In Pursuit of the Next Wonder 2-D Materials: An *ab initio* Study

M. Luisier[1], C. Klinkert[1], C. Stieger[1],
A. Szabo[1], Y. Lee[1], D. Campi[2], N. Marzari[2]

[1]*Integrated Systems Laboratory, ETH Zurich, 8092 Zurich, Switzerland*
[2]*Laboratory of Theory and Simulation of Materials, EPFL, 1015 Lausanne, Switzerland*
mluisier@iis.ee.ethz.ch

Daily progresses are made in the exfoliation and growth of high-quality two-dimensional (2-D) monolayers, in their reliable transfer onto different substrates, in the clean deposition of oxide dielectrics on top of them, in the incorporation of metallic contacts with low resistances, and in their chemical doping. A very appealing outlet of 2-D materials is the replacement of Si FinFETs, the currently manufactured transistor technology, at the end of Moore's scaling law. In effect, 2-D single-layer crystals benefit from their planar atomic structure that provides an excellent electrostatic control. This, in turn, allows to effectively turn off switches made out of them, even with gate lengths below 15 nm. Here, the most promising 2-D semiconductors as next-generation transistors beyond Si FinFETs will be identified via *ab initio* device simulations. A recently produced database containing more than 1,000 relatively easily exfoliable 2-D candidates [1] will be used as starting point. Not all materials are suitable for logic applications.

The transistor structure depicted in Fig. 1 has been chosen as benchmark to compare different 2-D channel materials. To model the "current vs. voltage" characteristics of the investigated components, an *ab initio* quantum transport approach has been developed. Its workflow is shown in Fig. 2. Starting from the atomic positions and lattice vectors found in the database of Ref. [1], the primitive unit cell of the considered 2-D material is constructed and its electronic structure calculated with a density functional theory (DFT) tool, e.g. VASP [2] or Quantum ESPRESSO [3]. By transforming the plane wave results into a set of maximally localized Wannier functions with the Wannier90 software [4], a Hamiltonian matrix in a localized orbital basis is obtained. It can be inserted into a quantum transport solver [5] to compute the figures of merit of transistors similar to the one in Fig. 1. Selected results are presented in Fig. 3. They demonstrate the existence of materials capable of producing high ON-currents for both n- and p-type device configurations. More than 100 2-D monolayers have so far been modeled.

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References: [1] N. Mounet et al., Nature Nano. **13**, 246 (2018). [2] G. Kresse et al., Phys. Rev. B **54**, 11169 (1996). [3] P. Giannozzi et al., J. Phys.: Condens. Matter **21**, 395502 (2009). [4] N. Marzari et al., Phys. Rev. B **56**, 12847, (1997). [5] M. Luisier et al., Phys. Rev. B **74**, 205323 (2006).

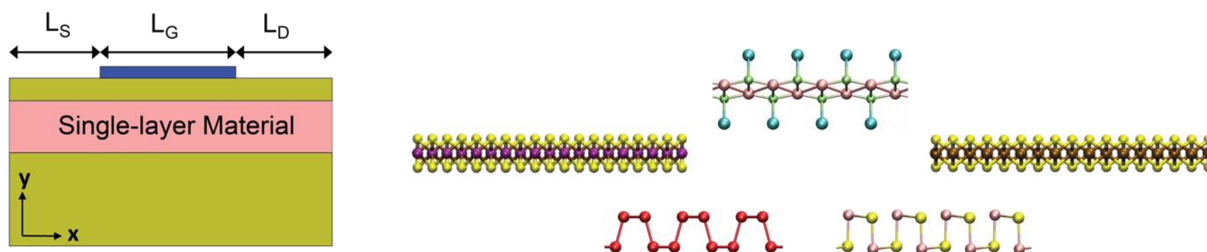

Figure 1: (left) Schematic view of a single-gate field-effect transistor with a 2-D monolayer as channel material. In this study, the gate length L_G ist set to 15 nm, the source and drain extensions measure L_S=L_D=12.5 nm each and are doped with a donor (N_D) or acceptor (N_A) concentration of 5e13 cm^{-2} for n- and p-type devices, respectively. The oxide separating the channel from the gate contact is assumed to be a 3nm thick HfO_2 layer with a relative dielectric constant ε_R=20. All simulations are performed at room temperature and include a phenomenological dissipative scattering mechanism to ensure convergence at high V_{GS} and to remove unphysical negative differential resistance behavior. (right) Example of 2-D monolayer crystals used in this work.

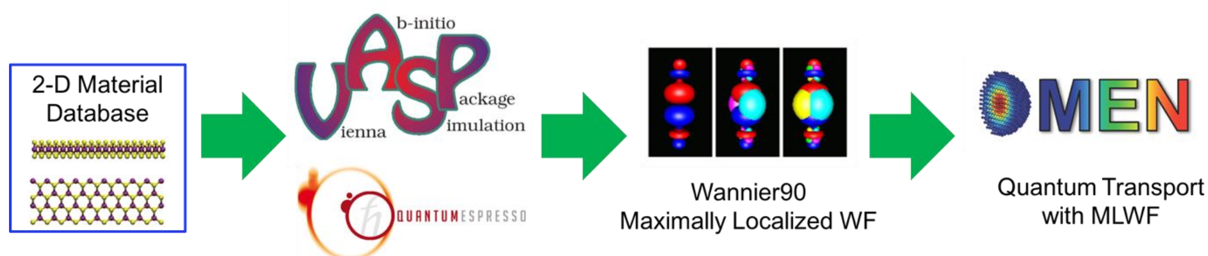

Figure 3: Illustration of the developed computational scheme to simulate the single-gate transistors from Fig. 1. Starting from a recently produced 2-D materials database that contains more than 1,800 monolayer candidates [1], the electronic structure of the selected crystal is calculated with density functional theory (DFT), e.g. with VASP [2] or Quantum ESPRESSO [3], for its primitive unit cell. The plane-wave results are converted into a set of maximally localized Wannier functions (MLWF), which gives rise to a Hamiltonian matrix with short range interactions. The latter is finally passed to a quantum transport solver called OMEN [5] to obtain the "current vs. voltage" characteristics of the considered transistor samples.

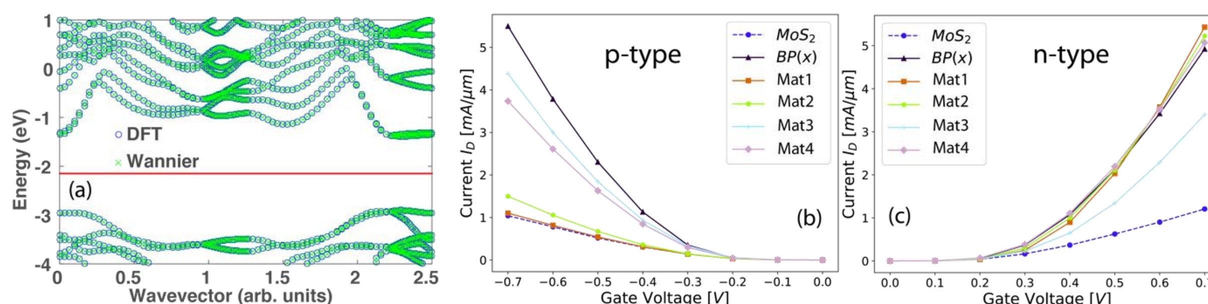

Figure 2: (a) Bandstructure of a single-layer 2-D material (P_8Si_4) as computed with density functional theory (blue circles) and after a transformation into MLWFs (green crosses). An excellent agreement between both methods is obtained. The red line in the middle of the band gap indicates the Fermi level. (b) I_D-V_{GS} transfer characteristics at V_{DS}=0.7 V of p-type single-gate 2-D transistors as in Fig. 1 with different 2-D monolayers as channel materials. The OFF-current of all devices is set to 0.1 μA/μm. The I-V characteristics of MoS_2 (dashed curve with circles) and black phosphorus (black curve with triangles) are given as references. They are compared to the those of transistors based on four other 2-D materials from the database of Ref. [1]. While none of them outperforms black phosphorus, at least two of them deliver promising ON-current values. (c) Same as (b), but for n-type transistors. All considered 2-D materials exhibit significantly higher ON-currents than MoS_2.