Single-Layer Dititanium Oxide Ti$_2$O MOene: Multifunctional Promises for Electride, Anode Materials, and Superconductor

Luo Yan, Tao Bo, Bao-Tian Wang, Sergei Tretiak, and Liujiang Zhou*

**ABSTRACT:** Using the first-principles calculations, we report the existence of the single-layer (SL) dititanium oxide Ti$_2$O (labeled as MOene) that constructs a novel family of MXenes based on transition-metal oxides. This MOene material strongly contrasts the conventional ones consisting of transition-metal carbides and/or nitrides. SL Ti$_2$O has high thermal and dynamical stabilities because of the strong Ti–O ionic bonding interactions. Moreover, this material is an intrinsic electride and exhibits extremely low diffusion barriers of ∼12.0 and 6.3 meV for Li and Na diffusion, respectively. When applied as anode materials in lithium-ion batteries and sodium-ion batteries, it possesses a high energy storage capacity (960.23 mAhg$^{-1}$), surpassing the traditional MXenes-based anodes. The superb electrochemical performance stems from the soft-mode of the first acoustic phonon branch and enhanced electron–phonon coupling in the low-frequency region. Furthermore, this soft-mode behaves much softer upon applying a compressive strain of 2%, leading to a higher $T_c$ of 11.9 K. Our finding broadens the family of MXenes and could facilitate more experimental efforts toward future nanodevices.

Recently, two-dimensional (2D) metal-shrouded crystals (MSC) (M$_x$X$_y$, M = metal and X = C, N) have triggered enormous interest because of their excellent mechanical and electronic (metallic and/or semiconducting) properties, providing promises for sensors, catalysts, energy storage, (topological) electrides, superconductors, and so on. These MSC have a trigonal structure with two layers of M atoms covering one layer of X atoms. This family encompasses both nontransition and transition metal shrouded carbides or nitrides. The former includes alkali-metal and alkali-earth-metal carbides and nitrides (e.g., Ca$_2$N, Mg$_2$C$^{14}$), which were mainly investigated by theory. The latter refers to transition-metal shrouded MXenes (TMSM), including Ti$_2$C$^{15}$ Mo$_2$C$^{16}$ Ti$_2$N$^{17}$ V$_2$C$^{18}$ Nb$_2$C$^{19}$ Y$_2$C$^{20}$ and so on, which have been widely explored over the past few years.

Following remarkable promises of conventional MSM, metal-shrouded monochalcogenides, such as single-layer (SL) Ti$_2$O$^{20}$ Al$_x$ (A = Na, K, Rb, or Cs; X = O, S, Se, or Te)$^{21}$ KTiO$^{22}$ and In$_x$X (X = O, S, Se)$^{23}$ have also showed fascinating physical and chemical traits, substantially enriching the family of 2D MSC. Considering the potential uses, the toxicity and scarcity of element Ti (as rare as gold) and the highly activity of alkali metals when exposed to ambient conditions seem to be detrimental. In contrast, Ti is a transition metal with a high abundance in the earth’s crust and multifarious uses in modern-day technologies. It is worthwhile to note that the bulk Ti$_2$O phase in a hexagonal lattice has been accessed in experiments since 1970, motivating us to explore the existence of SL or few-layer Ti$_2$O with atomic thickness. Addressing this issue would not only open the door to a new family of MXenes (i.e., metal-shrouded 2D transition-metal oxides) but also potentially enrich the physics of 2D materials.

In this work, the first-principles calculations suggest that SL dititanium oxide Ti$_2$O is a novel family of MXene based on transition-metal oxides (labels as MOene to underline the 2D morphology) rather than conventional ones consisting of transition-metal carbides and/or nitrides. This MOene is a stable material and an intrinsic electride with anionic electron on the surface. The anionic states of 2D Ti$_2$O enable the low diffusion barrier and large charge storage capacity when explored as an anode material of lithium-ion batteries (LIBs) and sodium-ion batteries (SIBs). Meanwhile, this MOene is a 2D superconductor with a $T_c$ of ∼9.8 K. Such a combination of stability and exceptional electronic features implies a number of potential applications of Ti$_2$O in the next-generation nanodevices.

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Intriguingly, FM, AFM-Stripy, and AFM-Zigzag tend to be stable configurations of SL Ti2O. The up and down arrows indicate spin-up and spin-down orientations, respectively. The dynamical stability of SL Ti2O with AFM-Néel configuration is confirmed by the phonon spectrum lacking unstable modes (Figure S1a). The ab initio molecular dynamics (AIMD) simulations were carried out next to assess the thermal stability. SL Ti2O is stable without Ti–O bonds breakage and geometric reconstructions up to 700 K (Figures S1b,c). The elastic constants are calculated to be $C_{11} = C_{22} = 133.7$ N/m, $C_{12} = 33.7$ N/m, and $C_{66} = 6.2$ N/m, satisfying the mechanical stability criteria for a rectangle unit cell.25,30 The in-plane Young’s modulus ($Y_x = Y_y$) is 125.2 N/m. The Poisson’s ratios along $x$ and $y$ directions ($\nu_x$ and $\nu_y$) are both determined to be 0.25 due to the isotropic nature. The cohesive $E_{coh}$ and formation $E_F$ energies are 5.20 and $-0.44$ eV/atom, respectively, indicating its exothermic feature in the chemical synthesis and high experimental feasibility. Fortunately, the SL Ti2O may be accessed via the chemical deposition on (0001)-oriented $\alpha$-Al2O3 single crystalline substrate, as observed in Ti2O thin films.28

Ti2O monolayer is expected to accommodate the anionic states, as observed in other SL TMSM.31–34 As shown in the ELF plot (Figure 2a), there are two excess electron pools localized above the SL Ti2O surfaces as verified by the delocalized electrode with anionic electrons. The chemical formula can thus be expressed as [Ti2O]3+ − 2e−, similar to the Y2C electride.33 The difference charge plot shows the charges are mainly transferred from less-electronegative Ti to more electronegative O atoms and the center sites of anionic electrons (denoted as X pseudo atoms) that reside above the SL Ti2O surfaces as verified by the ELF plot (Figure 2a). The dynamical stability of SL Ti2O with AFM-Néel configuration is confirmed by the phonon spectrum lacking unstable modes (Figure S1a). The ab initio molecular dynamics (AIMD) simulations were carried out next to assess the thermal stability. SL Ti2O is stable without Ti–O bonds breakage and geometric reconstructions up to 700 K (Figures S1b,c). The elastic constants are calculated to be $C_{11} = C_{22} = 133.7$ N/m, $C_{12} = 33.7$ N/m, and $C_{66} = 6.2$ N/m, satisfying the mechanical stability criteria for a rectangle unit cell.25,30 The in-plane Young’s modulus ($Y_x = Y_y$) is 125.2 N/m. The Poisson’s ratios along $x$ and $y$ directions ($\nu_x$ and $\nu_y$) are both determined to be 0.25 due to the isotropic nature. The cohesive $E_{coh}$ and formation $E_F$ energies are 5.20 and $-0.44$ eV/atom, respectively, indicating its exothermic feature in the chemical synthesis and high experimental feasibility. Fortunately, the SL Ti2O may be accessed via the chemical deposition on (0001)-oriented $\alpha$-Al2O3 single crystalline substrate, as observed in Ti2O thin films.28

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Table 1. Total Energy (eV) of per Unit Cell and Magnetic Moment (μB) of per Ti Atom for Different Configurations of SL Ti2O

<table>
<thead>
<tr>
<th>configuration</th>
<th>energy (eV)</th>
<th>magnetic moment (μB)</th>
</tr>
</thead>
<tbody>
<tr>
<td>nonmagnetic</td>
<td>$-35.59192$</td>
<td>0</td>
</tr>
<tr>
<td>FM</td>
<td>$-35.59188$</td>
<td>0</td>
</tr>
<tr>
<td>AFM-Néel</td>
<td>$-35.83279$</td>
<td>0.76</td>
</tr>
<tr>
<td>AFM-Stripy</td>
<td>$-35.59192$</td>
<td>0.76</td>
</tr>
<tr>
<td>AFM-Zigzag</td>
<td>$-35.59191$</td>
<td>0</td>
</tr>
</tbody>
</table>
To clearly determine the electronic states in the Ti$_2$O system, we further checked it in bulk Ti$_2$O. Intriguingly, the electronic states intrinsically reside within the interlayers (Figure S4), which helps to protect the electride states from oxygen or water contamination that destroys the anionic electride states of SL Ti$_2$O.

Since the electronic structures of conventional MXene are usually affected by surface functional groups, we here probe the functionalization on SL Ti$_2$O via fluoridation, hydrogenation, hydroxylation, and oxidization. Here, the four major possible functionalization configurations are considered (Figures S5, 6). After full structure optimizations, the F and OH groups locating on the top of O atoms are most energetically favorable (Figure S5c), while the most stable configurations for H and O groups locate above the hollow site of hexatomic ring of Ti and O atoms (Figure S6b). All of the functionalized Ti$_2$O show a nonmagnetic ground state because the dangling 3d orbitals of the Ti atoms are saturated by corresponding functional groups. The phonon spectra confirm that the fluorinated, hydrogenated, hydroxylated SL Ti$_2$O are dynamically stable, while oxidized Ti$_2$O contains the unstable imaginary modes (Figure S7). The optimized lattice constants for Ti$_2$OF$_2$, Ti$_2$OH$_2$, and Ti$_2$O(OH)$_2$ are $a = b = 2.85$, 2.83, and 2.89 Å, respectively. The band structures of Ti$_2$OF$_2$, Ti$_2$OH$_2$, and Ti$_2$O(OH)$_2$ are presented in Figures 2d and S8. Ti$_2$OH$_2$ and Ti$_2$O(OH)$_2$ are semimetal with finite electronic states crossing the Fermi level. In contrast, Ti$_2$OF$_2$ exhibits a semiconductor trait with a direct energy gap ($E_g$) of $\sim 0.5$ (PBE) and 1.1 eV (HSE) (Figure 2d), displaying great potentiality in optoelectronic devices. Thus, the electronic properties of SL Ti$_2$O can be efficiently tuned upon varying the surface functional groups.

Considering the promising application of conventional MXene materials in LIBs and SIBs, we here explore the feasibility of Ti$_2$O MOene as a suitable electrode for the rechargeable batteries. The capability of energy storage for Ti$_2$O monolayer was investigated by the adsorption energies. Three typical Li/Na adsorption sites (labeled as S1–S3) were considered (Figure 3a). Calculated adsorption energies of Li/Na adsorption identified S3 site to be the most stable site with the lowest adsorption energies of being $-0.75$ and $-0.96$ eV for Li and Na atoms, respectively (Figure 2b). These adsorption energies are lower than those on Mo$_2$C ($-0.58$ eV for Li, $-0.77$ eV for Na),$^{37}$ Ti$_3$C$_2$ ($-0.50$ eV for Li),$^{35}$ TiC$_3$ ($-0.50$ eV for Na),$^{38}$ and V$_2$C ($-0.16$ eV for Li)$^{36}$ and comparable to Ti$_2$N ($-0.75$ eV for Li, $-0.95$ eV for Na) monolayers,$^{39}$ indicating the strong interactions between the Li/Na atom and Ti$_2$O. Based on Bader analysis,$^{40}$ the net charge transfer from the adsorbed Li and Na atoms on the S3 site to the Ti$_2$O monolayer are 0.87 and 0.73 e/atom (Figure S9a,b), respectively, suggesting the ionic bonding feature stemming from the s–d hybridization between the Ti–3d and the metal s orbitals. Additionally, the Li and Na adsorbed systems maintain the metal trait (Figure S9c,d), indicating the good electronic conductivity in SL Ti$_2$O.

The charge–discharge rate was assessed via the energy barrier of Li/Na ion diffusion on Ti$_2$O monolayer using the climbing-image nudged elastic band (CI-NEB) method.$^{41}$ As shown in Figure 3c, the energy barrier for Li (Na) ion is low to
be about 12 (6.3) meV along the path I or III (I). The extremely low energy barrier indicates an ultrafast fast charge/discharge process when SL Ti$_2$O used as the anode materials. Such low diffusion barriers for Li and Na ions are lower than the previous values in other MXenes (≈14−70 meV$^{35,37,39}$), suggesting an ultra-efficient Li/Na ion diffusion and thus ultrafast fast charge/discharge process on the SL Ti$_2$O when used in rechargeable batteries. This unprecedentedly small diffusion barrier can be attributed to the surface-confined anionic electrons, which helps to smooth the surface potential effectively, as confirmed in SL Ca$_3$N electrode.$^{31}$

Four configurations of Li/Na adducts (i.e., Ti$_2$O,M$_n$(M = Li, Na), n = 1−4) (Figures S10a-d) on a 2 × 2 × 1 supercell were considered to evaluate the storage capacity via the concentration-dependent adsorption behaviors. All considered mixtures are energetically stable, confirmed by the negative formation energy and convex hulls (Figures 4a,c). Additionally, to estimate the volume effect, the geometries after full adsorption of Li and Na atoms are checked. The thicknesses of SL Ti$_2$O host after full adsorption of Li and Na atoms are 2.41 and 1.87 Å for the two-layer Li- and Na-adsorbed configurations, respectively. Compared with the pristine monolayer (2.82 Å), the volume of the fully Li (Na) adsorbed systems increases slightly to 2.73 (7.17) %. Meanwhile, the bond length of Ti−O has only a small change of ∼0.06 and ∼0.03 eV per atom for the one- and two-layer metal adsorption. Such a low absorption energy for the two-layer adatoms indicates a weak adsorption interactions. However, this value is still smaller than those of Mo$_2$C (−0.01 eV per atom)$^{37}$ and Nb$_2$C (−0.02 eV per atom)$^{42}$ and comparable to that V$_2$C (−0.06 eV per atom)$^{44}$ in LiBs. The layered $E_{\text{ave}}$ for the one- and two-layer Na adatoms are −0.27 and −0.03 eV per atom. It should be worthy noted that the two-layer $E_{\text{ave}}$ is still smaller than that of typical electrode materials in SIBs, such as MoN$_2$ (−0.02 eV per atom),$^{43}$ Ca$_3$N (−0.003 eV per atom)$^{31}$ and GeS (−0.02 eV per atom).$^{44}$ Therefore, the Li and Na atoms in the corresponding layer prefer to chemically bind to the host material (negative $E_{\text{ave}}$), rather than to form metal clusters (positive $E_{\text{ave}}$).$^{37,42,43}$ The theoretical capacities $C_\lambda$ for Ti$_2$O in LIBs and SIBs are 960.23 mAh g$^{-1}$, larger than those of conventional MXenes (100−542 mAh g$^{-1}$).$^{37,39,42,45}$ The ELF plots (Figure S11) upon Li and Na atoms adsorption reveal that the main origin of high capacity behavior is from the anionic electrons, which stabilize adsorbed Li/Na ions and favor the high adsorption concentration of Li/Na atoms.$^{37,46,47}$

In addition, the average open-circuit voltage (OCV) in the range of 0−1.0 V indicates the ability to prevent the dendrite formation of alkali metals during the discharge/charge process.$^{36,39,46}$ There are four main plateaus during the Li (Na) insertion process (Figures 4b,d), showing a steady decreasing trend from 0.64 to 0.28 V (0.63 to 0.13 V) upon increasing the concentration of Li(Na) adatoms. Moreover, the OCV for full sodiations of Ti$_2$O$_4$ and Ti$_2$O$_4$$_4$ are 0.28 and 0.13 V, respectively, which are rather low and comparable to the typical anode materials in LIBs and SIBs, such as Mo$_2$C,$^{37}$ MoS$_2$,$^{39}$ Ti$_2$O$_4$ and Ti$_2$C$_2$$_4$, among others. Therefore, given the above discussions, the SL Ti$_2$O should be an excellent candidate as anode material for rechargeable LiBs and SIBs.

The superconductivity of the metallic SL Ti$_2$O was further investigated. Figure 5a shows the resolved phonon spectra in terms of the displacement directions of Ti and O atoms, in agreement with the projected phonon density of states (PDOS) (Figure 5b). The out-of-plane modes of Ti atoms (Ti−z) dominate the low-frequency region (below 200 cm$^{-1}$). The mid-frequency region from 200 to 300 cm$^{-1}$ mainly consists of in-plane vibrations of Ti atoms. Figure 5c shows

![Figure 4](image-url) Figure 4. Hull of formation energies for the most stable configurations of (a) Li- and (c) Na-adsorbed Ti$_2$O monolayer. The OCV for each (b) Li and (d) Na concentration, respectively.

![Figure 5](image-url) Figure 5. (a) The phonon spectra of Ti$_2$O resolved in terms of the vibration directions of Ti and O atoms. The orange, pink, red, and green hollow circles indicate Ti in-plane, Ti out-of-plane, O in-plane, and O out-of-plane modes, respectively. (b) PDOS for Ti$_2$O. (c) The magnitude of the EPC $\lambda_{\text{EPC}}$. (d) The Eliashberg spectral function $\alpha^2 F(\omega)$ and the cumulative frequency-dependent EPC $\lambda(\omega)$. 497
that the relatively large strength of the electron–phonon coupling (EPC) (labeled by $\lambda_q$) are related to the soft-modes in the first acoustic branch with a frequency of $\sim 150 \text{ cm}^{-1}$. This soft-mode that stems from the Ti-$\pi$ contribution to the cumulative frequency-dependent EPC function $\lambda(\omega)$. The Eliashberg spectral function $\alpha^2F$ reveals that the two major peaks in the low frequency region of 100--200 cm$^{-1}$ lead to a rapid increase of the cumulative $\lambda(\omega)$ (Figure 5d), evidencing the jump of the total EPC in this range and pointing to a medium-coupling superconductor with $\lambda = 0.72$. Based on the McMillian–Allen–Dynes formula, the superconducting transition temperature $T_c$ is evaluated to be $\sim 9.8 \text{ K}$, higher than or comparable to that of MXene-based superconductors $\text{M}_{\text{X}}\text{C} (3.0 \text{ K})$, $\text{Ti}_4\text{C} (1.3 \text{ K})$, and $\text{Ti}_2\text{C} (4.5 \text{ K})$, $\text{Ti}_2\text{C} (4.5 \text{ K})$, $\text{Nb}_2\text{C} (4.5 \text{ K})$, $\text{Mo}_2\text{B}_2 (3.9 \text{ K})$, and $\text{Mo}_2\text{B}_2$ (3.9 K), $\text{W}_2\text{B}_3 (7.8 \text{ K})$, $\text{GaB}_6 (1.7 \text{ K})$, $\text{InB}_6 (7.8 \text{ K})$, $\text{Li}_2\text{B}_4$ (10.35 K), $\text{Li}_2\text{B}_4$ (10.35 K). Besides, the $T_c$ is associated with screened Coulomb repulsion constant ($\mu^*$). As shown in Figure S12a, the $T_c$ decreases monotonically from 11.4 to 6.3 K upon the increase of $\mu^*$ from 0.08 to 0.15. The superconductivity of $\text{Ti}_2\text{O}$ monolayer when subject to external strains were also investigated so as to describe the strain effects from substrates in the process of chemical deposition. Clearly, the tensile strains weaken the soft-mode vibrations of the first acoustic branch around the M point, thus producing a weaker EPC (Figure S12b). On the contrary, the compressive strains would enhance the EPC verified by a much softer mode at the M point (Figure S12b). The maximum value of $T_c$ of 11.9 K is achieved at a compressive strain of 2\% (Figure S12c). All in all, this superconductivity in $\text{Ti}_2\text{O}$ MOene enriches the 2D MXene-based superconductors that are only observed in $\text{M}_{\text{X}}\text{C}$, $\text{Ti}_4\text{C}$, and $\text{Nb}_2\text{C}$ materials.

In summary, we report a systematically theoretical investigation of a new SL metal-shrouded MOene, namely 2D dititanium oxide $\text{Ti}_2\text{O}$, in great contrast conventional MXenes that consists of transition-metal carbides and/or nitrides. This thermally and dynamically stable MOene is an electrode in monolayer and bulk form. $\text{Ti}_2\text{O}$ MOene can be used as an anode material in lithium and sodium battery technologies, owing to extremely low diffusion barriers (12.0 meV for LIBs and 6.3 meV for NIBs) and an excellent storage capacity (960.23 mAhg$^{-1}$). The anionic electrons intercalating the adsorbed Li/Na atoms and $\text{Ti}_2\text{O}$ monolayer make the significant contributions to the very fast charge/discharge process. Moreover, within the Bardeen–Cooper–Schrieffer microscopic theory, $\text{Ti}_2\text{O}$ is determined to be a intrinsic superconductor with a transition temperature $T_c$ of 9.8 K. The superconductivity mainly originates from the presence of soft modes in the first acoustic branch and a significant enhancement of EPC in the low-frequency region. The $T_c$ could reach a maximum value of 11.9 K when subject to a compressive strain of 2\%. These results endow $\text{Ti}_2\text{O}$ MOene with multifunctionality, promisingly suitable for future nanodevices and energy storage technologies and thus call for further experimental fabrication and characterization efforts.

First-principles calculations based on the density functional theory (DFT) calculations were performed according to the projector augmented wave (PAW) scheme. The exchange and correlation contributions were simulated within the generalized gradient approximation (GGA) as formulated by Perdew–Burke–Ernzerhof (PBE). A rapid dispersion-corrected DFT method (opt88-vdw) was adopted to model the van der Waals interaction. A subset of numerically expensive calculations were performed with an accurate screened exchange hybrid density functional by HSE06 and inclusion of spin–orbit coupling (SOC) terms. The plane-wave cutoff energy of 550 eV and Γ-centered 21 × 21 × 1 k-point mesh using the Monkhorst–Pack method were adopted in electronic structure calculations. To avoid the interactions between the nearest-neighbor unit cells, a vacuum thickness of 20 Å along the $z$ direction was applied. Some data analyses were done with the help of VASPKIT. See more details in Supporting Information.

**ASSOCIATED CONTENT**

**Supporting Information**

The Supporting Information is available free of charge at https://pubs.acs.org/doi/10.1021/acs.jpcl.0c03397.

- Detail methods; phonon spectrum; AIMD simulations; difference charge density; projected band structures; ELF plot of bulk $\text{Ti}_2\text{O}$; configurations and phonon spectra for fluorinated, hydrogenated, oxidized and hydroxylated SL $\text{Ti}_2\text{O}$; the most stable configurations with different Li/Na concentrations in $\text{Ti}_2\text{O}_n(M = \text{Li,Na})$ ($n = 1--4$); ELF plots for the Li/Na atoms adsorbed $\text{Ti}_2\text{O}$ monolayer; the changes of $T_c$ under the variable $\mu^*$; and variations of phonon spectra, $\lambda$, and $T_c$ under biaxial strains (PDF).

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**Notes**

The authors declare no competing financial interest.
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