Designing power efficient transistors using narrow bandwidth materials from the MA$_2$Z$_4$ monolayer series

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The subthreshold leakage current in transistors has become a critical limiting factor for realizing ultra-low-power transistors. The leakage current is predominantly dictated by the long thermal tail of the charge carriers. We propose a solution to this problem by using narrow bandwidth semiconductors for limiting the thermionic leakage current by filtering out the high energy carriers. We specifically demonstrate this solution in transistors with laterally confined monolayer MoSi$_2$N$_4$ with different passivation serving as channel material. Remarkably, we find that the proposed narrow bandwidth devices can achieve a large ON/OFF current ratio with an ultra-low-power supply voltage of $\sim 0.1$ V, even for devices with $\sim 5$ nm gate length. We also show that several other materials share the unique electronic properties of narrow bandwidth conduction and valence bands in the same series.

I. INTRODUCTION

The main bottleneck in the design of ultra-low-power transistors is the rate change of the ON current with the applied gate voltage. This is technically described as the lowering of the subthreshold slope (SS), which is a crucial figure of merit determining a transistor’s performance. The SS is the smallest change in gate voltage, $V_{GS}$ required to change the drain current, $I_{DS}$ by one order of magnitude. The dissipation of energy by thermally excited charge carriers is facilitated by a existence of electronic states at high energies, and it sets a natural limit on the subthreshold slope to be $SS < 60$ mV/decade. This is known as the thermionic limit and this thermodynamic dissipation problem is referred to as Boltzmann’s tyranny (see Fig. 1). Overcoming the Boltzmann tyranny by making $SS < 60$ mV/decade is currently one of the biggest challenges in conceptualizing ultra-low-power transistors.

Different strategies are being used to solve this problem. One strategy is to shorten the thermal tail, with tunnel field-effect transistors (FETs) being the most common device. Another strategy is to increase the barrier height’s steepness with gate voltages, with Landau’s FETs being the most common device. However, the tunneling transport limits the ON-state current to very low values in tunnel FETs, and there are several challenges in Landau FETs at both material and device levels. In fact, low hysteresis with the required ON-state current has not been achieved experimentally in Landau FETs. In recent years, the rise of layered materials has offered more opportunities to conceptualize and design energy-efficient logic devices. For subthermionic switching, the Dirac cone in the electronic band structures of layered materials like graphene has also been used to shorten the thermal tail.

Here, we present a solution to the problem of Boltzmann’s tyranny, by using narrow bandwidth semiconductors as channel material. The narrow bandwidth of the conduction/valance band naturally restricts the long thermal tail of the charge carriers, reduces the thermionic current in the OFF state [see Figure 1 (f)], and solves the problem of Boltzmann’s tyranny. We demonstrate that using this solution, the devices can achieve a large ON/OFF current ratio with an ultra-low-power supply voltage of $\sim 0.1$ V, down to $\sim 5$ nm gate length. While the concept is very general, we demonstrate this in the laterally confined monolayer of the recently synthesized MoSi$_2$N$_4$ monolayers. Monolayer MoSi$_2$N$_4$ is an excellent semiconductor with outstanding physical, mechanical, thermal, electronic, and metal contact properties, which are at par with most other 2D semiconductors. We assess the transistor performance of differently passivated monolayers of MoSi$_2$N$_4$, by using first principles-based nanoscale device simulations. All single and dual-gate devices show ultra-low-power steep slope transistor characteristics down to short channel lengths. Additionally, we show that other members of the MoSi$_2$N$_4$ family also show these unique electronic properties in their laterally confined structures. This opens up new avenues for exploring 2-D transistors for ultra-power-efficient computing.

This paper is organized as follows: In Sec. II A, we describe the origin of low power dissipation and subthermionic switching in transistors with narrow bandwidth source materials. As an example of this, we discuss the electronic properties of passivated MoSi$_2$N$_4$ nanoribbons, which host narrow bandwidth conduction band in Sec. II B. In Sec. II C, we describe the electrical properties of transistors made from these structures. In Secs. II D and II E, we show that several differently terminated MoSi$_2$N$_4$, and other materials in the MoSi$_2$N$_4$ series also host narrow conduction or valance bands. These can also serve as power efficient source or channel materials. Finally, we summarize our findings in Sec. III.
II. RESULTS AND DISCUSSIONS

A. Narrow bandwidth enabled subthermionic switching

Here, we highlight the idea of reduced power dissipation or subthermionic switching in transistors by using low bandwidth materials. The SS is defined as

$$SS = \frac{\partial V_{GS}}{\partial \log_{10} I_{DS}} = \frac{\partial V_{GS}}{\partial \phi_b} \times \frac{\partial \phi_b}{\partial \log_{10} I_{DS}}.$$  \hfill (1)

Here, $\phi_b$ is the barrier height from source-to-channel, and the first and second terms in Eq. (1) are the body factor ($m$) and the transport factor ($n$), respectively. To connect this to the electronic bandwidth, we note that the electron density in a n-type 3-D semiconductor at a given energy is specified by the product of the density of states and the Fermi function: $n(E) = D(E) \times f(E)$. Here, $f(E) = 1/[1 + \exp(E/k_B T)]$ is the Fermi function. For 3-D systems, we have $D_{3D}(E) \propto \sqrt{E}$. As a result, the carrier density in conventional bulk semiconductors like Si/Ge decays sub-exponentially with $E$, with an infinitely long thermal tail (see Figure 1). Similarly, the electron density in 2-D semiconductors is given by $D_{2D}(E) \propto E^0$ and we have $n(E) \propto f(E)$. This implies that the carrier density in 2-D systems also decays exponentially with $E$, and it also has an infinitely long thermal tail. Therefore, during the onset of conduction in conventional transistors comprised of 3D or 2D channel material, the current is determined by the thermally activated carriers and we have $I_{DS} \sim \exp(-\phi_t/\phi_b)$, with $\phi_t \equiv k_B T/q$ being the temperature scale. This yields, $n \cong \ln(10)\phi_t$. In conventional transistors, the electrostatic coupling between gate and channel dictates that $m > 1$. Thus, in conventional transistors, the $SS$ is limited to a value of $SS > 60$ mV/decade at room temperature (300 K), imposing a stiff limitation on their performance. It is typically referred to as the Boltzmann tyranny.

One possible solution to the problem of Boltzmann’s tyranny arising from the long thermal tail, is to have a narrow bandwidth conduction band separated from the higher conduction band by a large energy gap. This cuts off the thermal tail above the potential barrier in the channel and suppresses the thermionic injection at a low gate-to-source bias ($V_{GS}$) [see Figure 1]. In this scenario, direct source-to-drain tunneling (SDT) will leak a small amount of current in the OFF state ($I_{DS}$), which strongly depends on the tunneling carrier’s effective mass and width of the tunneling barrier (source-to-drain barrier). With the increase in $V_{GS}$, the potential barrier in the channel decreases, and the carrier density changes from SDT to thermionic, resulting in a sudden increase in the drain current. This enables $n$ to have much smaller values and consequently we can have $SS < 60$ mV/decade, opening up possibilities for designing very power efficient transistors. This is the main idea, and highlight of this paper. In the rest of the paper, we demonstrate this idea of narrow bandwidth 2-D semiconductors overcoming Boltzmann’s tyranny, using laterally confined MoSi$_2$N$_4$ as a channel material for realizing steep-slope and power-efficient logic electronic switches. To explicitly show this, we first establish the presence of a
Figure 2. (a) Unit cell of a laterally confined (in the $y$-direction) monolayer of MoSi$_2$N$_4$. We refer to it as $n$-MoSi$_2$N$_4$, depending on the number ($n$) of bulk unit cells along the confinement direction. (b) and (c) show the zoomed view of the top and bottom edge of the structure, respectively. (d) The electronic band structure of H-terminated 10-MoSi$_2$N$_4$. (e) Variation of the bandgap ($E_G$), the bandwidth of the conduction band ($E_{C,BW}$), and the gap of the first conduction band from the higher conduction band ($\Delta E_C$) with the width of the nanoribbon in the confinement direction. (f) The atom and orbital resolved density of states of the edge and inner Mo atoms. Clearly, the narrow conduction band states arise from the edge Mo atoms.

narrow bandwidth conduction band in laterally confined MoSi$_2$N$_4$ by calculating their electronic properties.

B. Electronic properties of H terminated MoSi$_2$N$_4$

We calculate the electronic properties of monolayer (2-D) MoSi$_2$N$_4$ for benchmarking our calculations [see Figure S1 and Table S1 in the Supporting Information (SI)]. The results are found to be consistent with those reported in the literature. We find the bandgap predicted by DFT with PBE functional ($E_G = 1.86$ eV) to be very close to the experimental value ($E_{G,exp} = 1.94$ eV). Orbital projected density of states (PDOS) reveals that in the vicinity of the conduction band minima (0.1 eV around CBM) $\sim 82\%$ and $\sim 15\%$ of the total DOS are contributed by the $d$-orbitals of molybdenum (Mo) and $p$-orbitals of nitrogen (N), respectively. Our charge distribution and orbital projected density of states (PDOS) analysis reveal that Mo-$d_{xz}$ and N-$p_z$ orbitals hybridize to form the $\sigma$-bonds. As a result, bonding and anti-bonding orbitals form VBM and CBM, respectively [see Figure S2 of SI for further details].

Starting from the optimized structure of 2-D monolayer, we construct $n$-MoSi$_2$N$_4$ nanoribbons (periodic along the $x$-direction) by stacking ($n/2$) number of unit cells along the $y$-direction [see Figure 2]. After creating the nanoribbon (say 10-MoSi$_2$N$_4$), the structure is relaxed once again before performing the electronic structure calculation. If dangling bonds of the edge atoms are left unpassivated, such a 10-MoSi$_2$N$_4$ nanoribbon is a semiconductor with a bandgap of $E_G \sim 0.9$ eV [see Figure S3 of SI and related discussion]. To eliminate the effect of the dangling bonds, we use hydrogen (H) atoms to terminate the edges. Hydrogen is commonly used for edge termination in experiments, as the process can be easily controlled by the pressure and temperature of the H$_2$ gas. To keep the coordination number unchanged, each of the edge Mo, N, and Si atoms is terminated by two H atoms, one H atom, and one H atom, respectively. The electronic band structure of the optimized structure is shown in Figure 2 (d), along the high symmetry path (-X - $\Gamma$ - X). The two lowest energy conduction bands have narrow bandwidth ($E_{C,BW}$), and they are separated from nearby bands by
a relatively large gap of $\Delta E_C$. The variation of $E_G$, $E_C$, $BW$, and $\Delta E_C$ with $n$ are plotted in Figure 2 (e) for H-terminated $n$-MoSi$_2$N$_4$. As $n$ increases, $E_G$, $E_C$, $BW$, and $\Delta E_C$ saturate to $\sim 0.7$ eV, $\sim 0.2$ eV, and $\sim 1.0$ eV, respectively. These localized conduction bands, in H-terminated 10-MoSi$_2$N$_4$, are predominated by $d$-orbitals of edge Mo atoms, as shown in Figure 2 (f). See Figure S4 of SI$^{14}$ for more details. Such a unique combination of electronic states can potentially achieve the target of sub-60 mV/decade switching in transistors by cutting off the thermionic current in the OFF-state.

C. Transistors based on H-terminated MoSi$_2$N$_4$

To evaluate the the transport properties and sub-60 mV/decade switching, we perform first-principles-based nanoscale device simulation of single-gate (SG) and double-gate (DG) devices composed of H-terminated 10-MoSi$_2$N$_4$. The schematics of devices are shown in Figure 3 (a) and (d), in which the main geometrical parameters are the gate length ($L_G$), source/drain length ($L_{S/D}$), source/drain-to-gate length ($L_{SG/DG}$), and oxide thickness ($t_{ox}$). SiO$_2$ is used as both gate oxide [$t_{ox} = 0.60$ nm] and box oxide [$t_{box} = 10$ nm]. The source/drain is electrostatically doped using source/drain gate with $L_{S/D} = 9.80$ nm, and $L_{SG/DG} = 0.20$ nm. The power
are the same as those of SG devices with L performance parameters of DG devices with L < 25 mV/decade down to 8 nm channel length. The is proportional to exp(−\text{ms}_{\text{eff}} \times l_t), where \text{ms}_{\text{eff}} is the effective mass along the transport direction and \text{l}_t is the tunneling length. Hence, the rate of increase of the drain current when going from the OFF state to the ON state degrades with the reduction of the channel length of the device. We find that the rate of degradation is lower in DG devices compared to SG devices due to better electrostatics in DG devices.

To counter the impact of increased source-to-drain tunneling, we increase the channel length of the double gate device with a gate length of 3 nm by adding ΔL_{SG} to L_{SG/DG}. The resulting device structure effectively increases the source-drain barrier width and height, thereby reducing the source-to-drain leakage and subthreshold leakage. However, there is a trade-off between ΔL_{SG} and ON-state performance due to reduced gate control over the extended channel.\textsuperscript{49,50} The simulated transport characteristics for various ΔL_{SG} values up to 3 nm [0, 0.5, 1.0, 1.5, 2.0, 3.0 nm] are shown in Figure S10 of the SI.\textsuperscript{44} We find that with increase in ΔL_{SG}, the source-to-drain leakage decreases. The device exhibits subthermionic behavior with a SS_{min} < 30 mV/decade, and SS_{avg} < 37 mV/decade over more than three decades of drain current at ΔL_{SG} ≥ 2.0 nm, with an ON-OFF ratio more than 10^3, as shown in Figure 3 (h) and (i).

**D. Edge Functionalization of MoSi_2N_4**

Having demonstrated efficient subthreshold switching below 60 mV/decade in laterally confined MoSi_2N_4 devices with hydrogen passivation, a natural question to ask is what happens on passivating with other atoms.\textsuperscript{51–54} To address this, we subject 10-MoSi_2N_4 to different edge functionalization, by passivating the dangling bonds with H, F, and O, which are commonly used for edge termination.\textsuperscript{51–57} In exploring edge functionalization, we keep the coordination number of edge atoms to be the same as in the bulk 2D sample. We investigate several possible combinations of edge functionalization, which are listed in Table I.

Among all the edge functionalized MoSi_2N_4 nanoribbons mentioned above, two of the band structures are shown in Figure 4. In case of O-H-H terminated 10-MoSi_2N_4 shown in Figure 4 (a), E_C (∼ 1.40 eV) is larger than the bandgap of 2H-H-H terminated 10-MoSi_2N_4. The two lowest energy conduction bands have a bandwidth of E_{CB, BW} ∼ 0.27 eV, and are separated from the next conduction band by ∼ 0.33 eV. Our Bader charge analysis\textsuperscript{58,59} shows that the charge on each Mo atom is reduced by 0.31\textit{e} in O-H-H terminated 10-MoSi_2N_4 compared to that in 2H-H-H terminated 10-MoSi_2N_4. As

**Table I. Different edge functionalization schemes for MoSi_2N_4.**

| S. No. | Edge Atoms Termination Scheme | Notation   |
|--------|-----------------------------|------------|
| 1      | (Mo, Si, N) → (2H, H, H)    | 2H-H-H     |
| 2      | (Mo, Si, N) → (2F, F, F)    | 2F-F-F     |
| 3      | (Mo, Si, N) → (2F, H, H)    | 2H-F-F     |
| 4      | (Mo, Si, N) → (O, H, H)     | O-H-H      |
| 5      | (Mo, Si, N) → (O, F, F)     | O-F-F      |
| 6      | (Mo-1, Mo-2, Si, N) → (H, F, H) | HF-H-H |
| 7      | (Mo, Si, N) → (N, H, H)     | N-H-H      |
| 8      | (Mo, Si, N) → (N, H, H)     | N-H-H      |
MoSi$_2$N$_4$ nanoribbon is its robust band structure, which has the same qualitative features irrespective of the choice of edge functionalization. Band diagrams of several possible combinations of edge functionalization are compared in Figure 5 (a), illustrating a wide range of values for $E_C$ (0.64 eV - 1.50 eV) and $\Delta E_C$ (0.18 eV - 1.08 eV), while $E_{CBW}$ value lies within a small range of 0.42 eV - 0.18 eV. The corresponding band structures are shown in Figure S5 of SI$^{44}$. Most of these structures have a narrow bandwidth conduction band which limits the long thermal tail of carriers and thermionic injection in the OFF state. This makes them suitable for low-power applications. Additionally, edge functionalization engineering offers a route to control their desired electronic properties. Amongst these, the 2F-F-F terminated nanoribbon is the only one having both narrow conduction and narrow valance bands. In addition, we find that the N-H-H terminated nanoribbon is metallic (see Figure S5 of SI$^{44}$). In fact, such ‘cold’ metals can be used as a cold source contact in FETs, which is another way to achieve sub-60 mV/decade switching and overcome Boltzmann’s tyranny$^{60}$.

### E. Transistors with functionalized MoSi$_2$N$_4$ and other materials in the series

The transfer characteristics of DG devices, with O-H-H terminated n-type, 2F-F-F terminated n-type, and 2F-F-F terminated p-type 10-MoSi$_2$N$_4$ as channel material is shown in Figure 4 (c-e). All the devices show subthermionic nature in drain current down to 5 nm channel length. More specifically, the drain current show subthermionic nature over more than five decades, eight decades, and three decades of drain current for devices with $L_{Ch} \leq 5$ nm based on n-type devices with O-H-H, and 2F-F-F termination, and p-type device with 2F-F-F termination, respectively.

The best performance of DG devices with $L_{Ch} = 5$ nm is shown in Figure 5 (b) and (c). All the devices show ON/OFF ratio of more than $10^3$ and an average subthreshold slope of less than 45 mV/decade. However, the best performing device is n-type comprised of 2F-F-F terminated 10-MoSi$_2$N$_4$, owing to flat conduction band minima and hence low SDT leakage, with $I_{ON}/I_{OFF} > 10^6$ and $SS_{avg} < 20 $ mV/decade. See Sec. E of the SI$^{44}$ for a more detailed analysis. The upper limit of devices’ performance is assessed as the ballistic nature of transport is considered. However, the presence of electron-phonon interaction could degrade the device’s performance, but the subthermionic nature of devices could be maintained$^{61,62}$.

Having demonstrated excellent low-power transistor characteristics for laterally confined and passivated MoSi$_2$N$_4$, we now explore other materials in the same series of compounds for ultra-low-power devices. Specifically, we extend the search in MA$_2$Z$_4$ the family, where M=Mo, Cr, Zr, Ti, Hf; A=Si, Ge; and Z=N, P, As. The calculated band diagrams for 2H-H-H terminated
10-MA$_2$Z$_4$ nanoribbon is shown in Figure 6. We find that there are several candidates in this family, having narrow bandwidth first valence or conduction bands, separated from nearby bands by a sizeable gap. This opens up the field for further exploration of MA$_2$Z$_4$ series of materials, for potential application in ultra-low power transistor applications as channel materials.

### III. CONCLUSION

One of the major bottlenecks for making ultra-power-efficient transistors is decreasing the applied gate voltage for a 10-fold increase in the source-to-drain current during the conduction process. The bottleneck is controlled by the long thermal tail of the charge carriers, which leads to a large thermionic current in the OFF state. We propose a solution to this problem by using narrow bandwidth semiconductors as channel material. The narrow bandwidth of the conduction/valance band naturally restricts the long thermal tail of the charge carriers, reduces the thermionic current in the OFF state, and solves the problem of Boltzmann’s tyranny.

We demonstrate this using the example of the laterally confined monolayer MoSi$_2$N$_4$. We show that passivated MoSi$_2$N$_4$ nano-ribbons have a narrow bandwidth conduction band, which is separated from nearby bands by a large bandgap. By combining first-principle calculations and nano-scale device simulations, we evaluate the performance of several transistors using differently terminated MoSi$_2$N$_4$ nano-ribbons as channel material. We find that devices with several differently terminated MoSi$_2$N$_4$ as channel material show a considerable performance improvement with a subthreshold slope much smaller than 60 mV/decade. Some of them can be used to realize both n- and p-type power-efficient transistors. We show that these unique electronic properties of narrow bandwidth are also shared by several other members of the MSi$_2$N$_4$ family of materials. Our work offers a new direction for engineering and exploring narrow bandwidth materials for enabling steep-slope transistors and ultra power-efficient computing.

### Appendix A: Methods

#### 1. Density Functional Theory Calculations

All the DFT-based first-principles calculations are performed using the projector augmented wave (PAW) potentials, as implemented in the Quantum ESPRESSO code suite.$^{63,64}$ A Perdew-Burke-Ernzerhof (PBE)$^{65}$ based generalized gradient approximation (GGA) is used to include the exchange and correlation effects. The kinetic energy cut-off of the wave function and the charge density is set to 60 Ry and 600 Ry, respectively. The magnetic energy cut-off of the wave function and the charge is 60 Ry and 600 Ry, respectively. The netic energy cut-off of the wave function and the charge

The electronic band structure of the system is represented by a set of Wannier functions to upscale the system for device simulation via the Wannier90 code suite.$^{66}$ The overlap matrix between the adjacent $k$ points and the projection matrix is used as the input to calculate the Wannier functions. The resulting transformed Hamiltonian matrix in the basis of MLWFs is sparse in nature. We calculate the transmission coefficients $T(E)$ and potentials at each bias ($V_{GS}$, $V_{DS}$), by solving the Poisson and Schrödinger equations self-consistently in the NEGF formalism.$^{67,68}$ The Landauer-Büttiker method is used to estimate the drain current, which can be expressed as

$$I_{DS} = \frac{2e}{h} \int_{-\infty}^{\infty} T(E,V_{GS},V_{DS})[f(E-\mu_S)-f(E-\mu_D)]dE.$$  

Here, $e$ is the elementary charge, $h$ is the Planck constant and $V_{GS}$ ($V_{DS}$) is the gate-source (drain-source) voltage. $T(E,V_{GS},V_{DS})$ is the transmission coefficient at a given energy $E$ and a bias ($V_{GS},V_{DS}$). $\mu_{S/D}$ and $f(E-\mu_{S/D})$ are the fermi energy level and the Fermi-Dirac distribution function at source/drain, respectively. The tunneling probability, $T(E,V_{GS},V_{DS})$ is calculated using

$$T(E,V_{GS},V_{DS}) = \text{Trace}[\Gamma_S G^R \Gamma_D G^A].$$  

(A1)

Here, $G^{R/A}$ is the retarded/advance Green functions, $\Gamma_{S/D}$ is the broadening from source/drain contacts and

![Figure 6. Pictorial representation of unique electronic properties different materials of the MA$_2$Z$_4$ series, with H termination. Going beyond MoSi$_2$N$_4$, several other materials in the same series also have similar bandstructure features as laterally confined MoSi$_2$N$_4$, which enable subthermionic switching for power efficient transistors.](image-url)
\( E \) is the energy. Additionally, we have

\[
\Gamma_{S/D}(E, V_{GS}, V_{DS}) = i[\Sigma_{S/D} - \Sigma^\dagger_{S/D}], \quad (A2a)
\]
\[
G^R(E, V_{GS}, V_{DS}) = [EI - H - \Sigma]^{-1}, \quad (A2b)
\]
\[
G^A(E, V_{GS}, V_{DS}) = [G^R(E, V_{GS}, V_{DS})]^\dagger. \quad (A2c)
\]

Here, \( I \) is the an identity matrix, \( \Sigma_{S/D} \) is source/drain contact self-energy, \( \Sigma = \Sigma_S + \Sigma_D \), and \( H \) is the Hamiltonian matrix representing the channel.

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