



International Workshop on Computational Nanotechnology

Session: 2D Semiconductors

(Invited) Transistors based on heterostructures of 2D materials

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Native graphene has a zero energy gap and it is therefore not suitable as a transistor channel material for digital electronics. However, recent advances based on materials engineering have demonstrated “*materials on demand*”, with tailored properties. *Vertical heterostructures* of graphene and 2D materials have been proven to be suitable for FETs and hot-electron transistors exhibiting large current modulation.

Inspired by recent progress in the growth of seamless *lateral 2D heterostructures*, lateral heterostructure (LH)-FETs have been proposed, exhibiting extremely promising switching behavior in terms of leakage current, propagation delay, and power-delay product.

We investigate the performance and the scaling perspectives of transistors based on heterostructures of two-dimensional materials against the requirements set by Semiconductor Industry Roadmaps for CMOS (first ITRS and then IRDS). We show that LH-FETs are very promising for high performance logic, down to the 3-5 nm gate length, depending on the types of materials. On the other hand, vertical heterostructure FETs exhibit intrinsic delay times higher by four orders of magnitude, due to large capacitance and poor electrostatics.

We also address some critical aspects related to the modeling of off-plane and in-plane transport in heterostructures of 2D materials.

Monte Carlo study of high field transport in some transition metal di-chalcogenides

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In recent years, there has been a push to find new materials which may have application in the electronics industry. The monolayer compounds came to the forefront when single layers of graphene were isolated [1]. The success of graphene for some applications has led to the investigation of the monolayer transition-metal di-chalcogenides (TMDCs) [2,3,4]. Indeed, field-effect transistors have been created in some of these TMDCs [5]. Of interest in these materials for device applications are specifically the saturated value of the velocity at high electric fields and the possibility of impact ionization within the channel of the device [5,6]. Recently, we have reported the theoretical study of transport in MoS₂ at moderate to high electric fields [7]. Here, we report the studies of transport at higher electric fields in both MoS₂ and WS₂ with the use of the ensemble Monte Carlo technique. These materials are monolayers in which each layer is composed of Mo or W atoms at the center of the layer and S atoms displaced above and below this center. In bulk form, they have an indirect band gap, which becomes direct only in the monolayer limit. The band extrema are located at the K and K' points of the Brillouin zone, so that there are two minima for the conduction band. Subsidiary valleys of the conduction arise from the residual valleys of what was the indirect gap. These valleys, referred to as the T valleys [8], lie midway between Γ and K on the connecting line between these two points. The conduction band mass is approximately 0.45(0.32) m_0 in the K valleys and 0.57(0.52) m_0 in the subsidiary valley for MoS₂(WS₂). These satellite valleys lie some 200(50) meV above the K valleys. These bands are non-parabolic, and this has to be taken into account for high field transport. We consider impact ionization initiated in both sets of conduction band valleys with a two-dimensional model based upon our