This value is significantly higher than that of commercial lithium-ion battery anode materials (such as graphite, with a theoretical value of approximately 372 mAh·g^{-1}), and far exceeds other reported calcium-ion battery anode materials, such as V_2CO_2 (335.49 mAh·g^{-1}) [24], phosphorene (865 mAh·g^{-1}) [25], and ZrS_2 (350 mAh·g^{-1}) [26]. Such a high theoretical capacity originates from the excellent accommodation capability of monolayer CrS_2 for Ca atoms, providing a key advantage for its application as an anode in high-energy-density energy storage devices.



(a) $Ca_{0.25}CrS_2$, (b)$Ca_{0.5}CrS_2$, (c)Ca_1CrS_2, (d)Ca_2CrS_2
Figure 6: Optimized structure after adsorption of multiple Ca ions

For rechargeable batteries, the open circuit voltage (V_{OC}) is another major factor affecting ion batteries. The U_{OC} can be obtained by calculating the average voltage, and its calculation formula is as follows:

$$V_{OC} = -\left[E_{Ca_2CrS_2} - E_{Ca_1CrS_2} - (X_2 - X_1)E_{Ca}\right] / (X_2 - X_1)e \quad (4)$$

where $E_{CaXCrS2}$represents the energy of monolayer CrS_2 after adsorbing Ca ions, and E_{Ca} is the energy of bulk Ca. X denotes the number of adsorbed metal cations. e=1.6*10^{-19}C. The average open circuit voltage (V_{OC}) of monolayer CrS_2 is 0.306 V, which is comparable to the open circuit voltages of anodes in conventional commercial lithium-ion batteries. For instance, the V_{OC} of TiO_2 is 1.5 V [27], and that of graphite is 0.11 V [28]. The low V_{OC} and superior theoretical storage capacity suggest that monolayer CrS_2 is a suitable electrode material.

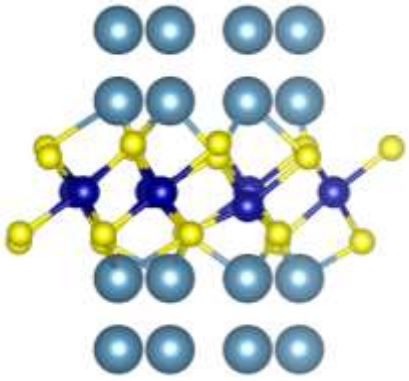


Figure 7: Optimized structure of Ca_4CrS_2

4.Conclusions

Based on first-principles calculations, this study systematically investigates the electrochemical performance of monolayer CrS_2 as a negative electrode material for calcium-ion (Ca^{2+}) batteries. The results show that Ca^{2+} can form stable adsorption configurations on the surface of monolayer CrS_2 (with an average adsorption energy of -1.74 eV), and its ultra-low diffusion barrier (0.14 eV) indicates excellent rate performance. The material also exhibits a high theoretical specific capacity of 1848.34 mAh·g^{-1}, significantly higher than that of mainstream commercial battery systems (For example, the graphite anode is approximately 372 mAh·g^{-1}). Combining its characteristics of high ion mobility, strong structural stability, and ultra-large calcium storage capacity, monolayer CrS_2 is confirmed to be a highly promising negative electrode material for calcium-ion batteries, holding significant application potential in vehicle energy storage.

References

[1] Yin, Z., Wang, H., Duan, W., et al. Research Status and Prospect Analysis of Key Technologies for Hydrogen Fuel Cell Vehicles [J]. Modern Chemical Industry, 2022, 42(10): 18-23.

[2] Fang, Y., Cheng, J., L. S., et al. Research Status and Prospect of China's Hydrogen Fuel Cell Vehicle Industry [J]. Contemporary Chemical Industry Research, 2022 (17):

[3] Goodenough, J, B., Park, K, S., The Li-ion rechargeable battery: a perspective [J]. Journal of the American Chemical Society, 2013, 135, 1167-1176.

[4] Liu, Y., Cao, R., Xia, J., Wang, J., et al. Research Progress on Low - temperature Performance of Cathode Materials for High - energy - density Sodium - ion Batteries [J]. Electric Power Science and Environmental Protection, 2025, 41(03).

[5] Chen, J., Zhang, R., Chen, Y. First-principles Study on Potential Applications of Monolayer GeTe in Lithium/Sodium/Potassium Ion Batteries [J].

Chem. J. Chinese Universities, 2024, 45(7): 20240148.
[6] Huang, Z., Zhai, C., Zhang, Y. Microstructure and Battery Performance of Mg-1Zn-1In-xCa Anode for Magnesium-Air Batteries [J]. The Chinese Journal of Nonferrous Metals, 2025, 1004-0609: 45411.
[7] Wang, R., C. D. Wessells, R. A. Huggins, et al, Highly reversible open framework nanoscale electrodes for divalent ion batteries [J]. Nano letters, 2013, 13(11), 5748-5752.
[8] Gao, J., Zeng, J., Jian, W., Mei, Y., Ni, L., Wang. H. High-valent cation (Al^{3+})-induced $Na_4Fe_3(PO_4)_2(P_2O_7)$ cathode for constructing all-climate sodium-ion full batteries [J]. Science Bulletin, 2024, 69(7): 772-783.
[9] Li, D., Liu, Y., Ma, Y., et al. Research Progress on Thermoelectric Transport Properties of Silicene [J/OL]. New Chemical Materials, 1-9 [2025-06-30]. http://kns.cnki.net/kcms/detail/11.2357.TQ.20241011.1520.001.html.
[10] Lu, Y., Dong, S., Cui, F., et al. Theoretical Study on Electronic Structure and High-Efficiency Photocatalytic Hydrogen Evolution Performance of Boron-Doped Fiber Red Phosphorene [J/OL]. Acta Physica Sinica, 1-26 [2025-06-30].
[11] Si, K., Meng, L., Gong, Y. Preparation and Physical Properties of Two-dimensional Group VB Transition Metal Dichalcogenides [J]. Chinese Journal of Rare Metals, 2019, 43(11): 1164-1178. DOI: 10.13373/j.cnki.cjrm.xy19080004.
[12] Wang, C., Guo, Z., Wang, Q., et al. First - principles Study on Thermoelectric Properties of BP/AsP Van der Waals Heterojunctions [J/OL]. Materials Review, 1-16 [2025-06-30].
[13] Choi, D, S., Yeom, M, S., Kim, Y, T., et al. Polyselenide Anchoring Using Transition-Metal Disulfides for Enhanced Lithium–Selenium Batteries [J]. Inorganic Chemistry, 2018, 57(4), 2149-2156.
[14] Shi, W., Wang, Z. Mechanical and electronic properties of Janus monolayer transition metal dichalcogenides [J]. Journal of Physics: Condensed Matter, 2018, 30(21), 215301.
[15] Chen. P., Ren. B., Zhang. C., et al. Energy Transfer and Photoluminescence Enhancement in WS_2/hBN/MoS_2 Heterojunctions (English) [J]. Chinese Journal of Luminescence, 2024, 45(12): 2021-2029.
[16] Yang, E., Ji, H., Jung, Y. Two-dimensional transition metal dichalcogenide monolayers as promising sodium ion battery anodes [J]. The Journal of Physical Chemistry C, 2015, 119(47), 26374-26380.
[17] Wang, Y., Li, W. Research on a Three-Phase High-Power ZCS-Buck Type On-Board Charger for Electric Vehicles [J]. Journal of Power Supply, 2017, 15(02): 85-93. DOI: 10.13234/j.issn.2095-2805.2017.2.085.
[18] You, S., Qin, Z., Ma, L, et al. Enhancement Mechanism of Magnetic Emission Performance of PZT MFC/Metglas Magnetoelectric Composites with MoS_2-Modified Adhesive Layer [J/OL]. Acta Physica Sinica, 1-22 [2025-06-30].
[19] Kresse, G. Ab initio molecular dynamics for liquid metals [J]. Journal of Non - Crystalline Solids, 1995, 192–193, 222–229.
[20] Kresse, G., Hafner, J. Ab initio molecular - dynamics simulation of the liquid - metal–amorphous - semiconductor transition in germanium [J]. Physical Review B: Condensed Matter and Materials Physics, 1994, 49, 14251–14269.
[21] Perdew, J, P., Burke, K., Ernzerhof, M. Generalized gradient approximation made simple [J]. Physical Review Letters, 1996, 77, 3865.
[22] Ding, Y., Deng, Q., You, C., Xu, Y. Li, J., Xiao., B. Assessing electrochemical properties and diffusion dynamics of metal ions (Na, K, Ca, Mg, Al and Zn) on a C2N monolayer as an anode material for nonlithium ion batteries [J]. Physical Chemistry Chemical Physics, 2020, 21208-21212.
[23] M. Arsentev, A. Missyul, A. V. Petrov, M. Hammouri, TiS3 magnesium battery material: atomic-scale study of maximum capacity and structural behavior [J]. The Journal of Physical Chemistry C, 2017, 121, 15509-15516.
[24] Aierken, Y., Sevik, C., Gülseren, O., Peeters, F, M., Çakır, D. MXenes/graphene heterostructures for Li battery applications: a first principles study [J]. Journal of Materials Chemistry A, 2018, 6, 2337-2345.
[25] Han, X., Liu, C., Sun, J., Sendek, A, D , Yang, W. Density Functional Theory Calculations for Evaluation of Phosphorene as a Potential Anode Material for Magnesium Batteries [J]. RSC Advances. 2018, 8, 7196-7204.
[26] RehmanS, U., Samad, A., Saeed, M., Amin, B., Hafeez, M., Mir, I, A. Computational insight of ZrS2/graphene heterobilayer as an efficient anode material [J]. Applied Surface Science, 2021, 551, 149304.
[27] Yang, Z., Choi, D., Kerisit, S., Rosso, K, M., Wang, D., Zhang, J., et al. Nanostructures and lithium electrochemical reactivity of lithium titanites and titanium oxides: A review [J]. Journal of Power Sources, 2009, 192, 588-598.
[28] Fan, X. Mao, J. Zhu, Y., Luo, C., Suo, L., Gao, T., et al. Superior stable self - healing SnP3 anode for sodium-ion batteries [J]. Advanced Energy Materials, 2015, 5, 1500174.