Insights on the physics and application of off-plane quantum transport through graphene and 2D materials

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Abstract— **Different proposals of graphene transistors based on off-plane (i.e., vertical) transport, have recently appeared in the literature, exhibiting experimental current modulation of a factor 10^4-10^5 at room temperature. These devices overcome the lack of bandgap that undermines the operation of graphene transistors, and positively exploit graphene's ultimate thinness, high conductivity, and low density of states. However, very little is known about vertical transport through graphene and two-dimensional materials, either in terms of experiments or theory.**

In this talk we will discuss the physics and the electronics of off-plane transport through hetero-structures of graphene and 2D materials. We investigate transport across vertical heterostructures of 2D materials with multi-scale simulations, including first-principle density functional theory and non-equilibrium Green's functions based on NanoTCAD ViDES. We show that unexpected behaviors emerge, which are not observed in the more

familiar semiconductor heterostructures based on III-V and II-VI materials systems, and that are not predicted by simplistic physical models. Such properties have a significant impact on the design and performance of transistors for digital or high frequency operations.

I. INTRODUCTION

Graphene and two-dimensional materials are the subject of interest by the electron device community. Graphene was isolated and characterised in 2004 [1], and can exhibit a very high mobility at room temperature (larger than 10^4 cm^2/Vs on a good substrate). This property, coupled to its single-atom thickness, make it very interesting for electron devices. However, graphene has no gap, and therefore FETs with a graphene channel cannot be switched off. One of the main objectives of research in graphene electronics is opening a gap in graphene, by geometrical or chemical modifications, without undermining its mobility.

In addition to graphene a whole new class of two-dimensional materials are under intense scrutiny for their applicability in electronics: they have a real semiconducting gap from few tenths of eV to few eV, but typically have lower mobility (Fig.1, left) [2]. More recently, the so-called "materials on demand paradigm" has been proposed [3], which is the possibility of obtaining a three dimensional material with tailored characteristics by combining layers of 2D materials (Fig. 1, left).

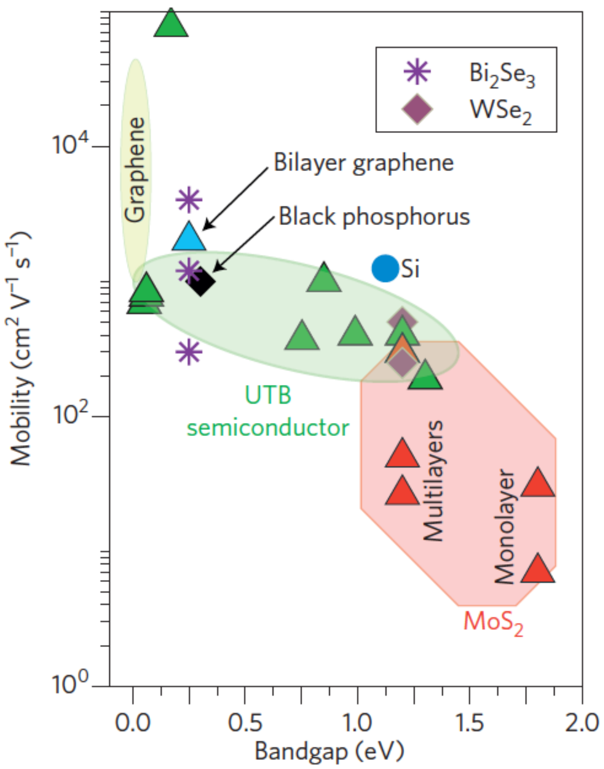

Figure 1: Left: mobility versus bandgap for several 2D materials. Figure from Ref. [2].

It is worth mentioning that the "materials on demand" paradigm is in many ways a modern version of the "bandgap engineering" technology that was proposed almost thirty years ago [4]. Fig. 2, left, shows a picture from a well known review on Science by Federico Capasso [4], then at Bell Labs. The word *paradigm* was not so in vogue at the time.

3D Materials naturally lead to vertical transport, because one wants to use the degree of freedom in device design offered by the third dimension. Of course, more knobs are always an opportunity, but one should ask why vertical transport can be of interest for applications, given that the rush to graphene-based electronics started precisely because graphene is the first truly two-dimensional material with exceptional in-plane mobility.

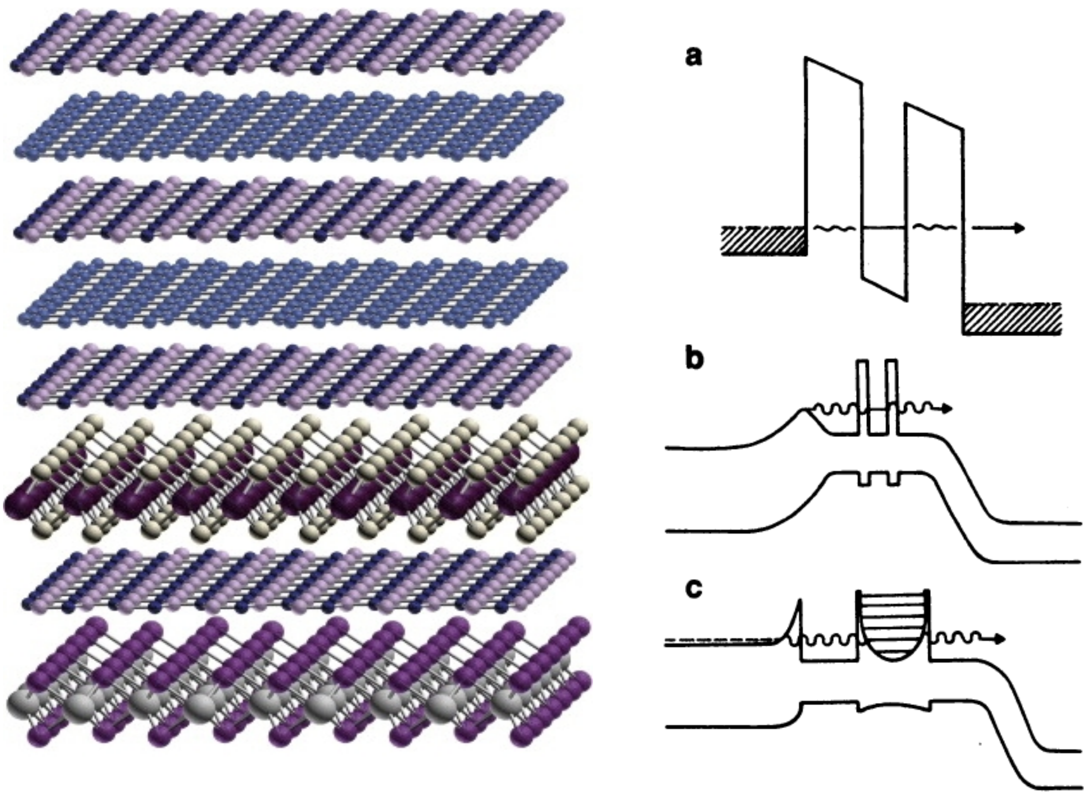

Figure 2: Left: Illustration of vertical heterostructrure of 2D materials (from Fig. 4 of Ref. [2]). Right: Examples of band-edge profiles of devices based on “bandgap engineering” (from Fig. 4 of Ref. [4]).

Actually, there are some good reasons to consider with interest vertical transport through a graphene layer: one the one hand, graphene is so thin that the transit time in the vertical direction can be very small; on the other hand, graphene can also have high mobility in the in-plane direction, and – if highly populated with carriers – also a low sheet resistivity.

Indeed, a few vertical devices have been proposed in the last few years. The so-called “barristor”, proposed in 2012 [5], is a controlled Schottky diode in which a top graphene layer is the emitter and a bottom silicon layer is the collector. An insulated gate on top of the whole structure modulates the Schottky barrier. The Vertical Heterostructure FET proposed by 2012 by Britnell et al. [6], is based on two graphene electrodes separated by a boron nitride layer. A gate on top of one of the graphene electrodes modulates the barrier, and therefore the current. Both types of devices exploit the fact that graphene is not an ideal metal, since it has a relatively small density of states, and cannot completely screen the electric field induced by the gate, which therefore can modulate the barrier and hence the current. However, there is still partial screening, which undermines the effectiveness of the electrostatic control mechanisms and suppresses device performance. This aspect is quantitatively addressed in Ref. [7], where some of us show that the lateral heterostructure FET [8]**Error! Reference source not found.**, which does not have such problem, can intrinsically outperform devices based on vertical heterostructures, and has the potential to meet requirements for CMOS in the sub-10nm technology nodes.

Another interesting vertical device is the graphene base transistor [9][10][11], in which a thin graphene layer acts as the controlling electrode and is sandwiched between insulating or semiconducting layers, connected with the emitter and collector electrode. As in the case of the hot electron transistor of the 80s [12], carrier injection is controlled by the base emitter voltage which modulates the barrier height. As mentioned above, this device exploits both the thinness and the high mobility of graphene in order to have a small transit time and a small base resistance.

After establishing the relevance of vertical transport, we now must clearly say that we have limited understanding of the mechanism: we have very few experimental data, and very few theoretical results. We can briefly summarize the main challenges to understanding vertical transport through two-dimensional materials:

- The Hamiltonian cannot be decoupled in a longitudinal and a transversal component, because the energy dispersion relations of adjacent layers can be very different. Also, Brillouin zones of adjacent layers are different and can be incommensurable. Transport must be computed for each injected wave vector in the 3D space. This is a significant difference with respect to the heterostructures of III-V or II-VI material systems, where adjacent layers had much more similar (though not equal) dispersion relations and Brillouin zones.

- Graphene is not transparent to charge carriers propagating normally to the layer: depending on the impinging wave vector it can offer a barrier of few eV. Basically, Bloch's theorem is not applicable: a graphene layer sandwiched between two semiconductor regions is a large scatterer.
- Alignment and coupling is important and very much dependent on the fabrication process. As of now, it is largely uncontrolled.

As we see, vertical transport involves complex issues for which we have very limited data points. Since we do not have a general approach to the problem, we can tackle it proceeding on a case-by-case basis, looking for cases within our reach. We can identify two possible approaches:

1. Focus on heterostructures for which lattice is quasi-matched, so that alignment between adjacent layers is in principle possible, and perform ab-initio calculations. The heterostructure hexagonal boron nitride (h-BN) – graphene is suitable to this case [13].
2. Use pseudoatomistic calculations, as an intermediate layer of abstraction between atomistic modeling and effective mass modeling, as some of us have proposed in Ref. [14].

In the following sections we consider three different cases based on these two approaches.

II. AB-INITIO CALCULATION OF TRANSPORT THROUGH VERTICAL HETEROSTRUCTURES OF 2D MATERIALS

We perform ab-initio calculations of the electronic properties using Quantum Espresso (density functional theory with local density approximation) [15], and then use the PWCOND module to project the Hamiltonian on a plane wave basis and therefore compute the transmission coefficients as a function of energy summing over all wave vectors in the Brillouin zone [16]. We consider the structures illustrated in Figure 3: Case 1 is a single barrier with a varying number of h-BN or h-BC_2N layers between graphite electrodes; case 2 is a double barrier of h-BN layers separated by one or more graphene layers.

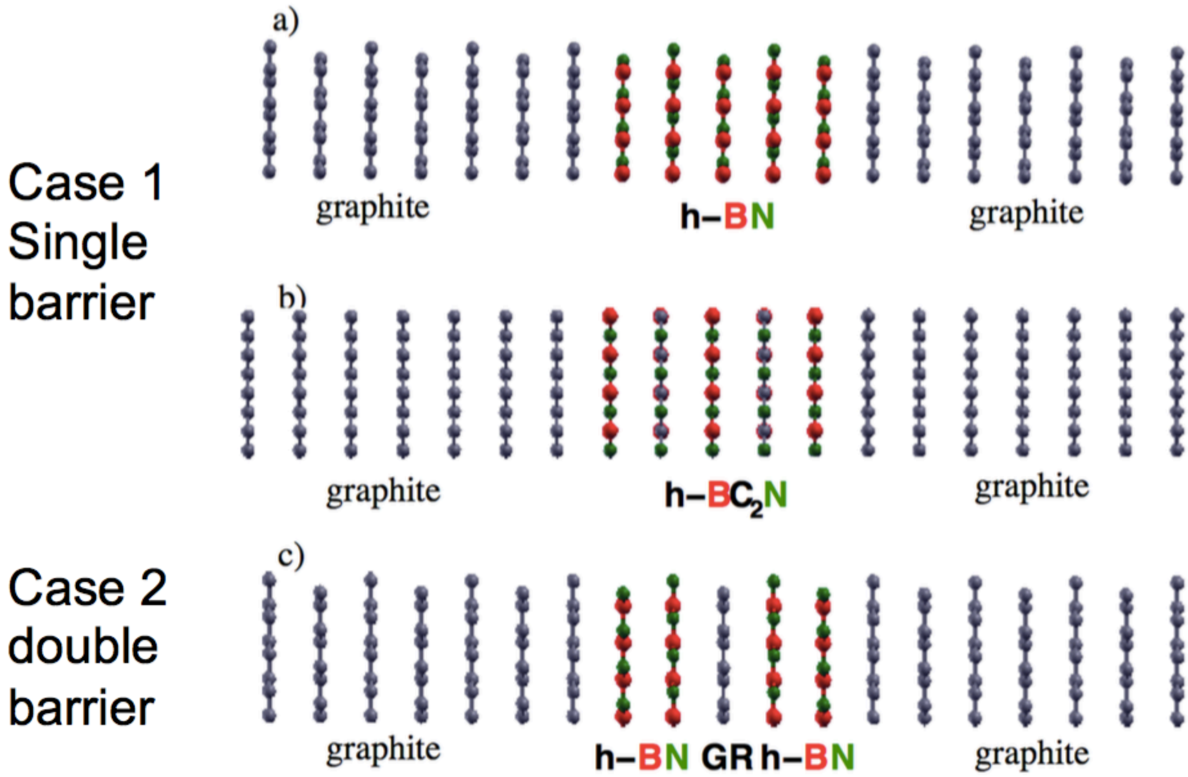

Figure 3. First two cases considered: a) and b) represent a few-layer h-BN or h-BC_2N barrier (case 1); c) represents a double barrier of h-BN layers separated by one graphene monolayer (or more). Figure adapted from Ref. [13]

Let us first consider the single barrier. In Figure 4, one can see the tunnelling probability as a function of energy for a different number of atomic layers. First, one should notice that the average tunnelling coefficient for energy in the bandgap depends exponentially on the number of layers, as we intuitively expect, but does not depend on energy, which - on the contrary - one would not expect. The reason can be easily understood if we look at the energy dispersion relation for imaginary wave vector: indeed, the wave vector is almost independent of energy in the gap, therefore also the tunnelling coefficient is independent on energy.

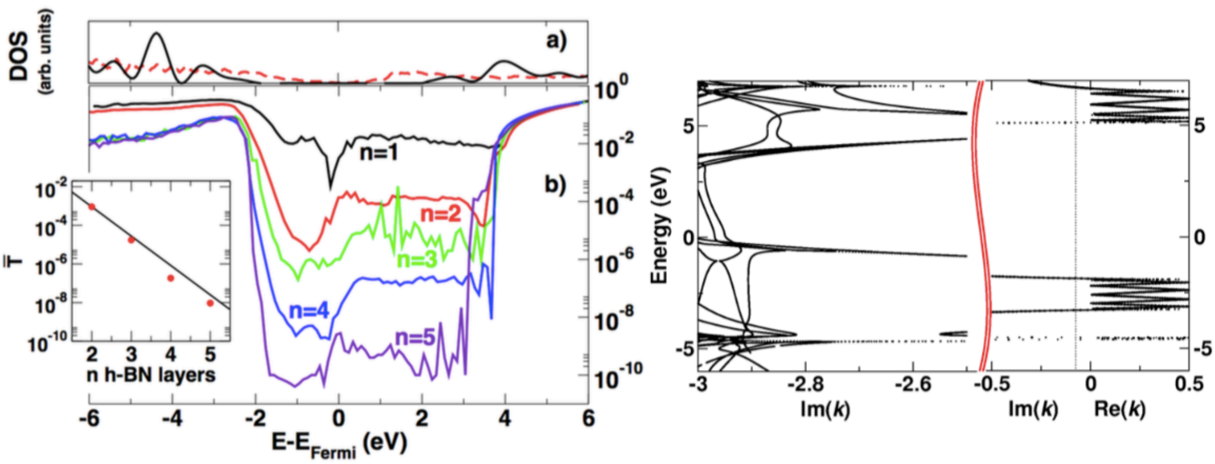

Figure 4: Left: tunneling probability as a function of energy for different number of h-BN layers; inset: average tunneling probability in the h-BN energy gap as a function of the number of layers; right: Energy dispersion relation of real and imaginary wave vectors: as can be seen, in the energy gap of h-BN the dispersion relations are almost vertical lines, which implies that the imaginary wave vector does not depend on energy. Both figures are extracted from Ref. [13]

Let us now consider the second case of a double barrier. We first discuss the plot of the transmission coefficient as a function of energy in the left of Figure 5. Three different types of barriers are considered: SB1 is a single barrier with one atomic layer of h-BN. If we add a second h-BN monolayer to the barrier, we obtain the plot indicated as SB2. In the flat region, corresponding to the energy gap of h-BN, the transmission coefficient is of order 10^{-2} for SB1, and 10^{-4} for SB2, in agreement with the fact that the transmission coefficient is exponentially dependent on thickness. However, if we put a graphene monolayer between the two h-BN monolayers, we see that the transmission coefficient actually increases significantly with respect to the SB2 case. The reason is that graphene has the effect of randomising the phase, so that a double barrier behaves almost as two barriers in series, and not as a barrier of double thickness. The effective phase randomization occurs because of a significant mismatch between the energy dispersion relations of graphene and boron nitride. The mismatch adds “quasi” random phase contribution to the electron wave.

In addition, one can also notice that there is no resonance in the current, as one would naively expect in the case of a double barrier. Again, the mismatch between energy dispersion relations does not allow to decompose the Hamiltonian in a longitudinal and a transversal components. Indeed, if we consider one specific transversal $\mathbf{k}_{\parallel}$ we see very nice resonance peaks, with maximum transmission coefficient of 1, as expected for symmetric double barriers (Figure 6). However, the energy of each peak changes when we change the transversal k, so when we integrate on all $\mathbf{k}_{\parallel}$, resonances get washed out.

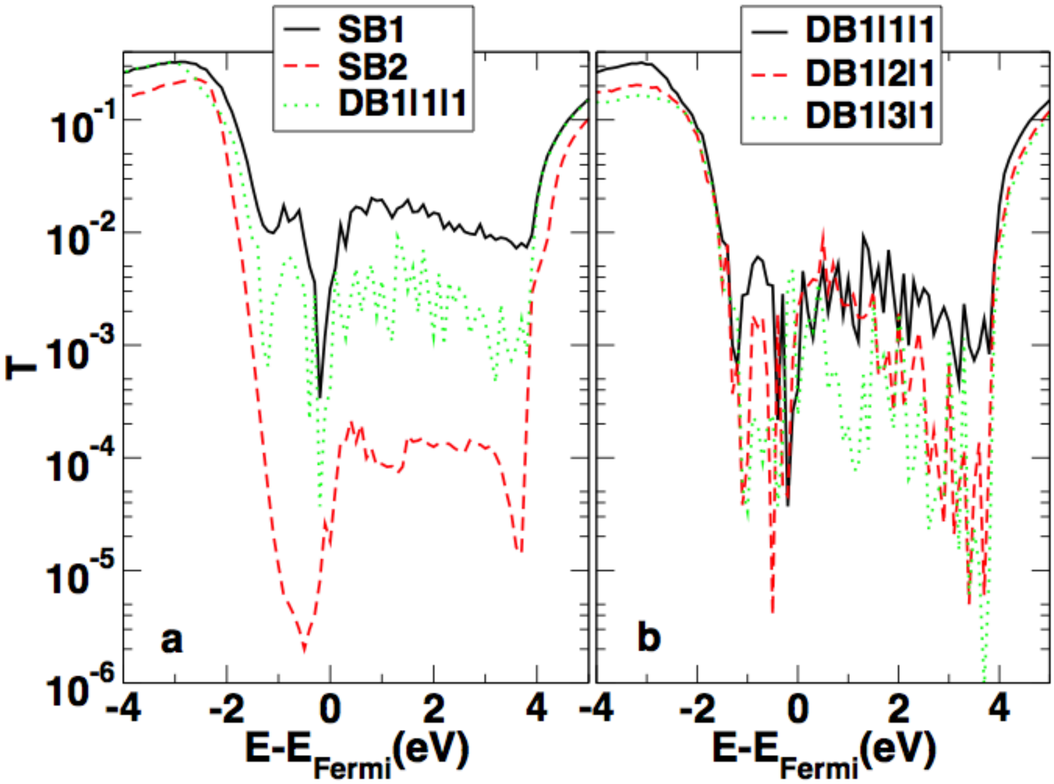

Figure 5. Left: transmission probability as a function of energy for a single barrier of one atomic layer of h-BN (SB1), a single barrier of two atomic layers of h-BN (SB2), a double barrier where monoatomic layers h-BN are separated by monolayer graphene. Right: transmission coefficient for double barriers consisting of monatomic layers of h-BN separated by one, two, or three atomic layers of graphene. Figure taken from Ref. [13]

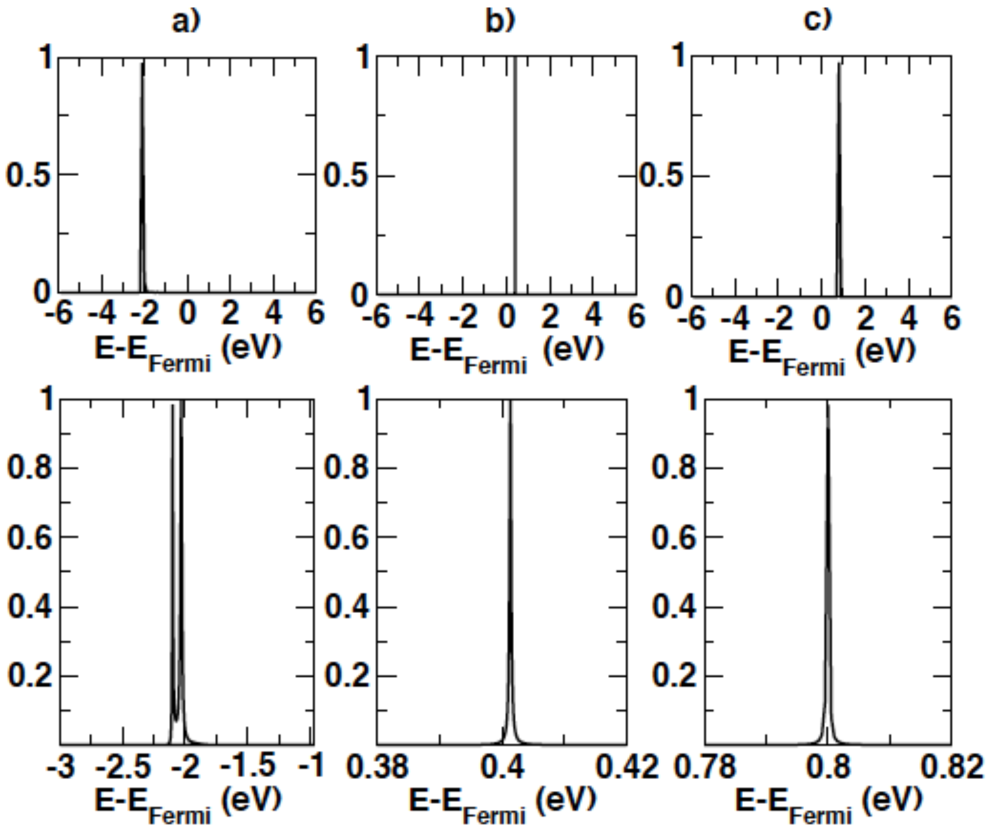

Figure 6. Transmission probability of the double barrier system as a function of energy for selected $\mathbf{k}_{\parallel}$: a) (0.28000;0.28867); b) (0.31000;0.32909); c) (0.28000;0.33486); in unit $2\pi/a$ with $a = 2.503$ Å.

III. PSEUDOATOMISTIC SIMULATION OF TRANSPORT THROUGH A GRAPHENE LAYER

The third case we consider is transport through a structure consisting of a graphene monolayer between two semiconducting regions. Here we use a pseudoatomistic Hamiltonian. Indeed, graphene and semiconductor lattices do not match, alignment cannot be obtained, coupling is unknown. Since the structure is largely unknown we prefer to use a model at a higher level of abstraction: for graphene we consider the actual lattice; for the semiconductor we consider a pseudo lattice, i.e. a lattice commensurable with graphene, but that provides the same energy gap and main band minima and maxima of the original semiconductor. In the case we consider (illustrated in Fig. 7), we only need three parameters to define the pseudo Hamiltonian of the semiconductor and two parameters to define coupling with graphene, which is unknown. It is an incomplete model, but at least we know it is incomplete, so we can still obtain useful information and evaluate sensitivity of transport properties to parameters. Unphysical conclusions are drawn if one uses an inadequate model without consideration. Since we are well aware of that, we can still obtain useful information.

Transport is then computed using the Non-equilibrium Green's Functions approach with the open-source atomistic device simulator NanoTCAD Vides [17][18]**Error! Reference source not found.**.

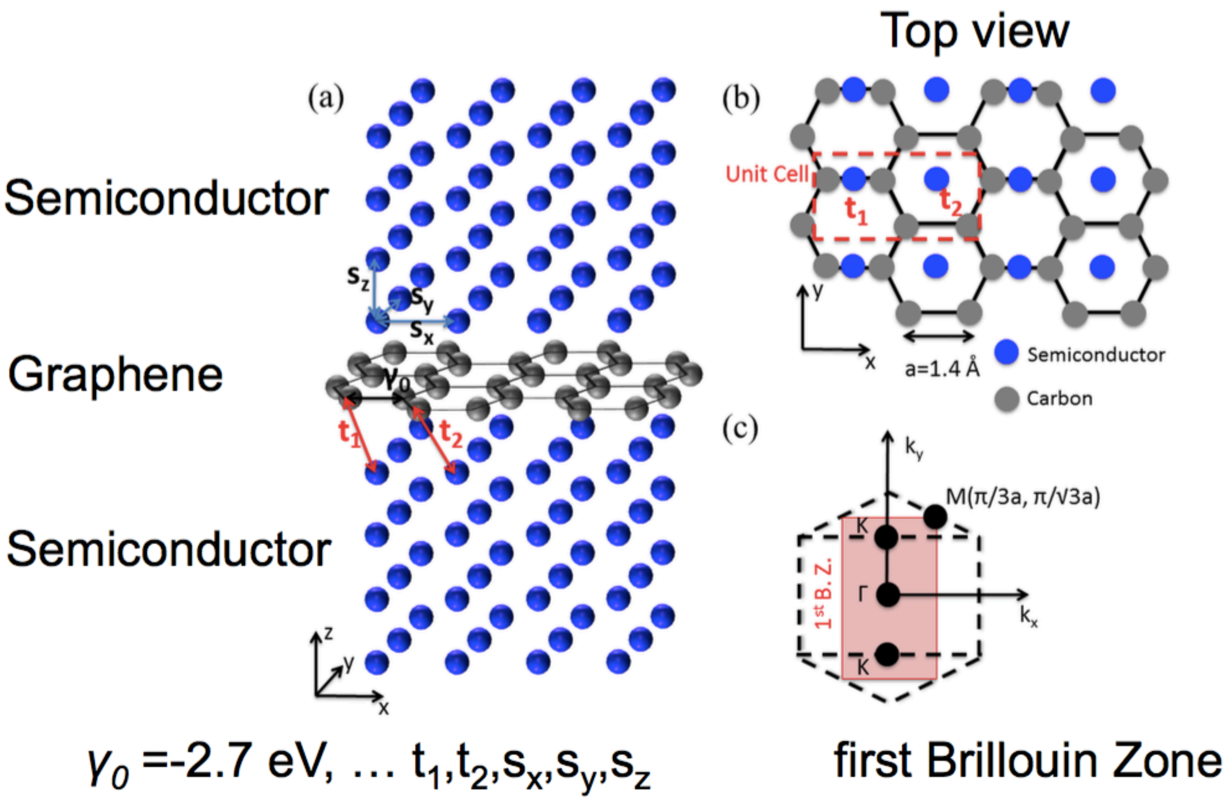

Figure 7. a) Illustration of the Pseudo-atomistic Hamiltonian considered for the semiconductor-

graphene-semiconductor structure, with indication of the main hopping parameters b) unit cell in the real space c) Brillouin zone. Figure adapted from Ref. [14].

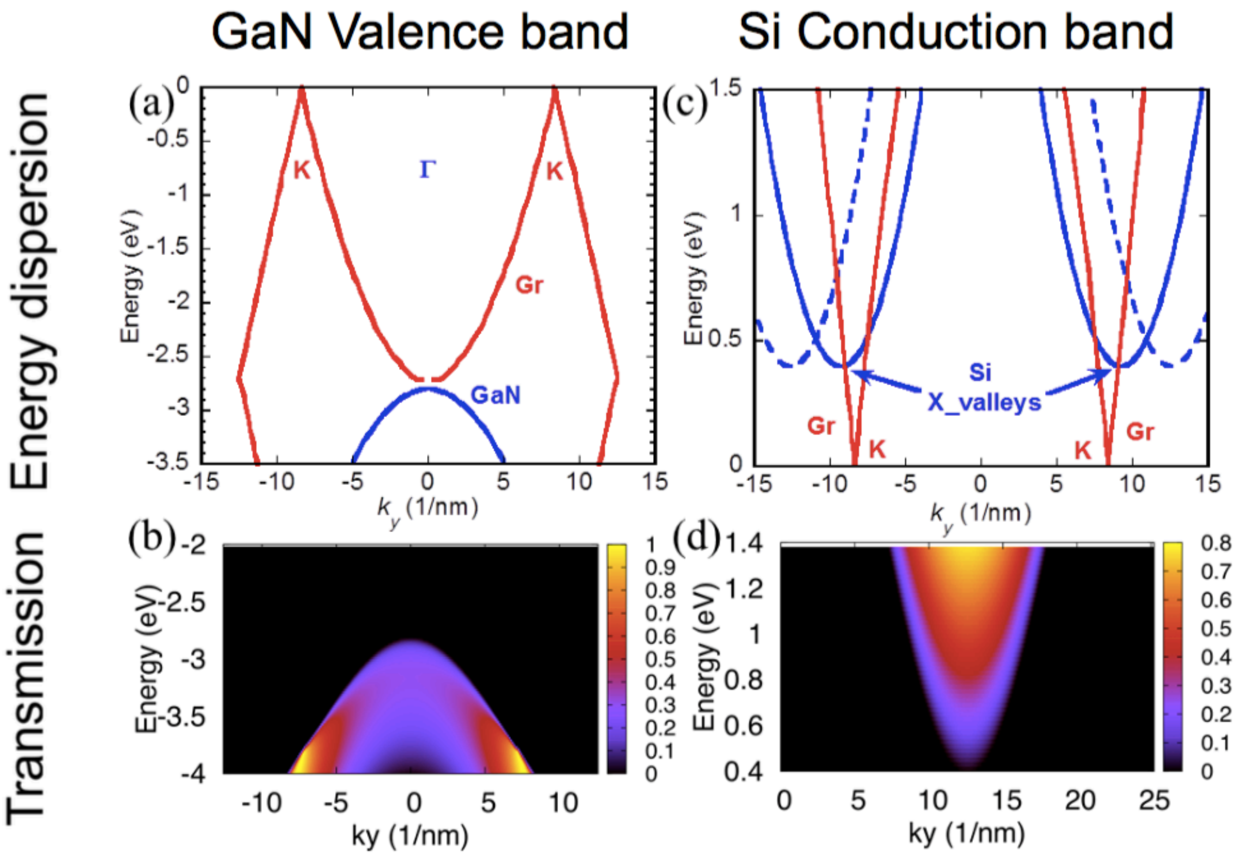

Figure 8. Energy dispersion and transmission through the structure in Fig. 7 as a function of k_y (one coordinate of the transversal $\mathbf{k}_{\parallel}$). Transport from and to GaN valence band is shown on the left, whereas transport from and to silicon conduction band is shown on the right. Figure adapted from Ref. [14].

The first thing we notice is that some materials are preferable to others for injecting carriers in graphene. This can be seen clearly in Fig. 8. For example from GaN we can easily inject holes in the graphene valence band, because the valence band of GaN lies below graphene conduction band. We can then expect higher tunneling coefficient. From two of the six minima in the conduction band of silicon we can inject electrons directly in the graphene conduction band. In both cases the tunnelling coefficient is larger than in the cases where such matching is not present.

We also understand that transmission strongly depends on the coupling between layers. In Fig. 9, for example we show the colour plots of the tunnelling probability as a function of the two coupling parameters between layers t_1 and t_2 indicated in Fig. 7. By changing such parameters in a reasonable range we can modulate the transmission probability by two orders of magnitude. Therefore coupling is extremely important, and as of now largely depends on the fabrication process and is extremely poorly controlled and understood. This is particularly critical for device operation: for example, in the case of the graphene base transistor, both the cutoff frequency and the maximum power gain frequency are proportional to the transmission probability through the graphene layers.

IV. CONCLUSION

We have highlighted the importance of understanding vertical transport through two-dimensional heterostructures and the associated challenges. Understanding vertical transport through graphene and 2D materials requires an atomistic approach (three dimensional in the wave vector space), since interfaces between layers and matching of energy dispersion relations have a strong effect on transport.

We need also new models that at the same time are simpler than a 3D atomistic description, and more physically correct than the classically used one-dimensional band profiles. Indeed, we need to consider that if we use approaches that are too simplistic we can draw unphysical conclusions (e.g. predicting resonant tunneling where it is not possible). Our pseudoatomistic simulation is a first step in that direction.

V. Acknowledgment

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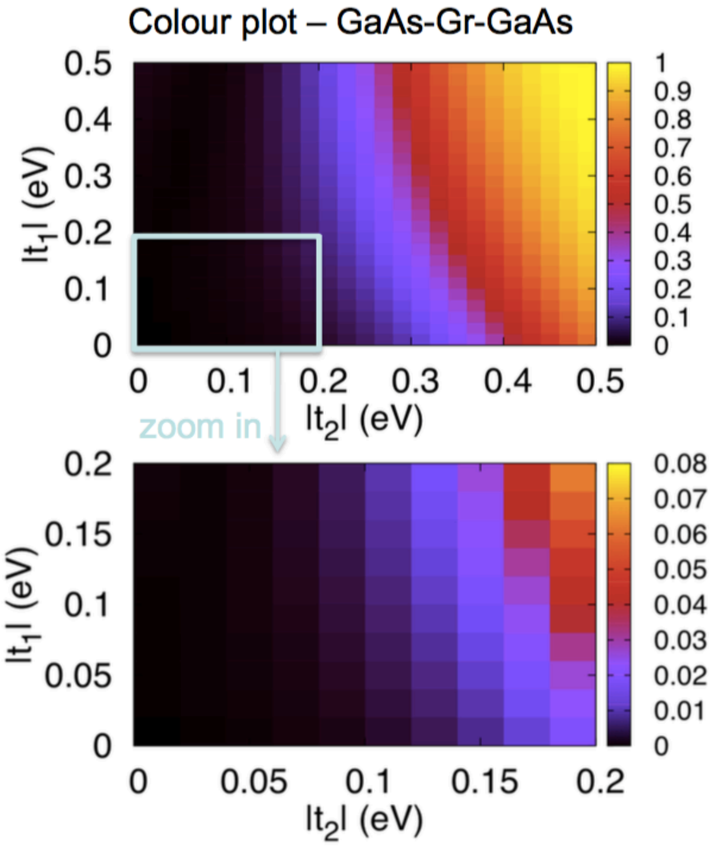

Figure 9. Colour plot of the transmission probability as a function of the coupling parameter t_1 and t_2 for a injected electron with wave vector close to the Gamma point of GaAs Brillouin zone. Figure adapted from Ref. [14].

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