

Assessment of Sc-, Ti- and V-based MBene Monolayers as High-Performance Anode Materials for Supercapacitors

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Abstract

It is highly expected that future energy inventions will use supercapacitors as a key energy storage device. The investigation of novel and/or high-capacity MBenes (Transition-metal borides) based supercapacitor electrode materials is an emerging area for the research community. Two-dimensional (2D) MBenes have outstanding electrochemical performances as electrodes for energy storage applications. In the present study, first-principles calculations were utilized to assess the electrochemical characteristics of a 2D Scandium boride (ScB), Titanium boride (TiB), Vanadium boride (VB) monolayers to determine their suitability as an electrode material for supercapacitors. The negative formation energies – 13.19 eV, -16.91 eV, -18.10 eV for ScB, TiB, VB monolayers, respectively, demonstrate their stability. The ScB, TiB and VB monolayers exhibit high quantum capacitance $3029 \mu F/cm^2$, $3450 \mu F/cm^2$ and $4447 \mu F/cm^2$ at 0.6 V, respectively. The metallic nature and high quantum capacitance make ScB, VB, and TiB monolayers efficient electrode materials for supercapacitors.

1. INTRODUCTION

The rising worldwide energy demand from industrialization and globalization has made energy generation and storage a top priority for technology and research advancements [1]. Renewable energy sources, such as wind, solar, tidal, biomass, and geothermal, are infrequent and scattered as compared to the standalone gigantic facilities currently producing the majority of electricity. To address these issues, efficient and long-lasting storage devices are viable need to store the energy [2]. According to International energy agency (IEA) statistics as shown in Fig. 1, the total primary energy supply from renewable sources is increased frequently from 1971 to 2023 and demand for energy services has expanded globally, from 416 EJ to 654 EJ at the end of 2024 [3].

Thus, electrochemical energy is a critical component of the clean energy portfolio. The fuel cells, batteries and supercapacitors are the major devices working on the electrochemical energy conversion principle. However, in order to meet demand, a lot of electricity must be swiftly stored and released. Consequently, high-power energy storage devices like supercapacitors or electrochemical capacitors are now being utilized [4]. The supercapacitors or ultracapacitors usually have high-power density as compared to common capacitors, and also fill the gap between conventional capacitors and batteries by providing high power performance in a compact design. They are recently used for applications where high-power bursts are needed, like hybrid vehicles, in wind turbine pitch, in UPS, in energy harvesting systems, etc., due to their affordability, compact size, high-power density and long cycle life [4–6], etc. A supercapacitor's performance depends on its manufacturing technique and components, including electrodes, electrolyte, binder, separator, and current collector. An electrode material, in particular, plays a crucial role in the operation of a supercapacitor [5]. To achieve large capacitance, the supercapacitor must have electrodes with a large surface area, so that it can hold the additional charge, as well as there are more favourable sites for the adsorption/desorption reactions [6]. The two-dimensional electrode materials with outstanding electronic conductivity, high surface to volume ratio, better mechanical

strength, large power and energy density might be the ideal option for electrodes used for supercapacitors [7]. The commercialized electrode materials like Graphene and its derivatives, hBN etc., have been identified as a fundamental block for supercapacitors due to their versatile properties [8–9, 40]. Owing to their low quantum capacitance, new materials are required for the better performance of supercapacitors [39–42].

One interesting post-MXene, a novel series of 2D materials named MBenes (Transition metal boride), is being extensively researched due to their remarkable properties like stability, conductivity, high carrier mobility, high surface area, diverse surface chemistry properties etc [10]. Three-dimensional MAB phases, in which 'A' is generally IIIA or IVA group element, M is a transition metal (Y, Mo, Sc, V etc.), and B is a boron atom, are chemically etched and exfoliated to create 2D multilayer MBenes [11–13]. Owing to the exceptional properties, these materials have attracted significant attention from the research community for a range of energy storage devices i.e batteries, supercapacitors, and various energy conversion applications [14, 15]. Gao et al.^[16] determined the electrochemical properties of CoB nanosheets using electrochemical impedance spectroscopy, cyclic voltammetry, and galvanometer charge-discharge technique. Their findings showed that CoB alloy acts as a high-performing supercapacitor electrode material with a specific capacitance of 411 F g^{-1} . The Ni-B alloys were synthesized and characterized by Wei et al. ^[17] using an easy-to-use method based on aqueous solutions and XRD technique. Their cyclic voltammetry results as a novel high-performance electrode material demonstrated that Ni-B alloy has a high specific capacitance of 2230 F g^{-1} at 1 A g^{-1} , and can be used in efficient supercapacitors. Using a fluorine-free diluted etching approach and energy-dispersive X-ray analysis (EDX) and scanning electron microscopy (SEM), Wei et al. ^[18] examined the multilayered $\text{MoAl}_{1-x}\text{B}$. Their outcomes showed that the $\text{MoAl}_{1-x}\text{B}$ and $1/24\text{-MoAl}_{1-x}\text{B}$ alloys has the capacitance 1003.30 mF/cm^2 and 2006 mF/cm^2 , respectively. Cao et al.^[19] synthesized the graphene oxide (GO) using the Hummers process from neutral graphite and characterized it by employing SEM and Transmission electron microscopy (TEM) techniques. They chemically reduced GO and nickel dichloride ($\text{NiCl}_2 / 6\text{H}_2\text{O}$) simultaneously in a single pot to create a highly linked nickel boride (Ni_2B)/reduced graphene oxide (RGO) hybrid. Their outcomes depicted that $\text{Ni}_2\text{B/RGO}$ has a specific capacitance of 1073.4 F/g at 1 A/g , high energy density of 22.1 Wh kg^{-1} and power density of 724.9 W kg^{-1} . In order to establish the understanding of the electrochemical behavior of MBenes monolayer, the quantum capacitance of functionalized Sc_2CT_2 monolayers ($\text{T} = \text{Se, Si, P, Cl}$) was theoretically investigated by Cui et al. ^[20]. They showed that functionalized monolayers have higher quantum capacitance than the bare Sc_2C monolayer. They claimed that Sc_2CT_2 monolayers have the potential to be utilized as electrode materials in aqueous symmetric supercapacitors. A First-principles calculations of Zr_2CO_2 based on density functional theory (DFT) were carried out by Xu et al. ^[21]. They analyzed the effect of doping on the electronic properties and quantum capacitance of Zr_2CO_2 monolayer and predicted that Zr_2CO_2 preserves its semiconductor behavior after doping of Sn, Si, Ge, whereas upon N, S and F doping, it shows metallic characteristics. Their results showed that the most promising electrode material is S-doped Zr_2CO_2 , which has a maximum quantum capacitance (C_{diff}) of $3293.7 \text{ }\mu\text{F/cm}^2$. Liu et al.^[22]

analyzed the optical and electronic properties of pristine Hf_2C and functionalised Hf_2CT_2 (where T = -OH, -Se, -S, -Cl, -F, -O) using DFT and found that Hf_2CO_2 has low C_Q of $16 \mu\text{F}/\text{cm}^2$ due to its semiconductor nature, whereas metallic Hf_2CF_2 has higher C_{diff} ($930 \mu\text{F}/\text{cm}^2$). They claimed that, due to their superior C_{diff} , Hf_2CT_2 (T = Cl, OH, F, S, Se) are promising anode materials for supercapacitors.

Based on the aforementioned experimental and theoretical insight on 2D materials, this work presents a comprehensive theoretical evaluation of MBenes as potential electrode materials for supercapacitor applications. The DFT-based calculations have been planned to conduct the electrochemical performance of 2D MBene (ScB, TiB, VB) monolayers. Furthermore, the ability of these monolayers for its use as an electrode material for a supercapacitor is also aimed to be by estimating their quantum capacitance and surface charge stored.

2. METHDOLOGY

The Projector augmented wave (PAW) method, as implemented in Vienna ab initio simulation package (VASP) software [23], was used to perform the first principles calculations of electrochemical characteristics of the MBene (M = Sc, Ti, B) monolayers with Perdew-Burke-Ernzerhof (PBE) parameterisation. The generalized-gradient approximation (GGA) was used to address exchange correlation potentials [24]. To calculate the value of C_Q , a $2 \times 2 \times 1$ supercell was used for the ScB, TiB, VB monolayers, which had eight transition metal (Sc, Ti, V) atoms and eight B atoms. A $11 \times 11 \times 1$ Monkhorst-Pack grid was utilized to sample the Brillouin zone for structure optimization. For the ab-initio molecular dynamic simulation (AIMD) and Phonopy calculations, $3 \times 3 \times 1$ and $2 \times 2 \times 1$ supercells are used with k-mesh $6 \times 6 \times 1$ and $9 \times 9 \times 1$, respectively. The force and energy convergence criteria were set up to 10^{-4} eV and 10^{-6} eV $\text{\AA}^{-1}$ per cell, respectively, and $18 \times 18 \times 1$ k-points were strategically taken for the accurate determination of density of states (DOS) and band-structures. To prevent interaction with periodic images, a significant $20 \text{\AA}$ vacuum layer was incorporated in the out-of-plane direction of the ScB, TiB, and VB unit monolayers.

3. RESULTS AND DISCUSSION

3.1 Structural Properties:

The structure of the MBene monolayer is orthorhombic, having space group Cmcm (No. 63) [25] and made up of one zigzag diatomic B layer in the middle and two outermost Sc, Ti, V layers, as shown in Fig. 2

After the geometry optimization of MB (where M = Sc, Ti, V) monolayers, the lattice constants were found to be $a = 3.34 \text{\AA}/3.17 \text{\AA}/3.26 \text{\AA}$, $b = 3.09 \text{\AA}/2.95 \text{\AA}/2.88 \text{\AA}$, for ScB/TiB/VB. These parameters are consistent with earlier results [26]. It is anticipated that the minimal bond lengths between Sc-B, Ti-B, V-B and B-B atoms were found to be $2.5 \text{\AA}$, $2.35 \text{\AA}$, $2.25 \text{\AA}$, and $1.7 \text{\AA}$, respectively.

3.2 Electrochemical properties

The electrochemical properties of electrodes have a direct impact on the supercapacitor's power and energy density, allowing for constant and reliable energy delivery. The electrode material must also have a high quantum capacitance in order to store more charge during the charging process. So, in order to check the reliability of the MBenes as an electrode material, it is essential to check their stability via formation energy, phonon simulation and AIMD calculation.

3.2.1 Formation energy:

The formation energy can be used as a stability scale because it describes the amount of energy that enters or exits during a chemical reaction. A negative formation energy (E_{form}) indicates an exothermic process, while a positive E_{form} indicates an endothermic reaction. Consequently, an exothermic reaction indicates that the formed compound is more stable than its constituent elements [27].

The E_{form} was calculated in order to check the stability of relaxed structures as :

$$E_{\text{form}} = E_{\text{ScB/TiB/VB}} - E_{\text{Sc/Ti/V}} - E_{\text{B}} \quad (1)$$

Here, $E_{\text{ScB/TiB/VB}}$ denotes the total energy of pure ScB/TiB/VB monolayers, $E_{\text{Sc/Ti/V}}$ represents the total energy of individual Sc, Ti, V atoms and E_{B} is the total energy of a boron atom. The calculated formation energy of these monolayers is listed in Table 1.

Table 1
Formation energies of ScB, TiB and VB monolayers.

Monolayers	Formation energy (eV)
ScB	-13.91
TiB	-16.91
VB	-18.10

All the studied monolayers (Table 1) have negative formation energies, which confirms their stability and VB is energetically most stable among others due to its more negative E_{form} .

3.2.2 Thermodynamic Stability:

Since the electrode materials work along with electrolytes in supercapacitors, they must be thermodynamically stable [28]. The thermal stability of monolayers (ScB, TiB, VB) is typically confirmed using AIMD simulations at the first-core level [29] at a constant temperature ($T = 300 \text{ K}$) for a set amount of time (5 ps) in the canonical ensemble (NVT).

As depicted in Fig. 3, there are no noteworthy changes in structure after the 5000 simulation steps, which validate the structural integrity in these monolayers, hence ScB, TiB, and VB monolayers are thermodynamically stable at 300K. The thermodynamic stability of the studied monolayers is further supported by the progressive convergence of their total energies throughout the relaxation period (5 ps).

Furthermore, the density functional perturbation theory-based PHONOPY code was used to precisely check the dynamic stability of ScB, TiB, and VB monolayers [30] as shown in Fig. 4. The frequency indicates that along the high symmetry-directions (-G, -X, -S, -Y, -G), every vibrational mode in the 1st Brillouin zone of all of these monolayers is positive and no imaginary frequencies appear, which confirm the dynamical stability of all monolayers.

3.3 Eletronic properties :

Once the structural, dynamical and thermal stabilities of the ScB, TiB and VB monolayers were confirmed, electronic properties were subsequently analyzed within the framework of DFT. In order to see the contribution of various orbitals at and near Fermi level (E_F), the total and projected orbital density of states (DOS) were examined in Fig. 5 for all studied monolayers. The DOS present at E_F confirms the metallic nature of all monolayers, which may lead to high C_Q and power density [31]. In all the cases, the contribution of M-d states dominates at and in the vicinity of E_F , whereas B-p states have a minor contribution only in total DOS.

To further elucidate the electronic properties and to support the DOS analysis, the electronic band structure of MBene monolayers is plotted in Fig. 6 along the high symmetry direction of Irreducible B.Z. In consistence with the DOS, the ScB, TiB, and VB monolayers exhibit no band gap and multiple band crossings of the E_F , which further confirm their metallic character.

3.4 Quantum Capacitance (C_Q)

A key feature of electrode materials in supercapacitors that determine how much charge can be collected on a conductor [32]. The notion of the C_Q for graphene, which was thought of as a 2D electron gas, was first defined by Lury [33]. The C_Q of a material is defined as the rate at which excessive charges/ions vary in response to changes in applied potential [34]. The concept of C_Q is fundamentally tied to the electronic energy configuration of the electrode materials. It can be effectively defined as the derivative of the net excess charge (Q) on the substrate or electrode with respect to electrostatic potential (φ) as given in Eq. (2). This relationship highlights the importance of understanding charge dynamics in optimizing electrode performance.

$$C_Q = \frac{dQ}{d\varphi} \quad (2)$$

The double-layer capacitance (C_D) and quantum capacitance (C_Q) are connected to the total interface capacitance (C_T) of electric double-layer capacitors (EDLCs) as [35]:

$$\frac{1}{C_T} = \frac{1}{C_D} + \frac{1}{C_Q}$$

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Here, C_D is due to the interaction between the electrode and electrolyte surface, which is determined through experiment, whereas C_Q is a material intrinsic property that comes from the kinetic energy, exchange-correlation energy, and electron-phonon interaction in the total energy functional [36].

A weighted average of the electronic DOS determines the overall charge. The excess charge (ΔQ) on the electrode can be represented by an integral term [37] as:

$\Delta Q = e \int_{-\infty}^{+\infty} D(E) [f(E) - f(E-\varphi)] dE$ (4) Here $D(E)$ denotes the DOS of the studied electrode material and $f(E)$ is the Fermi-Dirac distribution and φ is the chemical potential.

The C_Q of material is related to DOS given as [34];

$$C_Q = \frac{dQ}{d\varphi} = e^2 \int_{-\infty}^{+\infty} D(E) F_T(E-e\varphi) dE$$
 (5)

Here, $F_T(E)$ represents the thermal broadening function, which is expressed as [38] :

$$F_T(E) = (4kT)^{-1} \text{sech}^2(E/2kT)$$
 (6)

The surface charge density (Q), at a particular potential φ can be calculated using this formula;

$$Q = \int_0^{\varphi} C_Q(V) dV$$
 (7)

Figure 7 shows the C_Q curves of ScB, TiB and VB monolayers as a function of applied potential in the range -0.6 V to $+0.6$ V. The C_Q is directly related to DOS as shown in equ. 5, and its values for all studied monolayers are listed in Table 2.

As we can see in Fig. 7 that at E_F , TiB has a large $C_Q \sim 3177 \mu F/cm^2$ as compared to ScB ($2771 \mu F/cm^2$) and VB ($3137 \mu F/cm^2$), which is attributed due to higher DOS present at E_F , resulting from enhanced overlapping of M-d and B-p states.

Figure 7 Quantum capacitance (C_Q) of TiB, ScB and VB monolayers with varying potential.

In the negative bias region -0.6 V to 0 V, there is a gradual increase in C_Q of ScB and TiB as potential approaches toward 0 V, which shows that charge accumulation is more at 0 V whereas VB has a stable

and large capacitance value in this region due to the presence of more uniform DOS. In contrast to this, completely different behavior is observed in the positive bias region (0 V – 0.6 V). As depicted in Fig. 7, there is a sharp rise in C_Q of VB monolayer at 0.3 V and it reaches a maximum value $\sim 4447 \mu F/cm^2$ at 0.6 V. On the other hand, there is a gradual increase in C_Q for ScB and TiB. The calculated values of C_Q for all studied materials are larger than those of other reported materials Sc_2CP_2 ($3800.34 \mu F/cm^2$) [20], Zr_2CO_2 ($1938 \mu F/cm^2$) [21], Hf_2CF_2 ($930 \mu F/cm^2$) [22].

The C_Q of these monolayers is found to be distinct for positive and negative bias, which is responsible for the asymmetric performance of the supercapacitor. This finding suggests that ScB, TiB and VB monolayers are promising anode materials for a supercapacitor due to high C_Q value at positive bias [39].

3.5 Surface Charge Storage:

The aggregation of charge per unit area at various voltages is described by the surface charge density, which acts as an important criterion for selecting suitable electrode material for supercapacitor applications. The stored surface charge of ScB, TiB, VB monolayers can be calculated using the Eq. 7 and is plotted in Fig. 8 with respect to potential within the range – 0.6 V to 0.6 V.

As we can see from Fig. 8, within the negative bias region – 0.6 V to 0 V, the magnitude of accumulated charge gradually increases for all studied monolayers. Notably, the charge storage capacity is higher for VB monolayer as compared to ScB and TiB, which is consistent with its large C_Q , under applied bias relative to ScB and TiB monolayers.

In positive bias 0 V to 0.6 V, there is a stable and consistent increment in charge for ScB and TiB monolayers, which is due to the uniform and stable enhancement in their C_Q over this potential range. The VB attains the maximum charge storage ($2801 \mu C/cm^2$) at 0.6 V due to comparatively large C_Q .

Overall, the VB monolayer exhibits maximum charge storage capacity compared to TiB and ScB monolayers at both positive and negative bias conditions. At positive bias (0.6 V), the maximal stored charge (Q_a) is $1817 \mu C/cm^2$ (ScB), $2070 \mu C/cm^2$ (TiB), $2801 \mu C/cm^2$ (VB). In Contrast, the magnitude of charge storage (Q_c) is $1390 \mu C/cm^2$ (ScB), $1516 \mu C/cm^2$ (TiB), $1878 \mu C/cm^2$ (VB), under negative bias. Our predicted results indicate that at positive bias, all the investigated monolayers have a larger charge storage capacity than at negative bias. Moreover, the VB monolayer consistently exhibits high charge storage performance at the entire potential (-0.6 V to 0.6 V) as compared to other materials like Sc_2C ($304 \mu C/cm^2$) [20], B_Nyne/Graphene ($375 \mu C/cm^2$) [45], Boron carbide/graphene ($250 \mu C/cm^2$) [47].

The ratio of the storage charge at positive bias (Q_a) and negative bias (Q_c) i.e. $\frac{Q_a}{Q_c}$ serves as one of the indicators for the selection of electrode materials for a supercapacitor. In general, if $\frac{Q_a}{Q_c}$ Values lie in the

range 0.9–1.1, the material shows symmetric behavior. When $\frac{Q_a}{Q_c}$ value is > 1.1 and < 1.1 , the material exhibits anodic and cathodic characteristics, respectively [40].

In the present work, the ratio $\frac{Q_a}{Q_c}$ for ScB, TiB and VB monolayers lies within the acceptable range of 1.2–1.5, confirming their suitability as anode materials for asymmetric supercapacitors. The calculated results are consistent with the previously reported 2D electrode materials as listed in Table 2.

Figure 8 Stored surface charge of TiB, ScB and VB monolayers with respect to potential ranging from – 0.6 V to 0.6 V.

The differential capacitance C_Q , can be obtained from the slope of the charge vs potential (Q-V) curve (Fig. 8), because C_Q is related to the variation of storage charge (Q) with applied potential (V). As we can see, the VB monolayer has a steeper slope than ScB and TiB, which further confirms the superior charge storage performance of VB monolayer. The C_Q provides additional insight into the charge storage capability of the electrode materials.

Additionally, the area under the Q vs V curve gives the energy density of the supercapacitor using the fundamental relation [41];

$$E = \int V dQ \text{ or } \frac{1}{2} CV^2 \quad (8)$$

As we can see, the capacitance and energy density are directly correlated; an increase in the capacitance corresponds to a corresponding enhancement in the energy density. Based on the calculated C_Q values, the increasing order of energy density for the studied monolayers is;

$$VB > TiB > ScB$$

The VB monolayer exhibits the highest energy density due to its large C_Q compared to ScB and TiB, which indicates its excellent charge storage capacity.

Table 2

Key performance indicators used as electrode materials for supercapacitor and comparability with other materials at 0.6 V.

Material	Quantum capacitance ($\mu F/cm^2$)	Stored charge ($\mu C/cm^2$)	Reference
ScB	3029	1817	This work
TiB	3450	2070	This work
VB	4447	2801	This work
Sc ₂ CP ₂	3800	-	[20]
Sc ₂ CSe ₂	3030		
Graphene	10.33	-	[42]
FG-Ac	60.319		[43]
FG-N	256.42		
Br-hBN	1341.71		[44]
Si-hBN	852.12		
BNyne/Graphene	360.08	375	[45]
MoS ₂ /C	500	-	[46]
Boron carbide/graphene	280.41	250	[47]

Conclusion

The DFT calculations were performed to analyze the electronic properties, quantum capacitance (C_Q), and surface stored charge of MBene monolayers (ScB, TiB, and VB) for utilizing them as electrode materials in supercapacitors. The findings of the phonon spectra and AIMD simulation demonstrated the thermodynamic stability of these monolayers. The observed asymmetric behavior of the supercapacitor is due to the different C_Q values under the negative and positive bias. Owing to high DOS in the vicinity E_F , the VB monolayer exhibits the largest C_Q ($4447 \mu F/cm^2$) as compared to ScB ($3029 \mu F/cm^2$) and TiB ($3450 \mu F/cm^2$) at 0.6 V, which enhances its capability for charge storage. Aligning with the C_Q , the VB monolayer stores a higher specific charge Q ($2801 \mu C/cm^2$) than TiB ($2070 \mu C/cm^2$) and ScB ($1817 \mu C/cm^2$). Our analysis suggests that VB monolayer has excellent charge storage and accumulation capabilities even at low potential, compared to TiB and ScB monolayers. The high C_Q and charge storage analysis highlight that the MBenes (ScB, TiB, and VB) monolayers can act as cutting-edge anode materials for asymmetric supercapacitors.

Declarations

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Author Contribution

Author's Contributions: 1. Pooja Rani: Writing-original draft, calculations performed, Conceptualization, Methodology, 2. Dr. Hardev S. Saini: Supervision, Reviewing and editing 3. Dr. Veenu Mehta: Helping in conceptualization, visualization and writing 4. Dr. Rashmi Mittal: Calculations, Validation, analysis and interpretation of results, 5. Dr. Ramsaran Saini : Helping in Writing-original draft, prepared figures 6. Dr. Manish K. Kashyap: Supervision, Reviewing and editing All authors reviewed the results and approved the final version of the manuscript.

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Data Availability

The Ungdata surveys that support the findings of this study are available from Norwegian Social Research (NOVA), but restrictions apply to the availability of these data, which were used under licence for the current study and so are not publicly available. The data are, however, available upon request and with the permission of Norwegian Social Research (NOVA).

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Figures

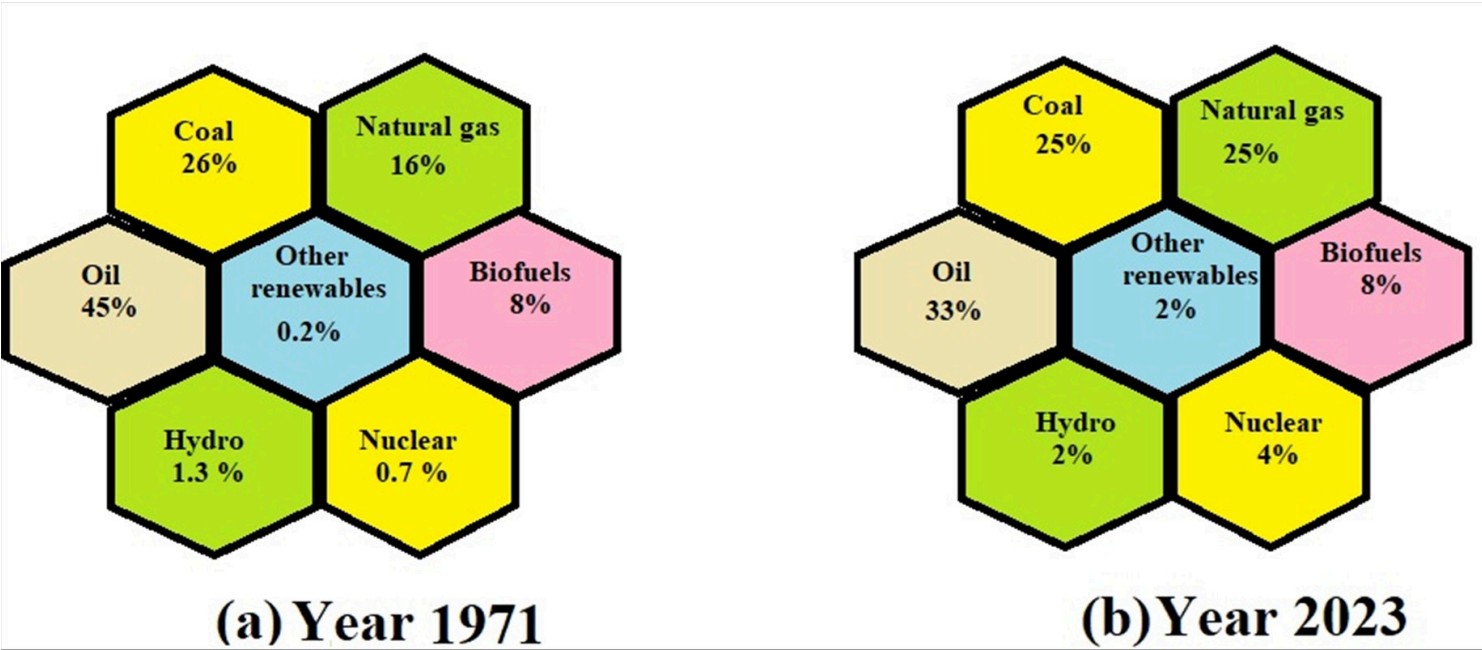


Figure 1

World total primary energy supply by various source.

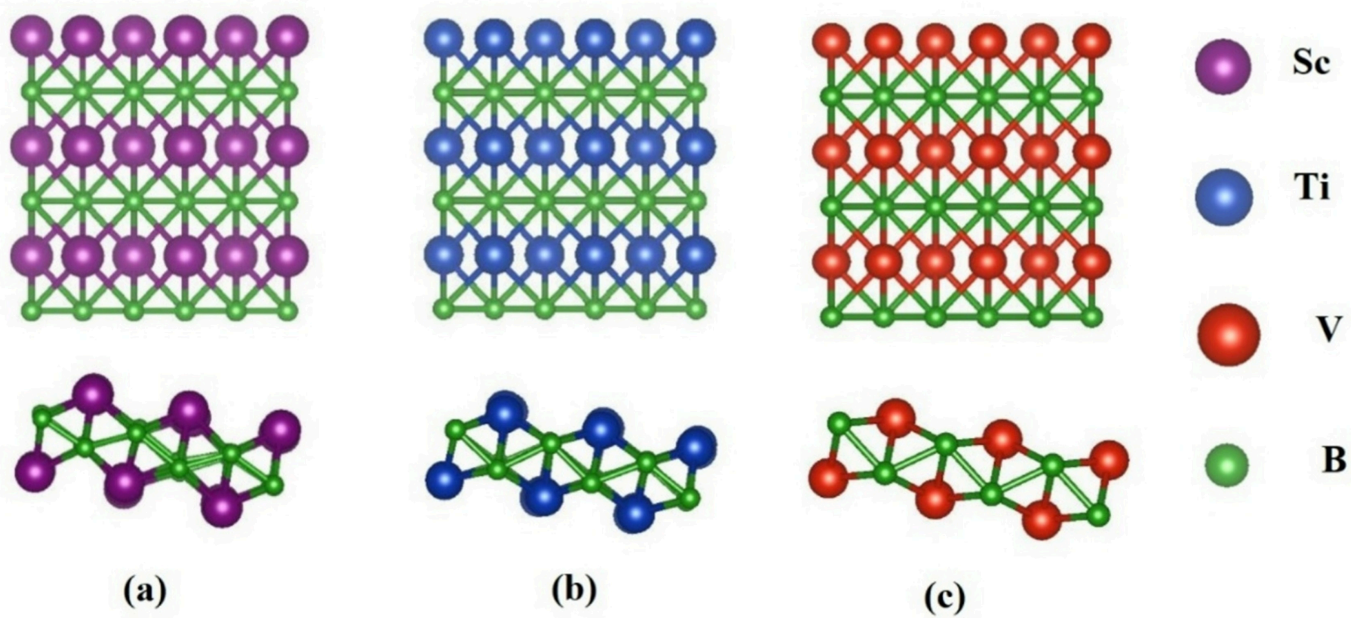


Figure 2

Top and side views of relaxed structure of (a) ScB (b) TiB (c) VB monolayers.

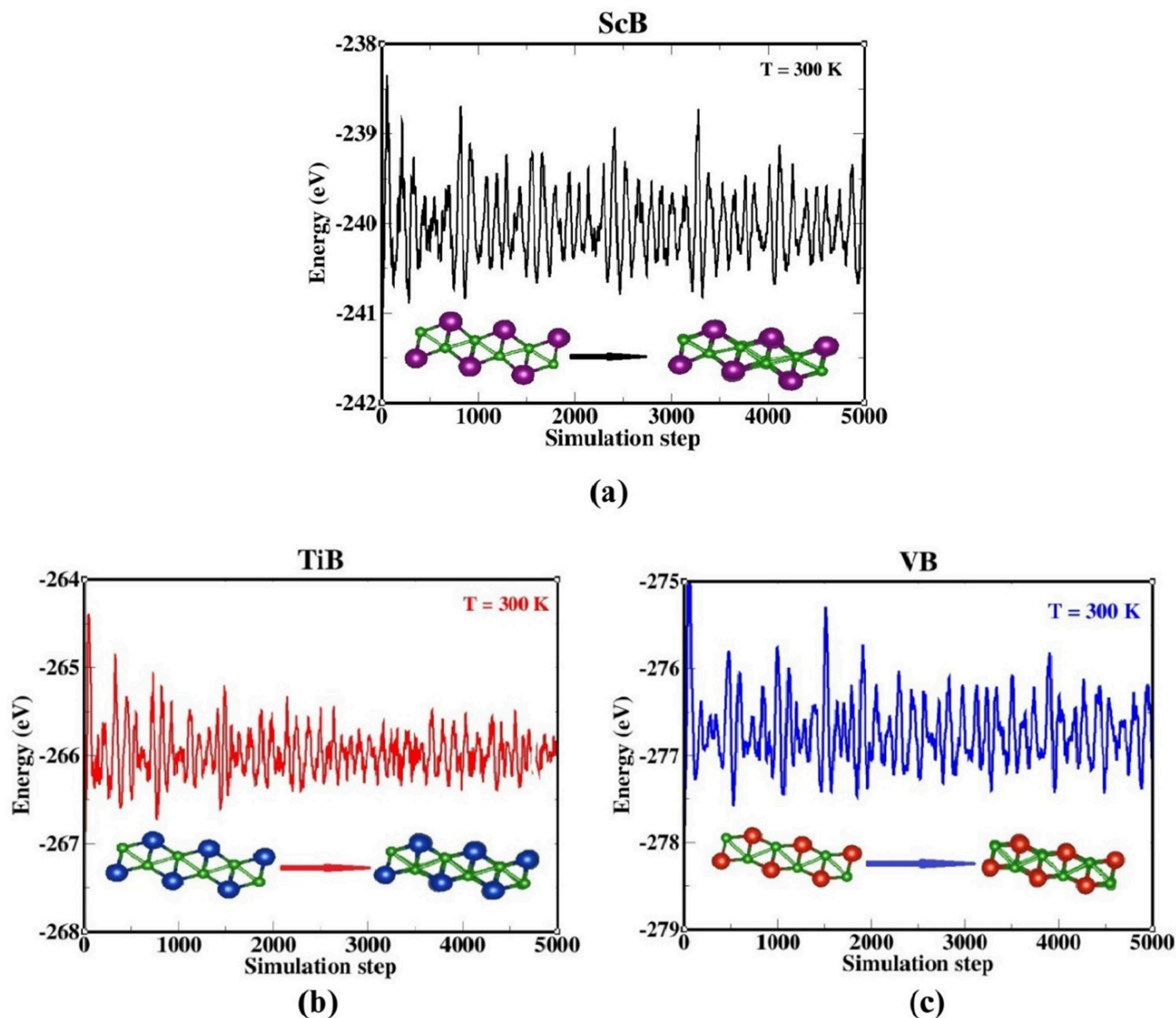


Figure 3

Energy variation of (a) ScB (b) TiB (c) VB monolayers during AIMD simulations at 300 K temperature with their corresponding structure before and after these simulations.

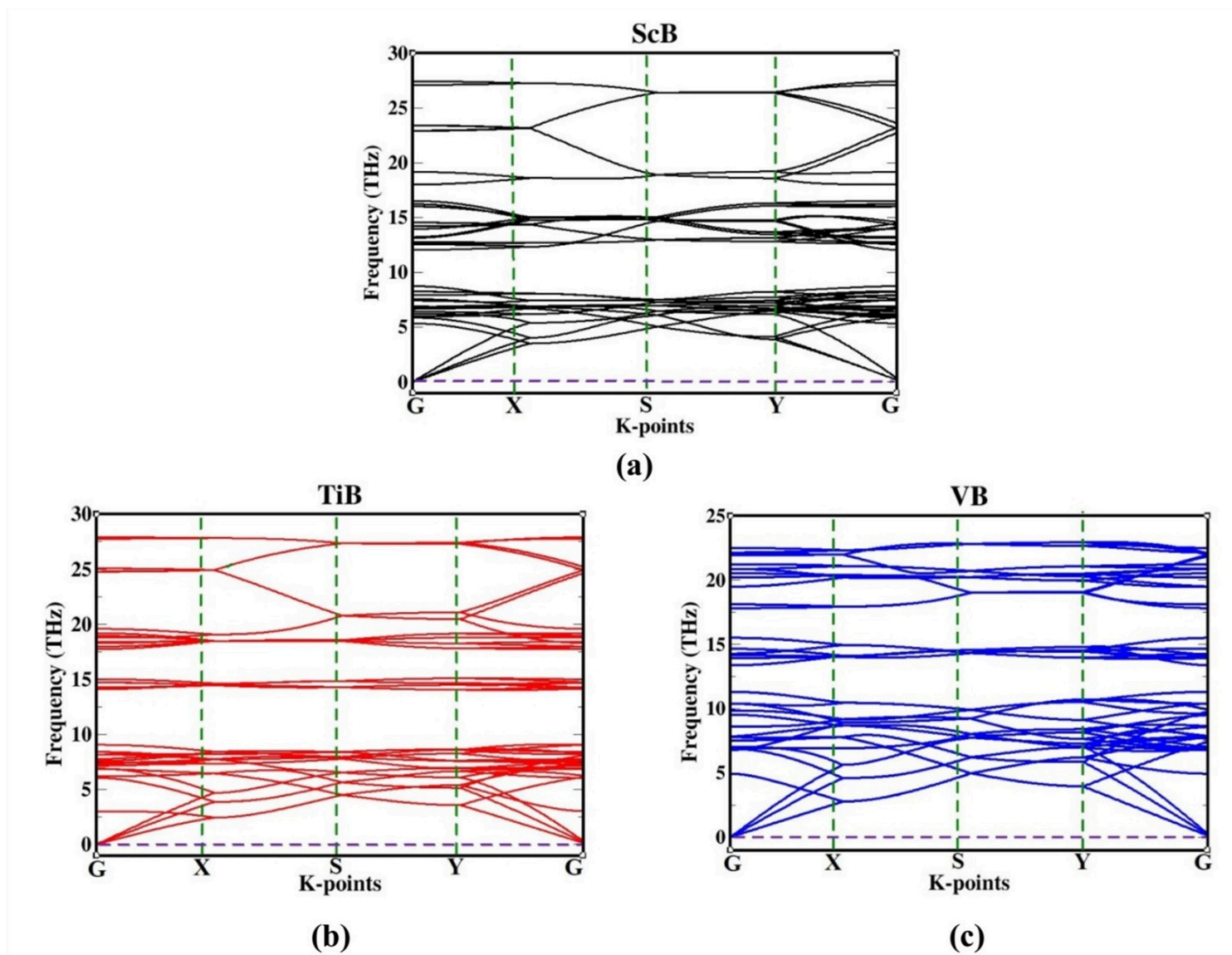


Figure 4

The phonon-dispersion spectra of (a) ScB (b) TiB (c) VB monolayers.

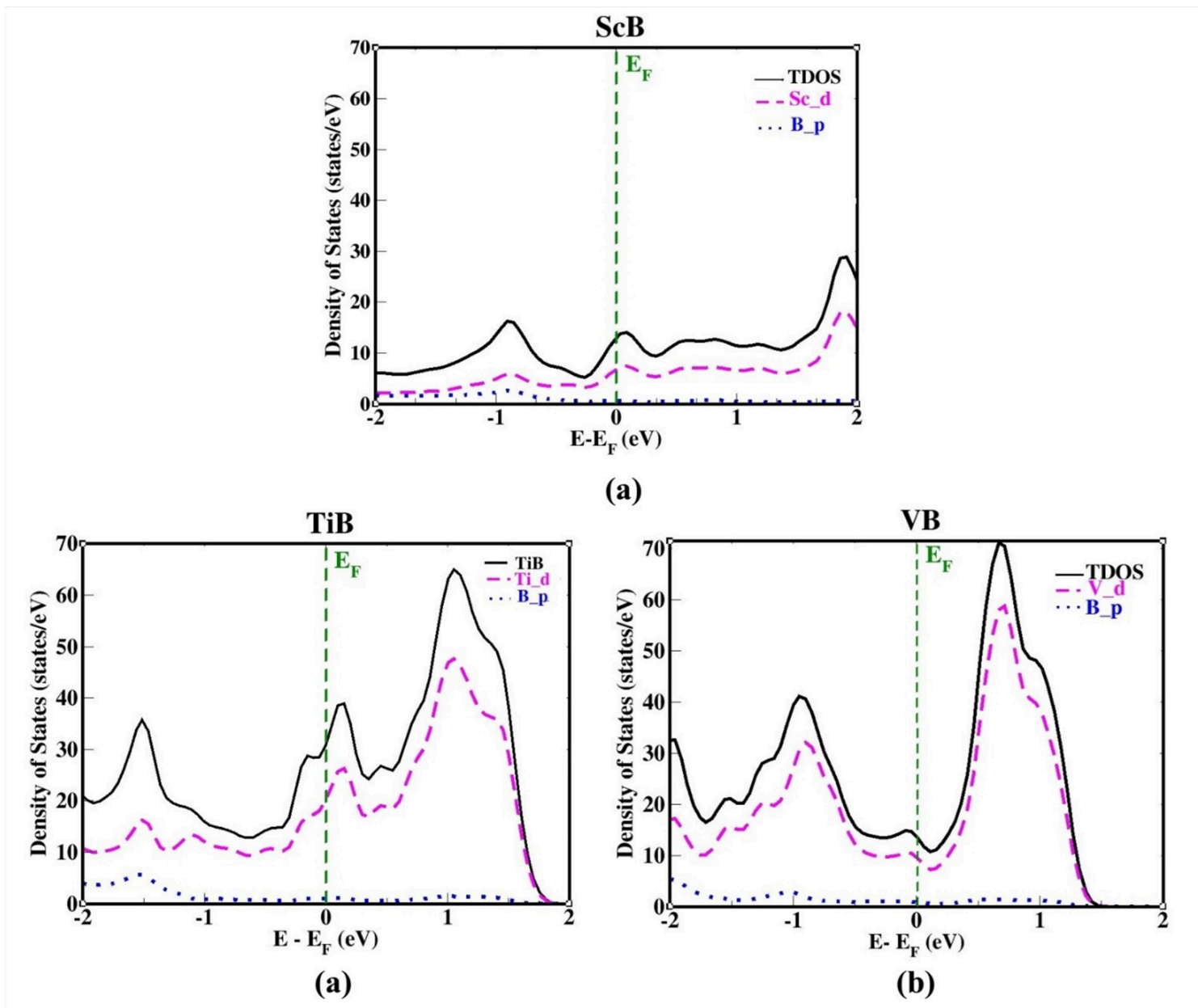


Figure 5

The total and projected density of states for (a) ScB (b) TiB (c) VB monolayers.

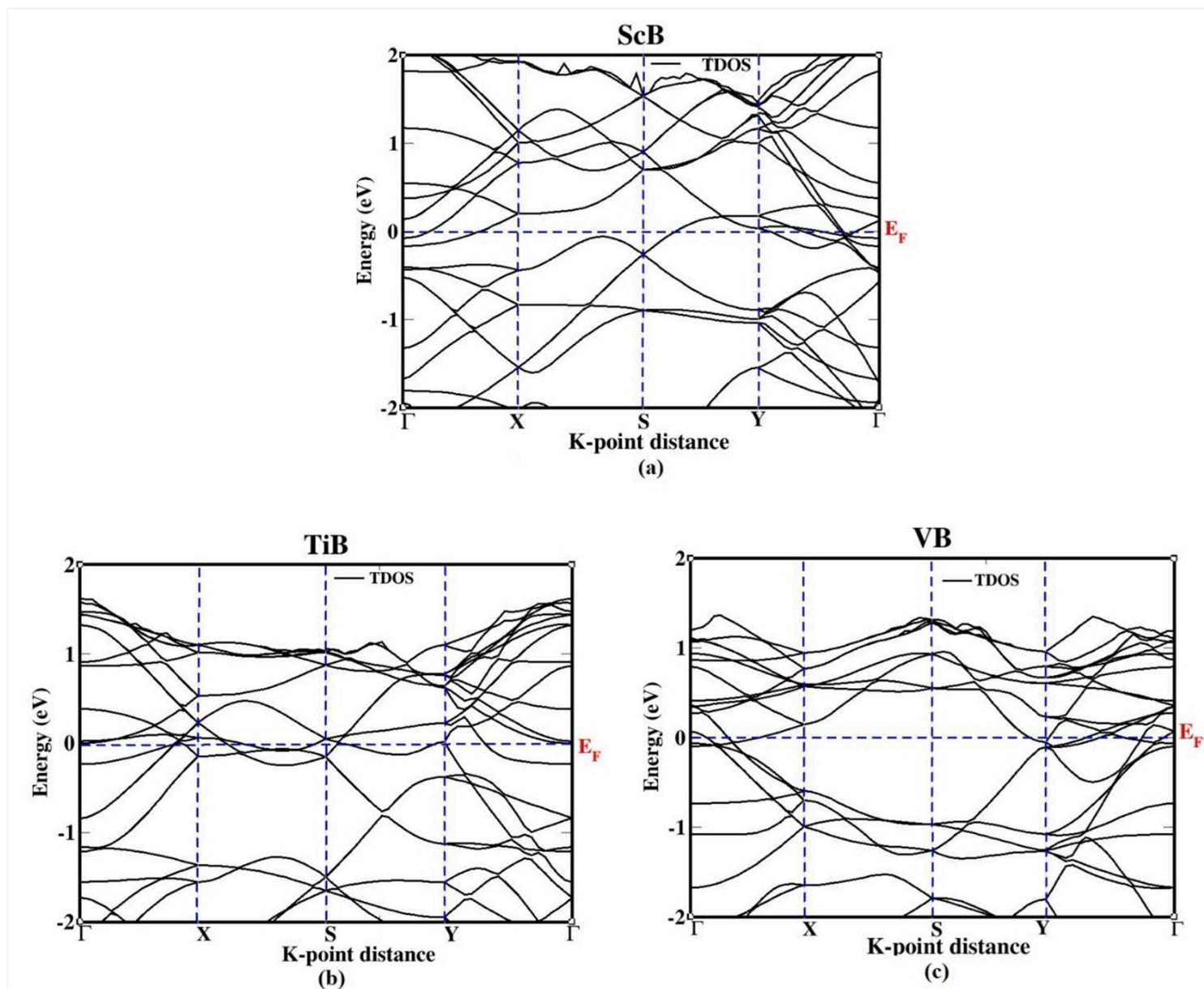


Figure 6

Calculated band structure of (a) ScB (b) TiB and (c) VB monolayers.

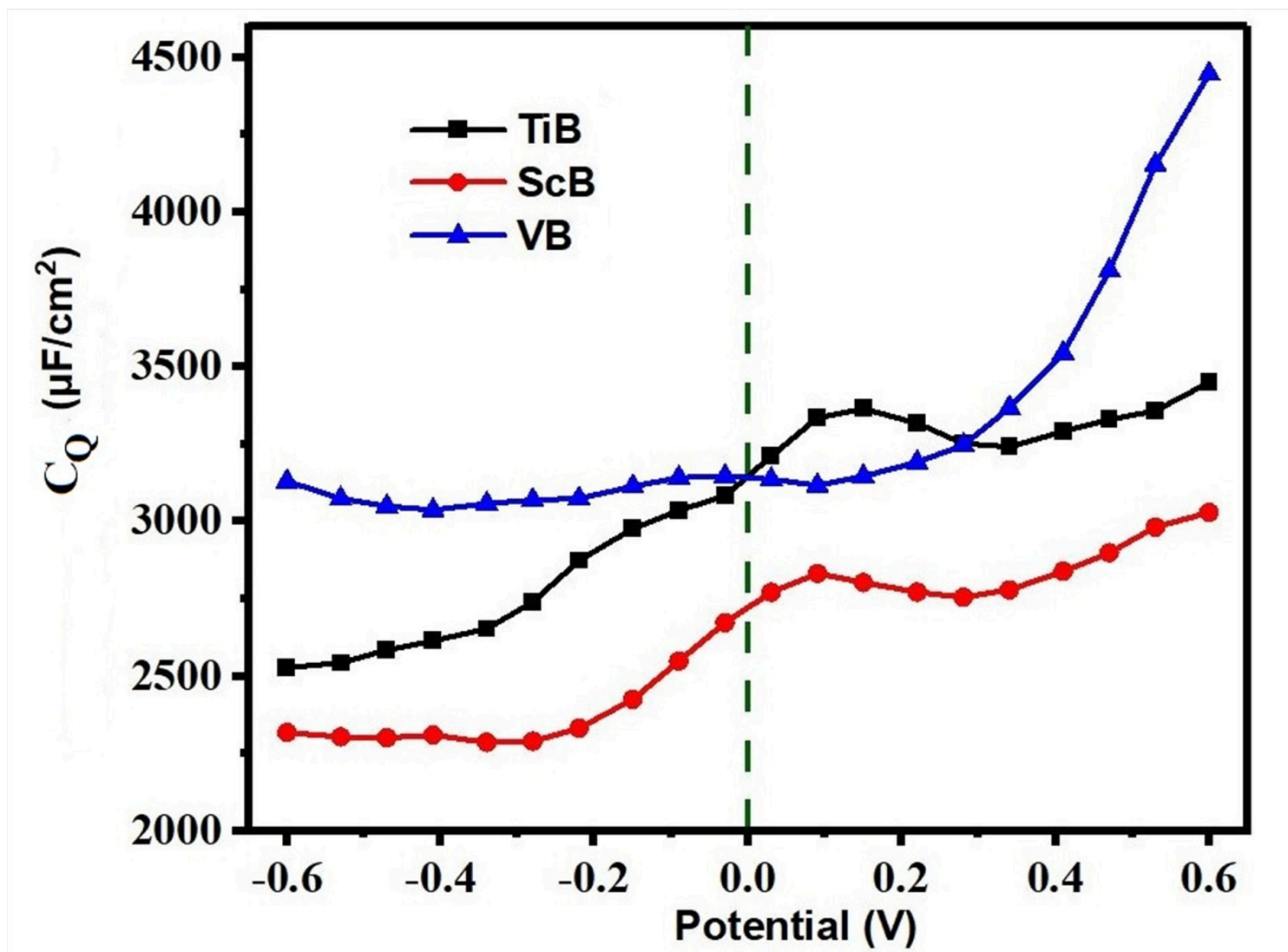


Figure 7

Quantum capacitance (C_Q) of TiB, ScB and VB monolayers with varying potential.

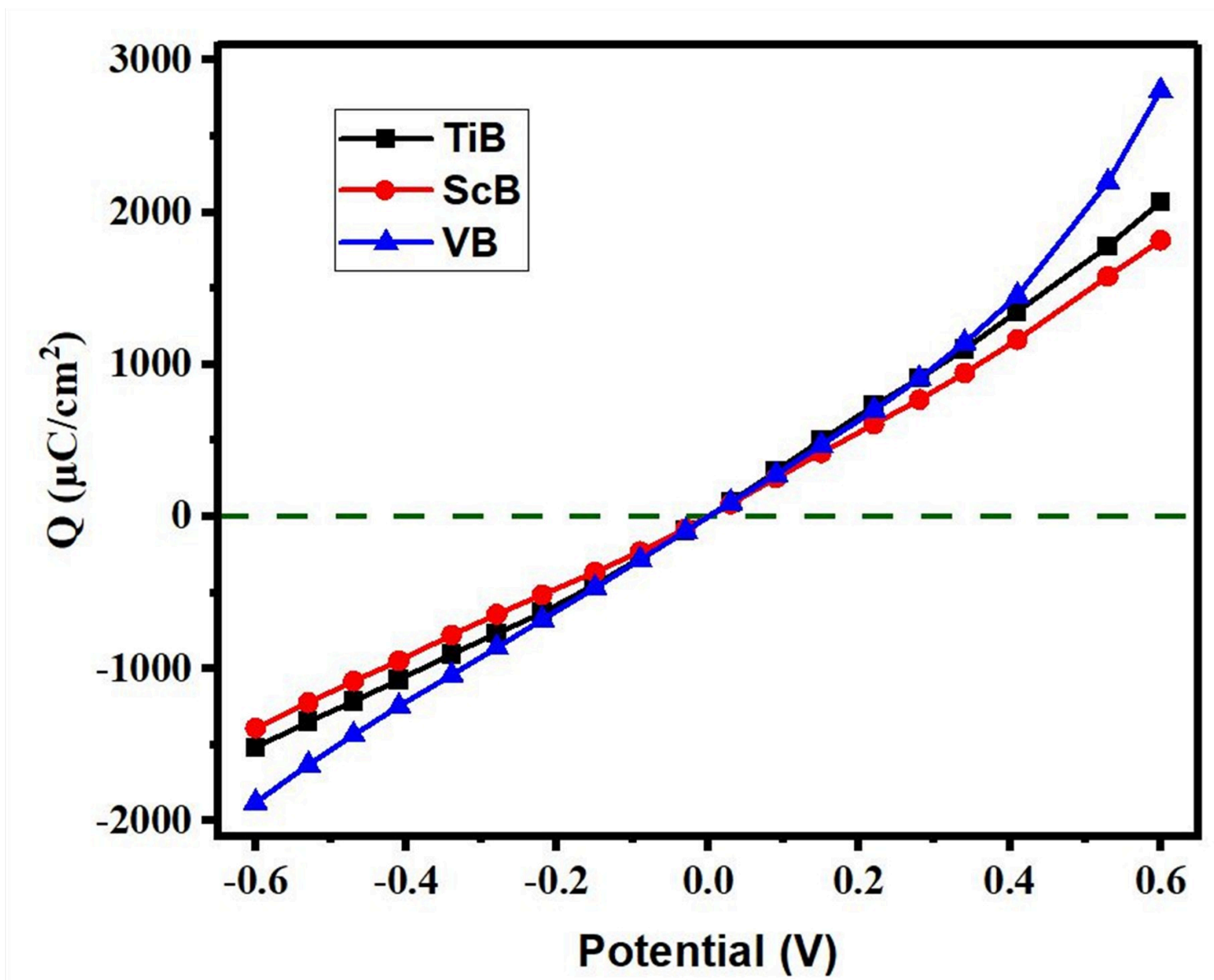


Figure 8

Stored surface charge of TiB, ScB and VB monolayers with respect to potential ranging from -0.6 V to 0.6 V.