2-D materials for ultra-scaled field-effect transistors: hundred candidates under the \textit{ab initio} microscope

Cedric Klinkert†, Áron Szabó†, Christian Stieger†, Davide Campi‡, Nicola Marzari‡, and Mathieu Luisier†∗

† Integrated System Laboratory, ETH Zurich, CH-8092 Zurich, Switzerland
‡ Theory and Simulation of Materials (THEOS) and National Centre for Computational Design and Discovery of Novel Materials (MARVEL), École Polytechnique Fédérale de Lausanne, CH-1015 Lausanne, Switzerland

E-mail: mluisier@iis.ee.ethz.ch

Abstract

Thanks to their unique properties single-layer 2-D materials appear as excellent candidates to extend Moore’s scaling law beyond the currently manufactured silicon FinFETs. However, the known 2-D semiconducting components, essentially transition metal dichalcogenides, are still far from delivering the expected performance. Based on a recent theoretical study that predicts the existence of more than 1,800 exfoliable 2-D materials, we investigate here the 100 most promising contenders for logic applications. Their “current vs. voltage” characteristics are simulated from first-principles, combining density-functional theory and advanced quantum transport calculations. Both \textit{n}- and \textit{p}-type configurations are considered, with gate lengths ranging from 15 down to 5 nm. From this unprecedented collection of electronic materials, we identify 13 compounds with electron and hole currents potentially much higher than in future Si FinFETs.
The resulting database widely expands the design space of 2-D transistors and provides original guidelines to the materials and device engineering community.

**Keywords:** 2-D materials, *ab initio* device simulation, next-generation field-effect transistors, performance comparison, materials and device parameters

For more than five decades the functionality of all electronic devices has not stopped growing driven by the continuous miniaturization of their active components, the transistors. As a consequence, the active region of the currently manufactured silicon Fin field-effect transistors (FinFETs) does not exceed a couple of nanometers along all directions. This renders their fabrication extremely difficult and gives rise to strong quantum mechanical effects such as inter-/intra-band tunneling that might negatively impact their switching behavior. Furthermore, with the resulting ultra-short gate lengths, $L_g \leq 20$ nm, maintaining good electrostatic properties has become really hard, even with multi-gate architectures.

Different options are therefore considered to extend Moore’s scaling law (More-Moore) or go beyond it (More-than-Moore). On the geometry side, nanowire and nanosheet FETs are attracting a lot of attention because of their excellent electrostatics and relative straightforward fabrication processes. On the material side, logic switches based on III-V compound semiconductors, germanium, and carbon nanotubes have long been investigated to replace silicon, all operating closer to their ballistic limit than Si.

The advent of graphene in 2004 brought another serious contender into this disputed race, two-dimensional (2-D) materials. The absence of band gap did not allow graphene to emerge as a rival to Si, but its discovery paved the way for other 2-D crystals, starting with MoS$_2$ in 2011. Other members of the transition metal dichalcogenide (TMDs) family have since then been used as single- or few-layer transistor channels. TMDs, like other 2-D materials, benefit from dangling-bond-free surfaces and from an excellent electrostatic integrity provided by their atomic-scale thickness. Sub-threshold swings close to the ideal value of 60 mV/dec at room temperature (RT) can be achieved with a single-gate contact. Moreover, TMDs exhibit reasonable mobilities, up to 50-100 cm$^2$/Vs at RT, and band gaps
compatible with logic operations ($E_g > 1$ eV). Taking advantage of these peculiar features, an ultra-scaled MoS$_2$ transistor with a carbon nanotube of diameter $d = 1$ nm as gate electrode was demonstrated.\textsuperscript{15}

While impressive, these results are still not sufficient to outperform Si FinFETs. On one hand, there remain several technology issues to address, notably the high contact resistance of monolayer TMDs.\textsuperscript{16} On the other hand, no drive current superior to 0.7 mA/$\mu$m has ever been reported.\textsuperscript{17} This shortcoming can be partly attributed to the large effective masses of these materials in comparison to Si, which limits their carrier injection velocities and their ON-state current. Hence, 2-D components with potentially better transport properties than TMDs have come under the spotlight, e.g. black phosphorus (P$_4$),\textsuperscript{19} silicene,\textsuperscript{20} germanene,\textsuperscript{21} antimonene,\textsuperscript{22} InSe,\textsuperscript{23} Bi$_2$O$_2$Se,\textsuperscript{24} and dozens of others.\textsuperscript{25–29}

An intense research activity on novel 2-D materials is on-going at the theoretical level too. A recent study based on density-functional theory (DFT) predicted the existence of more than 1,800 exfoliable 2-D candidates, among which several could play a major role as future, post Si FinFET transistors.\textsuperscript{30} Since most of them have not yet been experimentally isolated in their monolayer form, \textit{ab initio} device simulation is key to unlock their potential as ultimate FETs. Up to now, the modeling effort has mainly focused on known 2-D materials such as TMDs,\textsuperscript{31–33} P$_4$,\textsuperscript{34} Bi$_2$O$_2$Se,$\textsuperscript{35}$ monochalcogenides,$\textsuperscript{36}$ group IV\textsuperscript{37} and V\textsuperscript{38} monolayers, as well as on more exotic ones, e.g. Tl$_2$O\textsuperscript{39} whose electron mobility was studied.

Here, we significantly expand the design space and report the largest to date collection of simulated transistor characteristics together with the associated material parameters for electronic applications. The objective is to provide the community with a comprehensive atlas of 2-D materials capable of challenging Si FinFETs and to inspire the work of engineers exploring next-generation 2-D FETs. With this goal in mind, the 100 most promising entries from the database of Ref.\textsuperscript{30} are examined in their $n$- and $p$-type configuration, with gate lengths ranging from 15 nm down to 5 nm, assuming a simple, but realistic device geometry, beyond-ballistic transport, perfectly ohmic contacts, and ideally insulating dielectric layers.
All simulations are performed at the DFT level with a sophisticated *ab initio* quantum transport solver that relies on unique physical and numerical innovations. We determine the intrinsic transport properties of each 2-D material before comparing them to each other. The detrimental influence of contact resistances, interactions with charged impurities, structural defects, and surface optical phonon scattering is ignored because all these effects are expected to diminish as crystal quality and fabrication techniques improve.

In particular, we show that 13 2-D materials, among them 4 completely new ones, stand out, delivering an ON-state current larger than 3 mA/µm at a fixed OFF-state magnitude of 0.1 µA/µm, both as *n*- and *p*-type single-gate transistors. Three of these even have ON-currents above 4 mA/µm in their *n*- and *p*-type FET configuration. For each simulated 2-D compound, the electron/hole “current vs. voltage” characteristics, “sub-threshold swing vs. gate length”, unit cell, bandstructure, injection velocity, transport and density-of-states effective masses, as well as a novel physically relevant quantity called “pass factor” are presented in the Supporting Information (SI). A detailed analysis of these data follows.

**Results and Discussion**

**Device Test Structure.** As benchmark, the single-gate transistor structure of Fig. 1 is considered, as its fabrication is fully compatible with standard CMOS processes. Its design is loosely based on the specifications from the 2018 edition of the International Roadmap for Devices and Systems (IRDS) for the year 2025, the first technology node (2.1 nm) at which 2-D materials could eventually be inserted. The gate length is initially set to $L_g = 15$ nm (IRDS: 14 nm), the supply voltage to $V_{DD} = 0.7$ V (IRDS: 0.65 V), and the equivalent oxide thickness to $EOT = 0.6$ nm. The source and drain extensions are doped with a donor/acceptor concentration $N_{D/A} = 5e13$ cm$^{-2}$, which is required to ensure an excellent electrostatic control and access to the intrinsic properties of 2-D FETs. Such values might be difficult to reach experimentally, but they are definitively attainable. The 2-D materials investigated are
embedded between a SiO$_2$ box of thickness $t_{box}=20$ nm and relative permittivity $\epsilon_R=3.9$ and a HfO$_2$ dielectric layer with $t_{ox}=3$ nm and $\epsilon_R=20$ (see Fig. 1). These oxide regions do not participate in the electronic structure calculations, but they are nevertheless included indirectly through the solution of Poisson’s equation.

Every simulation starts by constructing the primitive unit cell of the selected 2-D material, which should have a band gap $E_g > 1$ eV to mitigate interband tunneling leakage. It continues with a relaxation of the atomic positions and a computation of the corresponding electronic structure; we use the Vienna Ab initio Software Package (VASP). Next, the plane-wave outputs of VASP are transformed into maximally localized Wannier functions (MLWFs) via the wannier90 code. The assembled MLWF Hamiltonian matrix is upscaled to match the targeted device dimensions. Finally, the I-V characteristics of the system are computed from first-principles with the OMEN quantum transport solver. The latter solves the Schrödinger and Poisson equations self-consistently in the Non-equilibrium Green’s Function (NEGF) formalism, taking the produced tight-binding-like MLWF Hamiltonian matrices as inputs. Electron-phonon interactions are accounted for through a fictitious scattering model that eliminates non-physical effects, e.g. negative differential resistance (NDR), and guarantees convergence of the electronic currents up to the desired gate-to-source voltage $V_{gs}=V_{DD}$. More details about the modeling approach can be found in the Methods Section. As it is the same for the 100 different 2-D channel materials simulated in this work, a direct comparison of their device properties is possible, opening up new avenues for 2-D electronics.

**Performance Analysis.** The IRDS expects individual high-performance (HP) Si FinFETs to reach ON-state currents $I_{ON}=1.67$ mA/µm by 2025, when neglecting the influence of the contact resistances, as assumed here. At the same time carrier injection velocities $v_{inj}=1.46\times10^7$ cm/s and sub-threshold swings $SS=80$ mV/dec should be achieved. Figures 2a and 2b report the I-V characteristics of five of the best 2-D FETs that we simulated at $L_g=15$ nm: P$_4$, GeS, As$_4$, Ag$_2$N$_6$, and SiH (silicane). They all deliver $I_{ON}>3$ mA/µm.
at $I_{OFF}=0.1 \mu A/\mu m$, in their $n$- and $p$-type configurations, and could thus outperform the projected Si FinFET currents by a factor $\sim 2$ and monolayer MoS$_2$ by a factor $>3$. In total we find 13 2-D materials that arrive at the same performance level, as shown in Fig. 2c and summarized in Table 1. None of the conventional TMDs (MX$_2$ with M=Mo or W and X=S, Se, or Te) belongs to this group, contrary to black phosphorus (P$_4$) with transport along its $\Gamma$-$X$ axis, which displays the highest “$n$-type $I_{ON}$ vs. $p$-type $I_{ON}$” combination. It should be noted that several 2-D candidates (39) exhibit an ON-current larger than 3 mA/$\mu m$ in their $n$-type form, e.g. P$_8$Si$_4$ (5.43 mA/$\mu m$), As$_8$Ge$_4$ (5.12 mA/$\mu m$), or Tl$_2$O (5.09 mA/$\mu m$), much less (17) as $p$-FET, e.g. C$_2$N$_4$Pb$_2$ (4.08 mA/$\mu m$).

From the simulated ON-state characteristics we then extract the charge at the top-of-the-barrier (ToB) potential, $\rho_{ToB}$, and the carrier injection velocity at the same location, $v_{inj}=I_{ON}/(q \cdot \rho_{ToB})$, where $q$ is the elementary charge (see Fig. 2d). These quantities are depicted in Figs. 2e and 2f, respectively. On average, the ToB charge is equal to $\rho_{ToB,avg}=1.55e13$ cm$^{-2}$, with few notable exceptions: several 2-D materials with a single $\Gamma$ electron valley, e.g. InX (with X=As, N, P, or Sb), Bi$_2$Se$_3$, or Bi$_2$Te$_3$Se, are characterized by $\rho_{ToB}<1e13$ cm$^{-2}$. Their low effective mass $m^* \simeq 0.1 m_0$, $m_0$ being the electron rest mass, is responsible for that and for causing a so-called density-of-states bottleneck effect: $\rho_{ToB}$ is no more determined by the oxide capacitance of the dielectric layer, $C_{ox}$, but limited by the quantum capacitance of the channel material, $C_Q$.\[6\

In terms of injection velocities, all 2-D components with an ON-state current larger than 4 mA/$\mu m$ exceed the strained silicon marks of both electrons (1.4e7 cm/s) and holes (1e7 cm/s) and therefore satisfy the IRDS objective. Some compounds in the ideal corner of Fig. 2d, for example HfS$_2$, $n$-GeS, or $p$-SiH do not fulfill this condition and have 10-20% lower velocities than expected. It can also be noticed in Fig. 2f that (i) up to $I_{ON}=2$ mA/$\mu m$, the ON-state currents and injection velocities are strongly correlated and (ii) the largest $v_{inj}$’s are found for the 2-D materials with the lowest isotropic effective masses, which are also those suffering the most from the DOS bottleneck.
These findings are the products of computationally intensive simulations. We also aim to provide a more straightforward methodology to predict the potential of 2-D materials without the need for complex calculations. It is widely accepted that a semiconductor should have a high concentration of fast carriers to deliver a large $I_{ON}$ at fixed $I_{OFF}$. In the absence of source-to-drain tunneling, a low transport ($m_{Trans}$) and a high density-of-states ($m_{DOS}$) effective mass are required to supply these favorable conditions. In 2-D materials the $m_{Trans}$ and $m_{DOS}$ parameters cannot always be unambiguously defined due to the presence of multiple band minima (pockets), low energy separations between principal and satellite valleys, and strong band non-parabolicities. Physically meaningful averaging methods are needed to compute $m_{Trans}$ and $m_{DOS}$. The proposed approach is described in the Methods Section. It relies on the analytical expressions that can be derived for single-valley semiconductors.

Figure 3a reports the ON-state currents of the 100 simulated $n$- and $p$-type 2-D transistors as a function of their $m_{Trans}$ and $m_{DOS}$ metrics. The best performing devices occupy the lower left corner of the plot, as anticipated. They either possess an extremely low $m_{Trans}$ and $m_{DOS}$, e.g. $n$-InAs, where $m_{Trans} \approx m_{DOS} \approx 0.1 m_0$, or (moderately) low $m_{Trans}$ and (relatively) large $m_{DOS}$ such as $n$-P$_8$Si$_4$ ($m_{Trans}=0.14 m_0$, $m_{DOS}=1.26 m_0$) or $p$-P$_4$ with transport along the $\Gamma$-X axis ($m_{Trans}=0.14 m_0$, $m_{DOS}=0.82 m_0$). While the shape in Fig. 2a encompasses almost all FETs with $I_{ON}>3$ mA/µm, it also contains several outliers that despite apparently suitable ($m_{Trans}, m_{DOS}$) combinations return poor ON-state currents. This is the case of $n$-PtSe$_2$ with transport in the $\Gamma$-K direction ($m_{Trans}=0.32 m_0$, $m_{DOS}=1.92 m_0$, $I_{ON}=1.82$ mA/µm) or $n$-Au$_4$I$_4$Te$_4$ ($m_{Trans}=0.33 m_0$, $m_{DOS}=1.19 m_0$, $I_{ON}=0.88$ mA/µm).

The reason why $n$-PtSe$_2$ or $n$-Au$_4$I$_4$Te$_4$ show low $I_{ON}$'s can be traced back to their bandstructure, which is characterized at its bottom (conduction) or top (valence) by a single band with an energy width smaller than the applied source-to-drain voltage $V_{ds}$, as illustrated in Fig. 3b. In the ballistic limit of transport such narrow bands contribute only partly to the electrical current because a wave leaving the source contact cannot find a matching state on
the drain side (Fig. 3c). It follows that the transmission function $T(E, k_z)$, as computed with NEGF, is not only shifted by the gate-to-source voltage, as in conventional FETs, but also changes its shape and magnitude as the potential drop between source and drain increases (Fig. 3d). The inclusion of electron-phonon scattering reduces the negative impact of narrow bands by connecting them to conducting channels through phonon emission and absorption. However, even under realistic conditions, i.e. in the presence of dissipative scattering, narrow bands still limit the transport properties of several 2-D materials.

To quantify the influence of these narrow bands, we introduce a third metric called the pass factor ($PF$). It describes the ratio between the ballistic current that flows when a linear potential drop is applied to a device, $I_{\text{drop}}$, and under flat band conditions, $I_{\text{flat}}$, i.e. $PF = I_{\text{drop}} / I_{\text{flat}}$ (see Methods Section). In $I_{\text{drop}}$ the current contributions coming from the narrow bands are filtered out, whereas they are accounted for in $I_{\text{flat}}$. It is important to note that the smaller the $PF$ is, the more perturbed by narrow bands is the propagation of electrons and holes through 2-D devices. When $PF$ is 1, transport becomes optimal. The pass factor of the considered $n$- and $p$-type FETs is depicted in Fig. 3e. It can be seen that all 2-D materials with a large ON-current have a $PF$ greater than 0.75. To reflect this observation we plot again in Fig. 3f the “$I_{\text{ON}}$ vs. $m_{\text{Trans}}$ and $m_{\text{DOS}}$” data from before, this time keeping only the components with $PF > 0.75$. All outliers in the lower left corner of Fig. 3a have now disappeared, demonstrating that besides the transport ($m_{\text{Trans}}$) and density-of-states ($m_{\text{DOS}}$) effective masses, a third parameter, the pass factor ($PF$), is necessary to reveal the most promising candidates as ultimate 2-D logic switches and remove “false positive” contenders.

**Gate Length Scalability.** After studying the performance of 2-D FETs at $L_g=15$ nm, we turn to their scalability down to 5 nm. To bring insight into this critical issue, the subthreshold swing (SS) of all simulated transistors is extracted at different gate lengths (15, 12.5, 10, 7.5, and 5 nm) over a voltage range $\Delta V_{gs}=0.1$ V at $V_{ds}=0.7$ V. The results are reported in the form of a histogram in Fig. 4a, whereas the median “SS vs. $L_g$” data
averaged over all 2-D n- and p-FETs is presented in Fig. 4b. Down to a gate length of 10 nm, the SS distribution is very localized, with average values of 72 mV/dec at \( L_g = 15 \) nm, 77 mV/dec at \( L_g = 12.5 \) nm, and 88 mV/dec at \( L_g = 10 \) nm, with relatively narrow standard deviations of 3.4, 11.9, and 15.1 mV/dec, respectively. Starting at \( L_g = 7.5 \) nm, the SS spread drastically increases, indicating that single-gate 2-D FETs might not work optimally below 10 nm gate lengths. It should however be emphasized that with SS\(_{avg} = 72\) mV/dec at \( L_g = 15 \) nm and SS\(_{avg} = 77\) mV/dec at \( L_g = 12.5 \) nm, these devices surpass the 2025 IRDS targets for multi-gate Si FinFETs (80 mV/dec).

As already mentioned, 2-D materials with a high \( I_{ON} \) typically have a low transport effective mass \( m_{Trans} \), which can lead to large source-to-drain (S-to-D) tunneling leakages and poor sub-threshold swings at short gate lengths. No such correlation is noticed in Fig. 4c, where SS at \( L_g = 15 \) nm is reported as a function of the transistor ON-currents. It can thus be inferred that S-to-D tunneling plays a minor role at this gate length for the 2-D semiconductors considered and that the calculated band gaps, even if underestimated by DFT, do not impact SS at this scale, except for Bi$_2$GeTe$_4$ and InSb. Their narrow \( E_g \) of 0.99 and 1.07 eV, respectively, combined with a low \( m_{Trans} = 0.11 m_0 \) for electrons in InSb, push SS above 80 mV/dec. Note that at gate lengths \( L_g = 7.5 \) and 5 nm, when S-to-D tunneling starts to severely limit SS, \( E_g \) becomes a crucial parameter. Hence, from a quantitative point of view, the simulation results below \( L_g = 10 \) nm should be taken with precautions as the present DFT+NEGF approach may overestimate the sub-threshold swing of certain 2-D materials, especially those with a DFT band gap smaller than 1.2 eV and a low \( m_{Trans} \). It remains that even for compounds with band gaps larger than 1.5 eV, the average SS goes beyond 100 mV/dec at \( L_g = 5 \) nm, which calls for alternative device designs.

The scalability of transistors down to \( L_g = 5 \) nm can be improved by using gate-underlapping, i.e. by keeping undoped regions around the gate contact. This technique allows to increase the effective gate length without modifying its physical footprint. Lower ON-currents usually result from this process. Alternatively, the bottom SiO$_2$ substrate in Fig. 1a can be
replaced by a thin HfO$_2$ layer of the same thickness as the top one ($t_{ox}$=3 nm) and a second gate electrode can be inserted below it, symmetric with the first one. Such double-gate (DG) architectures, as illustrated in Fig. 4, are more complex and expensive to fabricate than single-gate ones, but they substantially reduce SS over the whole gate length range of interest, as demonstrated in the SI for selected 2-D materials. This phenomenon can be explained by examining the dependence of SS on the oxide capacitance $C_{ox}$, when S-to-D tunneling is ignored. It is given by $SS=(1+C_Q/C_{ox})\times60$ mV/dec, at room temperature, where $C_Q$ is the quantum capacitance of the channel material. By adding a second gate contact acting in parallel with the first one, $C_{ox}$ increases by a factor up to 2, the term $1+C_Q/C_{ox}$ gets closer to 1, and SS approaches 60 mV/dec.

Double-gate FETs do not only scale better than their single-gate counterparts; they also show higher ON-currents since their SS is steeper than in SG configurations (more rapid increase of the current) and their $C_{ox}$ is larger (more mobile charges are generated at the top-of-the-barrier location). The combined influence of these effects can more than double the ON-state current of DG transistors, as compared to SG ones, as can be seen in Figs. 4e and 4f for a GeS $n$- and $p$-type FET. Results for other 2-D materials with high ON-currents are presented in Table 2. As expected, in all cases, the DG $I_{ON}$ is between 1.9 and 2.3 times larger than the SG one, attaining values above 10 mA/$\mu$m in few materials (As$_4$, P$_4$, and As$_8$Ge$_4$). If such devices could be successfully fabricated and their contact resistance kept below 100 $\Omega$·$\mu$m, they would outplay the IRDS projections for Si FinFETs by a factor 6. More DG results can be found in the SI.

To complete the analysis of Table 2 it should be underlined that $\rho_{ToB}$ does not increase by the same amount as the current ($1.6\times$ for $\rho_{ToB}$ vs. 1.9 to 2.3$\times$ for $I_{ON}$) when going from single- to double-gate transistors. From this observation it can be deduced that the injection velocity at the ToB, $v_{inj}$, is greater in the DG structures too. This does not come as a surprise since higher-energy states get populated when $\rho_{ToB}$ increases. These states are usually characterized by a steeper band dispersion than those situated close to a band
extremum and therefore by a higher injection velocity, 30% on average for the considered logic devices.

Conclusions

We performed *ab initio* quantum transport simulations of 100 different single-gate *n*- and *p*-type field-effect transistors using stable 2-D monolayers taken from the computational database of Ref.\(^{30}\) as channel materials. For each of them, the *I*-*V* characteristics at a gate length \(L_g=15\) nm were calculated and their scalability was investigated down to \(L_g=5\) nm. The ON-current of 13 2-D materials was found to be larger than 3 mA/\(\mu\)m in both their *n*- and *p*-type configuration, even exceeding 4 mA/\(\mu\)m in three cases. Excellent sub-threshold swings down to \(L_g=10\) nm were obtained, confirming the great scalability potential of the 2-D technology. Finally, the compounds delivering the highest ON-currents were further tested with a double-gate architecture, which increased their \(I_{ON}\) by a factor 2 and might be required to go below \(L_g=10\) nm. These findings clearly indicate that 2-D materials could enable the continuation of Moore’s scaling law beyond Si FinFETs, provided that their contact resistances improve and their structural as well as interfacial defect density is reduced. Our results should be seen as the starting point for the exploration of novel 2-D materials with better transport properties than the known ones. We hope that they will motivate experimental groups to exfoliate new compounds, e.g. \(\text{As}_8\text{Ge}_4\), \(\text{O}_6\text{Sb}_4\), or \(\text{C}_2\text{N}_4\text{Pb}_2\) that are expected to outperform the popular transition metal dichalcogenides and challenge Si-based transistors.

On the simulation side, the design space will be extended with 2-D materials coming from other databases\(^{54,55}\) and from on-going searches conducted by some of the co-authors of this study. The proposed metrics (\(m_{\text{Trans}}, m_{\text{DOS}},\) and \(PF\)) will be extracted first. This will limit the number of 2-D systems that must be simulated at the quantum transport level and reduce the computational burden. The current 13 best-performing 2-D materi-
als will go through a second round of analysis where electron-phonon, defect, and surface optical phonon scattering will be added to accurately model their carrier mobility. The dielectric environment surrounding the 2-D monolayers will be explicitly accounted for in the Schrödinger equation; when possible, GW corrections and spin-orbit coupling will be included as well. Contact resistances will also be evaluated with different metal electrodes. Altogether this will help refine the predictions made in this paper.

**Methods**

**Selection of 2-D Materials.** The database of Ref. containing more than 1,800 entries was pre-screened to select 100 2-D materials that were then investigated as single-gate planar transistors. Based on their bandstructure characteristics we singled out the semiconductors with less than 30 atoms in their primitive unit cell, a layer thickness smaller than 1.5 nm, a band gap larger than 1 eV and, if possible, anisotropic conduction band minima and/or valence band maxima so that a low transport and high density-of-states effective mass can be obtained. We also eliminated 2-D materials where the lowest conduction or highest valence subband had a very narrow energy width of 0.5 eV or less and was completely isolated from the other bands. Finally, we inspected the structural stability of the chosen 2-D components by verifying that their phonon bandstructure did not exhibit negative branches.

**DFT Calculations.** The first step of each DFT calculation consists of identifying the primitive unit cell of the considered 2-D material. The lattice vectors and atomic positions are taken from Ref. A vacuum space of 20 Å is added along the confined direction to remove fictitious interactions between a 2-D layer and its periodic image. For the \( k \)-point sampling of the Brillouin Zone \( \Gamma \)-centered Monkhorst-Pack grids are employed with equal densities of \( k \)-points in all directions, except for the confined one. The plane-wave cutoff is set to at least 1.5 times the default value found in the exchange-correlation potential. For computational reasons spin-orbit coupling is neglected. Its influence on the transport
properties of the simulated 2-D materials can therefore neither be quantified nor estimated.

Most electronic structures were calculated within the generalized gradient approximation (GGA) of Perdew, Burke, and Ernzerhof (PBE) with the DFT-D3 parameterization of van der Waals forces from Grimme. At the beginning of this work, few 2-D materials were treated with the optPBE-vdW functional of Klimes, Bowler, and Michaelides before realizing that this model sometimes leads to the presence of valence states in the vacuum region of the simulation domain. For this reason optPBE-vdW was later on abandoned and 2-D materials whose electronic structure was obtained with it are specifically marked in the SI. Note that it has been verified that in case of perfectly empty vacuum, optPBE-vdW and PBE give the same bandstructure results.

For each 2-D sample, three consecutive DFT calculations are performed with the Vienna Ab initio Software Package (VASP). First, the atomic positions within the unit cell are relaxed until the force acting on each ion is converged to below \(10^{-3}\) eV/Å. The electronic structure is determined in a second step based on a very fine \(k\)-point grid so that the final energies vary by less than 1 meV per atom when increasing the number of \(k\)-points. Finally, the bandstructure along a path through the high-symmetry points of the Brillouin Zone is calculated with the charge density from the second simulation.

Although DFT is an ab initio method its results may depend on the choice of the exchange-correlation functional, basis set, or pseudo-potential parameterization. As a ground-state theory it tends to underestimate the band gap of semiconductors, which might lead to inaccurate predictions when source-to-drain tunneling becomes important, at gate lengths of 10 nm and below. GW corrections usually improve the situation, but with 2-D materials, this is not necessarily the case as their band gaps, effective masses, and valley splitting may depend on the surrounding dielectric environment. As such they are currently not known exactly, preventing a validation of the obtained bandstructures. Despite these drawbacks, in the vast majority of the cases, the fact that the precise band gap value remains uncertain does not impact the presented results, especially when \(L_g > 10\) nm. This is why the simula-
tion data proposed in this paper give a unique overview on the functionality of 100 different 2-D FETs.

**Wannier Functions.** The plane-wave results produced by VASP are transformed into a basis of maximally-localized Wannier functions (MLWFs) with the wannier90\(^{[22]}\) tool. An energy window encompassing 0.7 to 1 eV around the band gap of each material is defined. All bands originating from within this interval are retained in the MLWF Hamiltonian. Next the latter is diagonalized for the same \(k\)-point path as the original VASP simulation. The resulting VASP and MLWF bandstructures can then be compared to each other. The Wannierization process is considered as successful if all occupied bands, according to the chosen doping concentration (5e13 cm\(^{-2}\)), are reproduced within a maximum tolerance of 20 meV and if the errors around the conduction and valence band edges are below 5 meV. As last step the MLWF Hamiltonian blocks corresponding to the primitive unit cell of the studied 2-D materials are scaled up according to the techniques presented in Ref.\(^{[62]}\) to yield the Hamiltonian matrix of the full device, \(H_{MLWF}\) (see Fig. 1a for the dimensions).

**Quantum Transport Simulations.** The OMEN code is used as quantum transport simulator.\(^{[40]}\) The approach is very similar to the one described in the Supporting Information of Ref.\(^{[62]}\) After upscaling the MLWF Hamiltonian the \(I-V\) characteristics of the investigated 2-D transistors are computed with the NEGF formalism at room temperature. The retarded \((G^R(E,k_z))\), lesser \((G^<(E,k_z))\), and greater \((G^>(E,k_z))\) Green’s function are evaluated for all possible carrier energies \(E\) and momentum points \(k_z\) using

\[
\left( E - H_{MLWF}(k_z) - \Sigma^{RB}(k_z, E) - \Sigma^{RS}(k_z, E) \right) \cdot G^R(k_z, E) = I, \tag{1}
\]

\[
G^<(k_z,E) = G^R(k_z,E) \cdot \left( \Sigma^{>B}(k_z,E) + \Sigma^{>S}(k_z,E) \right) \cdot G^A(k_z,E). \tag{2}
\]

The advanced Green’s Function \(G^A(E,k_z)\) is the transpose of \(G^R(E,k_z)\). The Hamiltonian matrix \(H_{MLWF}\) is expressed in a MLWF basis and constructed according to the prescriptions described above. The size of \(H_{MLWF}\) as well as of all Green’s Functions is equal to \(N_A \times N_{wf}\),
where $N_A$ is the total number of atoms in the simulated system and $N_{wf}$ the average number of Wannier functions per atom.

In Eqs. (1) and (2), the energy vector is homogeneously discretized with a distance $dE=1$ meV between two adjacent points. The momentum dependence, which is a consequence of the assumed-periodic out-of-plane direction $z$ in Fig. 1a, is modeled via $N_{kz}=15$ points. Orthorhombic unit cells are used in our transport calculations. Their width along the $z$ direction is chosen to be larger than 1 nm so that $N_{kz}=15$ is sufficient to obtain accurate results. The open boundary conditions and all scattering sources are cast into the self-energies $\Sigma^{TB}(E,k_z)$ and $\Sigma^{TS}(E,k_z)$, respectively. They are of the same type $T(R, <, or >)$ and size as the Green’s Functions.

Non-physical behaviors may occur in 2-D materials in the ballistic limit of transport due to the presence of narrow bands. To avoid them and provide realistic simulation results, an energy relaxing mechanism is introduced into the NEGF equations. We opted for a phenomenological electron-phonon scattering model where two parameters can be freely chosen, the phonon frequency $\omega$ and the deformation potential $D_{e-ph}$.

$$\Sigma^{S}(k_z, E) = D_{e-ph}^2 \left(n_\omega G^S(k_z, E + \hbar \omega) + (n_\omega + 1)G^S(k_z, E - \hbar \omega)\right).$$  \hspace{1cm} (3)

In Eq. (3) $n_\omega$ is the Bose-Einstein distribution function. We use a phonon energy $\hbar \omega=40$ meV and a scattering strength $D_{e-ph}$ comprised between 25 and 125 meV, depending on the width of the narrow bands. The resulting equations are solved within the so-called self-consistent Born approximation till convergence is reached, i.e. till the electronic current is conserved all along the device structure. By considering these (pseudo) electron-phonon interactions, energy bands with a narrow width get connected to each other, either through phonon emission or absorption, which opens additional conduction channels and eliminates ballistic modeling artifacts. Furthermore, non-idealities such as inter-valley scattering are accounted for to a certain extent. Still, all investigated 2-D transistors operate close to their
ballistic limit: the used scattering strength causes a decrease of the electrical current by no more than 20%. Note however that for the 2-D materials with narrow energy bands, an increase of the current is typically observed when dissipative interactions are turned on. Effective Mass and Pass Factor Extraction. To extract the transport \((m_{Trans})\) and density-of-states \((m_{DOS})\) effective masses of 2-D materials and allow for meaningful comparisons of different components, the average ToB charge density \(\rho_{ToB,avg}=1.55e13\) cm\(^{-2}\) from Fig. 1e is recalled. All calculations are done assuming that the bandstructure of the 2-D materials is filled with that specific density, which sets a reference to establish the potential of a crystal before running any device simulation.

First, the bandstructure \(E(k_x,k_z)\) of the 2-D semiconductor under investigation is computed for all \((k_x,k_z)\) wave vectors belonging to its Brillouin Zone (BZ), see the SI. Here, \(k_x\) refers to the axis aligned with the transport direction, \(k_z\) models the one assumed periodic, i.e. the out-of-plane direction in Fig. 1a. In this study, an orthorhombic unit cell is used as starting point. With the knowledge of \(E(k_x,k_z)\) the Fermi level \(E_f\) that corresponds to \(\rho_{ToB,avg}\) can be numerically acquired from

\[ \rho_{ToB,avg} = \frac{1}{A} \sum_{k_x,k_z \in BZ} f(E(k_x,k_z),E_f), \]  

where \(A\) is the area of the unit cell and \(f(E,E_f)\) the Fermi-Dirac distribution function. The sum goes over the entire Brillouin Zone, which is rectangular for orthorhombic unit cells. In case of holes, \(E(k_x,k_z)\) is first multiplied by -1 so that all equations derived for electrons can be directly applied. From now on, no distinction is made in the treatment of electrons and holes.

Next, the bandstructure-limited ToB electronic current \(I_{d,BS}\) that flows through an idealized device at a charge concentration \(\rho_{ToB,avg}=1.55e13\) cm\(^{-2}\) is evaluated with the following
equation

\[ I_{d,BS} = \frac{1}{2A} \sum_{k_x,k_z \in BZ} |v_x(k_x,k_z)| f(E(k_x,k_z), E_f) \]  (5)

with the \(E_f\) value from Eq. (4). The factor 1/2 indicates that only half of the Brillouin Zone carries current, the one where the electronic states have a positive velocity \(v_x(k_x,k_z)=1/\hbar dE(k_x,k_z)/dk_x\) along the transport axis \(x\) in Fig. 1a. The variable \(\hbar\) is Planck’s reduced constant.

If a single parabolic band with an anisotropic dispersion \(E(k_x,k_z)=E_{min}+\hbar^2/2(k_x^2/m_x+k_z^2/m_z)\) and an energy minimum \(E_{min}\) is assumed, then quasi-analytical expressions can be found for the solution of Eqs. (4) and (5)

\[ \rho_{ToB,avg} = \frac{\sqrt{m_x m_z}}{\pi \hbar^2} \int_{E_{min}}^{\infty} dE f(E, E_f), \]  (6)

\[ I_{d,BS} = q\sqrt{2m_z/\pi^2 \hbar^2} \int_{E_{min}}^{\infty} dE \sqrt{E - E_{min}} f(E, E_f). \]  (7)

We observe that \(m_{DOS}=\sqrt{m_x m_z}\) and by definition, \(m_{Trans}=m_x\), the effective mass along the transport direction. For comparison purpose, the bandstructure of all considered 2-D materials is reduced to these two highly relevant quantities that can be interpreted as occupancy-aware, averaged masses. First, \(E_f\) is computed in Eq. (4), then \(I_{d,BS}\) in Eq. (5), \(m_{DOS}\) in Eq. (6), and finally \(m_{Trans}=m_{DOS}^2/m_z\) in Eq. (7). The obtained effective masses indirectly account for all valleys situated close to the band extrema, non-parabolic effects, and band filling according to the average ON-state charge at the ToB location, \(\rho_{ToB,avg}\). No QT simulation is needed to evaluate Eqs. (4) to (7), only bandstructures.

The last metrics that we used to assess the potential of a given 2-D material is a new quantity called pass factor (\(PF\)). It is defined as

\[ PF = \frac{\sum_{k_z} \int_{E_{min}}^{\infty} dE T_{Vd_s=V_{DD}}(E,k_z) f(E, E_f)}{\sum_{k_z} \int_{E_{min}}^{\infty} dE T_{Vd_s=0}(E,k_z) f(E, E_f)} , \]  (8)
where $T_{V_{ds}}(E, k_z)$ is the energy- and momentum-dependent transmission function calculated when a linear potential drop of amplitude $qV_{ds}$ is applied between both ends of a 2-D material, as in Fig. 2d. Note that determining $T_{V_{ds}}(E, k_z)$ requires a non-self-consistent QT simulation involving $N_E=1,000$ energy- and $N_{k_z}=15$ momentum-points, which remains computationally very affordable.

The $m_{\text{Trans}}, m_{\text{DOS}},$ and $PF$ values of the simulated 2-D materials can be found in the SI.

**Acknowledgement**

This research was supported by ETH Zurich (grant ETH-32 15-1) and by the Swiss National Science Foundation (SNSF) under grant no. 200021_175479 (ABIME) and under the NCCR MARVEL. We acknowledge PRACE for awarding us access to Piz Daint at CSCS under Project pr28, PRACE for the allocated computational resources on Marconi at CINECA under Project 2016163963, and CSCS for Project s876.

**Supporting Information Available**

The following files are available free of charge. Electron/hole “current vs. voltage” characteristics, “sub-threshold swing vs. gate length”, unit cell, bandstructure, injection velocity, transport and density-of-states effective masses, and “pass factor” of the 100 2-D materials considered in this work.

**References**

(1) Kuhn, K. Considerations for Ultimate CMOS Scaling. *IEEE Trans. Elec. Dev.* **2012**, 59, 1813-1828.
(2) Appenzeller, J.; Knoch, J.; Borg, M. T.; Riel, H.; Schmid H.; and Riess, W. Towards Nanowire Electronics. *IEEE Trans. Elec. Dev.* **2008**, *55*, 2827-2845.

(3) Loubet N. et al. Stacked nanosheet gate-all-around transistor to enable scaling beyond FinFET. *2017 Symposium on VLSI Technology (VLSIT)* **2017**, *230*-231.

(4) del Alamo, J. A. Nanometre-scale electronics with III-V compound semiconductors. *Nature* **2011**, *479*, 317-323.

(5) Sistani, M.; Staudinger, P.; Greil, J.; Holzbauer, M.; Detz H.; Bertagnolli, E.; and Lugstein, A. Room-Temperature Quantum Ballistic Transport in Monolithic Ultrascaled Al-Ge-Al Nanowire Heterostructures. *Nano Letters* **2017**, *17*, 4556-4561.

(6) Javey, A.; Guo, J.; Wang, Q.; Lundstrom, M.; and Dai, H. Ballistic carbon nanotube field-effect transistors. *Nature* **2003**, *424*, 654-657.

(7) Novoselov, K. S.; Geim, A. K.; Morozov, S. V.; Jiang, D.; Zhang, Y.; Dubonos, S. V.; Grigorieva, I. V.; and Firsov, A. A. Electric Field Effect in Atomically Thin Carbon Films. *Science* **2004**, *306*, 666-669.

(8) Radisavljevic, B.; Radenovic, A.; Brivio, J.; Giacometti, V.; and Kis, A. Single-layer MoS$_2$ transistors. *Nat. Nanotech.* **2011**, *6*, 147-150.

(9) Tosun, M.; Chuang, S.; Fang, H.; Sachid, A. B.; Hettick, M.; Lin, Y. J.; Zeng, Y. P.; and Javey, A. High-gain inverters based on WSe$_2$ complementary field-effect transistors. *ACS Nano* **2014**, *8*, 4948-4953.

(10) Ovchinnikov, D.; Allain, A.; Huang, Y.-S.; Duncenco, D.; and Kis, A. Electrical Transport Properties of Single-Layer WS$_2$. *ACS Nano* **2014**, *8*, 8174-8181.

(11) Pradhan, N. R.; Rhodes, D.; Feng, S.; Xin, Y.; Memaran, S.; Moon, B. H.; Terrones, H.; Terrones, M.; and Balicas, L. Field-effect transistors based on few-layered $\alpha$-MoTe$_2$. *ACS Nano* **2014**, *8*, 5911-5920.
(12) Meng, Y.; Ling, C.; Xin, R.; Wang, P.; Song, Y.; Bu, H.; Gao, S.; Wang, X.; Song, F.;
Wang, J.; Wang, X.; Wang, B.; and Wang, G. Repairing Atomic Vacancies in Single-Layer MoSe\textsubscript{2} Field-Effect Transistor and Its Defect Dynamics. *NPJ Quant. Mater.* \textbf{2017}, 2, 16.

(13) Mleczko, M. J.; Zhang, C.; Lee, H. R.; Kuo, H. H.; Magyari-Köpe, M.; Moore, R. G.;
Shen, Z.-X.; Fisher, I. R.; Nishi, Y.; and Pop, E. HfSe\textsubscript{2} and ZrSe\textsubscript{2} : Two-Dimensional Semiconductors with Native High-$\kappa$ Oxides. *Science Adv.* \textbf{2017}, 3, e1700481.

(14) Liu, E. et al. Integrated Digital Inverters Based on Two-Dimensional Anisotropic ReS\textsubscript{2} Field-Effect Transistors. *Nat. Commun.* \textbf{2015}, 6, 6991.

(15) Desai, S. B. et al. MoS\textsubscript{2} transistors with 1-nanometer gate lengths. *Science* \textbf{2016}, 354, 99-102.

(16) Allain, A.; Kang, J.; Banerjee, K.; and Kis, A. Electrical contacts to two-dimensional semiconductors. *Nature Mat.* \textbf{2015}, 14, 1195-1205.

(17) McClellan, C. J.; Yalon, E.; Smithe, K. K. H.; Suryavanshi, S. V.; and Pop, E. Effective n-type doping of monolayer MoS\textsubscript{2} by AlO\textsubscript{x}. 2017 \textit{75th Annual Device Research Conference (DRC)} \textbf{2017}, DOI: 10.1109/DRC.2017.7999392.

(18) Suh, J.; Park, T.; Lin, D.; Fu, D.; Park, J.; Jung, J.; Chen, Y.; Ko, C.; Jang, C.;
Sun, Y.; Sinclair, R.; Chang, J.; Tongay, S.; and and Wu, J. Doping against the Native Propensity of MoS\textsubscript{2} : Degenerate Hole Doping by Cation Substitution. *Nano Lett.* \textbf{2014}, 14, 6976.

(19) Li, L. et al. Black phosphorus field-effect transistors. *Nat. Nanotech.* \textbf{2014}, 9, 372-377.

(20) Tao, L.; Cinquanta, E.; Chiappe, D.; Grazianetti, C.; Fanciulli, M.; Dubey, M.; Molle, A.; and Akinwande D. Silicene field-effect transistors operating at room temperature. *Nat. Nanotech.* \textbf{2015}, 10, 227-231.
(21) Derivaz, M.; Dentel, D.; Stephan, R.; Hanf, M. C.; Mehdaoui, A.; Sonnet, P.; and Pirri, C. Continuous germanene layer on Al(111). *Nano Letters* **2015**, *15*, 2510-2516.

(22) Ji, J. P. et al. Two-dimensional antimonene single crystals grown by van der Waals epitaxy. *Nat. Commun.* **2016**, *7*, 13352.

(23) Bandurin, D. A. et al. High electron mobility, quantum Hall effect and anomalous optical response in atomically thin InSe. *Nat. Nanotech.* **2017**, *12*, 223-227.

(24) Wu, J. et al. High electron mobility and quantum oscillations in non-encapsulated ultrathin semiconducting Bi$_2$O$_2$Se. *Nat. Nanotech.* **2017**, *12*, 530-534.

(25) Fiori, G. et al. Electronics based on two-dimensional materials. *Nat. Nanotech.* **2014**, *9*, 768-779.

(26) Franklin, A. D. Nanomaterials in transistors: From high-performance to thin-film applications. *Science* **2015**, *349*, aab2750.

(27) Tan, C. et al. Recent Advances in Ultrathin Two-Dimensional Nanomaterials. *Chem. Rev.* **2017**, *117*, 6225-6331.

(28) Zeng, M.; Xiao, Y.; Liu, J.; Yang, K.; and Fu L. Exploring Two-Dimensional Materials toward the Next-Generation Circuits: From Monomer Design to Assembly Control. *Chem. Rev.* **2018**, *118*, 6236-6296.

(29) Liu, Y.; Duan, X.; Huang, Y.; and Duan, X. Two-dimensional transistors beyond graphene and TMDCs. *Chem. Soc. Rev.* **2018**, *47*, 6388.

(30) Mounet, N. et al. Two-dimensional materials from high-throughput computational exfoliation of experimentally known compounds. *Nat. Nanotech.* **2018**, *13*, 246-252.

(31) Chang, J.; Register, L. F.; and Banerjee, S. K. Ballistic performance comparison of monolayer transition metal dichalcogenide MX$_2$ (M = Mo, W; X = S, Se, Te) metal-oxide-semiconductor field effect transistors. *J. Appl. Phys.* **2014**, *115*, 084506.
(32) Luisier, M.; Szabó, Á.; Stieger, C.; Klinkert, C.; Brück, S.; Jain, A.; and Novotny, L. First-principles simulations of 2-D semiconductor devices: mobility, $I$-$V$ characteristics, and contact resistance. *Proceedings of the 2016 International Electron Device Meeting (IEDM)* 2016, 5.4.1-5.4.4.

(33) AlMutairi, A. A.; Yin, D.; and Yoon, Y. PtSe$_2$ Field-Effect Transistors: New Opportunities for Electronic Devices. *IEEE Elec. Dev. Lett.* 2017, 39, 151-154.

(34) Ilatikhameneh, H.; Ameen, T.; Novakovic, B.; Tan, Y.; Klimeck, G.; and Rahman R. Saving Moore’s Law Down To 1nm Channels With Anisotropic Effective Mass. *Scientific Reports* 2016, 6, 31501.

(35) Quhe, R. et al. High-performance sub-10 nm monolayer Bi$_2$O$_2$Se transistors. *Nanoscale* 2019, 11, 532-540.

(36) Das, P.; Wickramaratne, D.; Debnath, B.; Yin, G.; and Lake, R. K. Charged impurity scattering in two-dimensional materials with ring-shaped valence bands: GaS, GaSe, InS, and InSe. *Phys. Rev. B* 2019, 99, 085409.

(37) Gaddemane, G.; Vandenberghe, W. G.; Van de Put, M. L.; Chen, E.; and Fischetti, M. V. Monte-Carlo study of electronic transport in non-$\sigma$-h-symmetric two-dimensional materials: Silicene and germanene. *J. Appl. Phys.* 2018, 124, 044306.

(38) Pizzi, G.; Gibertini, M.; Dib, E.; Marzari, N.; Iannaccone, G.; and Fiori, G. Performance of arsenene and antimonene double-gate MOSFETs from first principles. *Nat. Comm.* 2016, 7, 12585.

(39) Ma, Y.; Kuc, A.; and Heine, T. Single-Layer Tl$_2$O: A Metal-Shrouded 2D Semiconductor with High Electronic Mobility. *J. Am. Chem. Soc.* 2017, 139, 11694-11697.

(40) Ziogas, A. N.; Ben-Nun, T.; Fernández, G. I.; Schneider, T.; Luisier, M.; and Hoefler, T. A Data-Centric Approach to Extreme-Scale *Ab Initio* Dissipative Quantum Trans-
port Simulations. *Proceedings of the International Conference for High Performance Computing, Networking, Storage and Analysis 2019*, Article 1.

(41) Ong, Z. Y. and Fischetti, M. V. Mobility enhancement and temperature dependence in top-gated single-layer MoS$_2$. *Phys. Rev. B* **2013**, *88*, 165316.

(42) Hong, J. et al. Exploring atomic defects in molybdenum disulphide monolayers. *Nat. Comm.* **2015**, *6*, 6293.

(43) Ma, N. and Jena, D. Charge Scattering and Mobility in Atomically Thin Semiconductors. *Phys. Rev. X* **2014**, *4*, 011043.

(44) https://irds.ieee.org/editions/2018

(45) Kresse, G. and Furthmüller J. Efficient iterative schemes for *ab initio* total-energy calculations using a plane-wave basis set. *Phys. Rev. B* **1996**, *54*, 11169.

(46) Marzari, N. and Vanderbilt, D. Maximally localized generalized Wannier functions for composite energy bands. *Phys. Rev. B* **1997**, *56*, 12847.

(47) Mostofi, A. A. et al. wannier90: A Tool for Obtaining Maximally-Localised Wannier Functions. *Comp. Phys. Comm.* **2008**, *178*, 685-699.

(48) Szabó, Á.; Rhyner, R.; and Luisier, M. *Ab initio* simulation of single- and few-layer MoS$_2$ transistors: Effect of electron-phonon scattering. *Phys. Rev. B* **2015**, *92*, 035435.

(49) Lundstrom M.; and Ren, Z. Essential Physics of Carrier Transport in Nanoscale MOS-FETs. *IEEE Trans. Elec. Dev.* **2002**, *49*, 133-141.

(50) Fischetti, M. V.; Wang, L.; Yu, B.; Sachs, C.; Asbeck, P. M.; Taur, Y.; and Rodwell, M. Simulation of Electron Transport in High-Mobility MOSFETs: Density of States Bottleneck and Source Starvation. *Proceedings of the 2007 International Electron Device Meeting (IEDM)* **2007**, 109-112.
(51) Khakifirooz, A. and Antoniadis D. A. MOSFET performance scaling-Part I: Historical trends. *IEEE Trans. Elect. Dev.* **2008**, 55 1391-1400.

(52) Luisier, M.; Lundstrom, M.; Antoniadis, D. A.; and Bokor, J. Ultimate device scaling: Intrinsic performance comparisons of carbon-based, InGaAs, and Si field-effect transistors for 5 nm gate length. *Proceedings of the 2011 International Electron Device Meeting (IEDM)* **2011**, **11.2.1-11.2.4**.

(53) Rahman, A.; Guo, J.; Datta, S.; and Lundstrom, M. Theory of Ballistic Nanotransistors. *IEEE Trans. Elec. Dev.* **2003**, 50, 1853.

(54) https://www.ctcms.nist.gov/~knck6/JVASP.html

(55) https://cmr.fysik.dtu.dk/c2db/c2db.html

(56) Lee, Y.; Fiore, S.; and Luisier, M. *Ab initio* Mobility of Single-layer MoS$_2$ and WS$_2$: Comparison to Experiments and Impact on the Device Characteristics. *Proceedings of the 2019 International Electron Device Meeting (IEDM)* **2019**, **24.4.1-24.4.4**.

(57) Perdew, J. P.; Burke, K.; and Ernzerhof, M. Generalized Gradient Approximation Made Simple. *Phys. Rev. Lett.* **1997**, 77, 3865.

(58) Grimme, S.; Antony, J.; Ehrlich, S.; and Krieg, H. A consistent and accurate ab initio parametrization of density functional dispersion correction (DFT-D) for the 94 elements H-Pu. *J. Chem. Phys.* **2010**, 132, 154104.

(59) Klimes, J.; Bowler, R. B. and Michaelides, A. Chemical accuracy for the van der Waals density functional. *J. Phys. Matt.* **2010**, 22, 022201.

(60) Qiu, D. Y.; da Jornada, F. H.; and Louie, S. G. Optical Spectrum of MoS$_2$: Many-Body Effects and Diversity of Exciton States. *Phys. Rev. Lett.* **2013**, **111**, 216805.
(61) Jiang, X.; Kharche, N.; Kohl, P.; Boykin, T. B.; Klimeck, G.; Luisier, M.; Ajayan, P. M.; and Nayak, S. K. Giant quasiparticle bandgap modulation in graphene nanoribbons supported on weakly interacting surfaces. *Appl. Phys. Lett.* 2013, 103, 133107.

(62) Szabó, Á.; Jain, A.; Parzefall, M.; Novotny, L.; and Luisier, M. Electron Transport through Metal/MoS$_2$ Interfaces: Edge- or Area-Dependent Process? *Nano Letters* 2019, 19, 3641-3647.
Figure 1: Schematic view of the single-gate field-effect transistors (SG FETs) investigated in this work. The total device length measures 40 nm, with a gate length $L_g$ varying between 15 and 5 nm. The source and drain extensions are doped with a donor $N_D$ or acceptor $N_A$ concentration of $5 \times 10^{13} \text{ cm}^{-2}$ for the $n$- and $p$-type configuration, respectively. The doping abruptly stops at the channel-source/drain interfaces. A $t_{ox}=3 \text{ nm}$ thick high-$\kappa$ dielectric layer ($\text{HfO}_2$) separates the 2-D channel from the gate contact. The 2-D material (here $\text{PdS}_2$) is deposited on a $\text{SiO}_2$ box of thickness $t_{box}=20 \text{ nm}$. Perfectly ohmic contacts are assumed (no resistance). All simulations are performed at room temperature with the metal gate work function adjusted to fix the OFF-current to $0.1 \mu\text{A}/\mu\text{m}$. Transport occurs along the $x$-axis, $y$ is a direction of confinement, while $z$ is assumed periodic. The primitive unit cells of few representative 2-D materials are plotted around the transistor structure.
Figure 2: (a) Transfer characteristics $I_d-V_{gs}$ at $V_{ds}=V_{DD}=0.7$ V of 6 selected 2-D $p$-type FETs similar to the one in Fig. 1: P$_4$, As$_4$, GeS, Ag$_2$N$_6$, SiH, and MoS$_2$. (b) Same as (a), but for the $n$-type configuration. (c) “$n$-type $I_{ON}$ vs. $p$-type $I_{ON}$” for the 100 simulated 2-D materials. Green triangles refer to components with both current types larger than 3 mA/µm, red squares to standard TMDs (MX$_2$ with M=Mo or W and X=S, Se, or Te). (d) Illustration of the method used to extract the top-of-the-barrier location from 2-D devices as well as the corresponding charge $\rho_{ToB,avg}$ and injection velocity $v_{inj}$. (e) ON-state charge density extracted at the top-of-the-barrier location as a function of the ON-current. The dashed line indicates the average charge over all devices, $\rho_{ToB,avg}=1.55e13$ cm$^{-2}$. Filled (empty) symbols correspond to electron (hole) conduction. (f) ON-state carrier injection velocity $v_{inj}$ at the ToB location with respect to the ON-current. The values for electrons and holes in strained silicon are given as references.\[51]
Figure 3: (a) ON-current of the 100 simulated n- and p-type 2-D FETs as a function of their transport $m_{\text{Trans}}$ and density-of-states $m_{\text{DOS}}$ effective masses. Filled (empty) symbols refer to electron (hole) configurations, whereas squares represent TMDs and triangles the 13 most promising 2-D materials. The color of each symbol indicates the magnitude of the corresponding $I_{\text{ON}}$. The shape in the lower left corner includes almost all best performing materials, i.e. those with a suitable ($m_{\text{Trans}}, m_{\text{DOS}}$) combination, but also several outliers. (b) Bandstructure of AuITe around its conduction band minimum, along the X-Γ-M path. The lowest band has an energy width of $\sim 0.5$ eV only, which is smaller than the applied source-to-drain voltage $V_{\text{ds}} = 0.7$ V. (c) Schematic representation of the electron transmission through a device with an applied voltage $V_{\text{ds}}$. Only bands with an energy width larger than $qV_{\text{ds}}$ can directly carry current, those with a narrower width must absorb or emit a phonon to be (partly) transmitted. (d) Energy-resolved transmission function $T(E, k_z = 0)$ through a 40 nm long AuITe monolayer with a linear potential drop of 0, 0.4, and 0.7 V between both its extremities. Due to the presence of a narrow band, the transmission function strongly depends on the applied bias. (e) Pass factor $PF$ of all considered 2-D FETs as a function of their ON-current. The same plotting conventions as in sub-plot (a) are used. (f) Same as (a), but after eliminating the 2-D materials with $PF < 0.75$. All components with a poor ON-state performance have disappeared from the shape in the lower left corner.
Figure 4: (a) Histogram of the sub-threshold swing (SS) of all investigated n- and p-type FETs at a gate length $L_g=15, 12.5, 10, 7.5,$ and $5 \text{ nm}$. The mean value is indicated for each $L_g > 5 \text{ nm}$. (b) Box plot summarizing the distribution of the sub-threshold swings for the considered gate lengths. Each box contains 50% of the extracted SS. The mark in the middle of the box is the median. The ends of the whiskers represent one standard deviation above and below the mean of the data. (c) Sub-threshold swing at $L_g=15 \text{ nm}$ as a function of the ON-current at the same gate length. Green triangles refer to the 13 best 2-D materials, red squares to conventional TMDs, while filled (empty) symbols represent n-type (p-type) transistors. (d) Schematic view of a double-gate GeS FET. As compared to the structure in Fig. 1, the bottom SiO$_2$ substrate was replaced by a HfO$_2$ layer of thickness $t_{ox}=3 \text{ nm}$ and a second gate contact was added at the bottom. (e) Transfer characteristics $I_d-V_{gs}$ at $V_{ds}=0.7 \text{ V}$ of the GeS p-FET in (d) with $L_g=15 \text{ nm}$, using a single- and double-gate architecture. The $I-V$ curves are plotted on a linear and logarithmic scale. (f) Same as (e), but for the GeS n-FET.
Table 1: ON-state current ($I_{ON}$), charge at the top-of-the-barrier ($\rho_{ToB}$), injection velocity at the same location ($v_{inj}$), and sub-threshold swing (SS) for the 13 2-D single-gate FETs with $I_{ON} > 3$ mA/µm in both their n- and p-type configuration at $L_g = 15$ nm.

|   | n-FET |   |   | p-FET |   |   |
|---|---|---|---|---|---|---|
|   | $I_{ON}$ (mA/µm) | $\rho_{ToB}$ (cm$^{-2}$) | $v_{inj}$ (cm/s) | SS (mV/dec) | $I_{ON}$ (mA/µm) | $\rho_{ToB}$ (cm$^{-2}$) | $v_{inj}$ (cm/s) | SS (mV/dec) |
| Ag$_2$N$_6$ | 3.91 | 1.45e13 | 1.68e7 | 67 | 3 | 1.46e13 | 1.28e7 | 66.6 |
| As$_2$ | 4.17 | 1.7e13 | 1.53e7 | 67.4 | 3.77 | 1.47e13 | 1.59e7 | 69.7 |
| As$_4$ | 4.37 | 1.65e13 | 1.65e7 | 67.7 | 5.12 | 1.47e13 | 2.18e7 | 73.2 |
| Ge$_2$S$_2$ | 4.45 | 1.77e13 | 1.57e7 | 67.8 | 4.08 | 1.67e13 | 1.52e7 | 65.8 |
| Ge$_2$Se$_2$ | 3.4 | 1.86e13 | 1.14e7 | 69.1 | 4.38 | 1.8e13 | 1.52e7 | 68 |
| HfS$_2$ | 3.27 | 1.97e13 | 1.04e7 | 69.1 | 3.59 | 1.77e13 | 1.26e7 | 68.8 |
| O$_6$Sb$_4$ | 4.47 | 1.61e13 | 1.73e7 | 67.6 | 3.07 | 1.51e13 | 1.27e7 | 62.6 |
| P$_4$ | 4.9 | 1.49e13 | 2.05e7 | 69.3 | 5.21 | 1.58e13 | 2.05e7 | 70.4 |
| Sb$_2$ | 5.11 | 1.78e13 | 1.79e7 | 67.5 | 3.8 | 1.57e13 | 1.51e7 | 70.1 |
| Si$_2$H$_2$ | 4.46 | 1.8e13 | 1.55e7 | 69.5 | 3.2 | 1.6e13 | 1.25e7 | 69.5 |
| Ti$_2$Br$_2$N$_2$ | 3.49 | 9.38e12 | 2.32e7 | 71.6 | 3.25 | 1.04e13 | 1.95e7 | 75.8 |
| Ti$_2$N$_2$Cl$_2$ | 3.44 | 1.07e13 | 2.01e7 | 69.9 | 3.48 | 9.85e12 | 2.2e7 | 70.4 |
| ZrS$_2$ | 3.24 | 2.25e13 | 9e6 | 66.4 | 3.37 | 1.76e13 | 1.19e7 | 68.5 |
Table 2: ON-state current ($I_{ON}$), charge at the top-of-the-barrier ($\rho_{ToB}$), sub-threshold swing at $L_g=15$ nm ($SS_{15nm}$) and $L_g=5$ nm ($SS_{5nm}$) for selected 2-D materials with a high n- and/or p-type current, with a single- and a double-gate architecture. The $I_{ON}$ and $\rho_{ToB}$ quantities are extracted at $L_g=15$ nm.

| Single-Gate | Double-Gate |
|-------------|-------------|
|             | $I_{ON}$ (mA/µm) | $\rho_{ToB}$ (cm$^{-2}$) | $SS_{15nm}$ (mV/dec) | $SS_{5nm}$ (mV/dec) | $I_{ON}$ (mA/µm) | $\rho_{ToB}$ (cm$^{-2}$) | $SS_{15nm}$ (cm/s) | $SS_{5nm}$ (mV/dec) |
| n-As$_4$    | 4.37         | 1.65e13       | 67.7          | 339.7        | 9.06         | 2.66e13       | 61.3            | 229.7        |
| p-As$_4$    | 5.12         | 1.47e13       | 73.2          | 689.3        | 10.19        | 2.38e13       | 64.4            | 286.5        |
| n-As$_4$Ge$_4$ | 5.12       | 1.54e13       | 71.8          | 254.4        | 11.42        | 2.48e13       | 61.3            | 159.2        |
| p-C$_2$N$_4$Pb$_2$ | 4.08    | 1.69e13       | 68.8          | 159.5        | 9.28         | 2.66e13       | 61.6            | 114.2        |
| n-GeS       | 4.45         | 1.77e13       | 67.8          | 156.3        | 8.4          | 2.76e13       | 62              | 111          |
| p-GeS       | 4.08         | 1.67e13       | 65.8          | 168.4        | 8.67         | 2.79e13       | 61.1            | 119.7        |
| n-O$_6$Sb$_4$ | 4.47      | 1.61e13       | 67.6          | 207.7        | 10.73        | 2.61e13       | 62.8            | 136          |
| n-P$_4$     | 4.90         | 1.49e13       | 69.3          | 226.9        | 9.44         | 2.36e13       | 62.7            | 161.5        |
| p-P$_4$     | 5.21         | 1.58e13       | 70.4          | 231.4        | 10.72        | 2.5e13        | 63.6            | 155.5        |