Atomistic Quantum Transport using Empirical Pseudopotentials

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We have recently developed a technique to calculate ballistic electron transport through atomic structures using empirical pseudopotentials that is numerically tractable for devices containing more than a thousand atoms. [1] Our technique offers a competitive alternative to the commonly used tight-binding approximation.

To attain this efficiency, we exploit the Bloch waves of the underlying material. To do so, we consider atomic structures consisting of a repeated supercell, as shown in Fig. 1. Without external potentials, the solutions are Bloch waves that are calculated using a standard plane-wave empirical pseudopotential solver [2]. To account for the potential variations seen in devices, we employ the partition-of-unity method [3], where the wavefunctions are expanded using finite-elements shape-functions enhanced with the Bloch waves. The finite-element mesh, defined by nodes between each supercell (shown in Fig. 1), captures the device scale. The combination of Bloch waves captures the atomic scale within a supercell. Specifically, we use a limited set of Bloch-waves at high symmetry points. Use of the Galerkin method transforms the Schrödinger equation into a sparse generalized eigenvalue problem in the expansion coefficients. Thanks to the shape functions, the Hamiltonian contains only nearest neighbors coupling between adjacent nodes, resulting in a high computational efficiency and scalability.

The quantum transmitting boundary method (QTBM) is used to describe the open system in the presence of contacts and the travelling wavefunctions are calculated self-consistently with the Poisson equation. We have used our method to simulate various field-effect transistors (FETs) based on graphene nanoribbons (GNRs) and silicon nanowires (Si-NWs). We show, in Fig. 2, the structure and transfer characteristics of a GNR FET containing 960 atoms. For this device, we include the Bloch waves at the center and edge of the first Brillouin zone of 42 valence and 20 conduction bands. In Fig. 3, we demonstrate the accuracy of our method by reconstructing the complete band structure. Note that, unlike for methods based on envelope-functions [4], there are no spurious solutions in the energy range covered by the basis. A single self-consistent solution for the GNR FET in the off state (as shown in Fig. 4) is obtained in 20 minutes on a single CPU core, which is two orders of magnitude faster than a previous plane-wave approach [4]. In Fig. 5, we also show the transfer characteristics of an extremely scaled Si-NW FET with 2048 atoms, to demonstrate the generality of our method.

[1] M.L. Van de Put *et al.,* IEEE SISPAD 2018, 71-74 (2018)
[2] M.L. Van de Put *et al.*, J. Appl. Phys. **119**, 214306 (2016)
[3] I. Babuska and J.M. Melenk, Int. J. Numer. Meth. Eng. **40**, 727–758 (1998)
[4] J. Fang *et al.*, J. Appl. Phys. **119**, 035701 (2016)

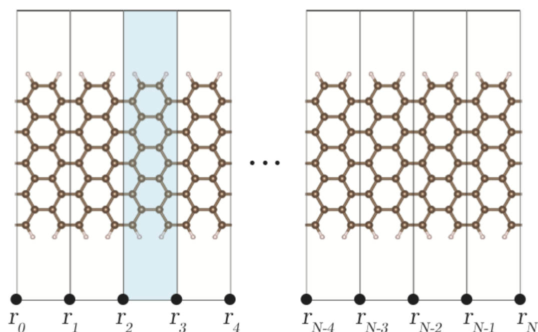

Fig. 1: The atomic structure of a graphene nanoribbon, where the supercells and nodes (r_i) are indicated. The Bloch waves are calculated assuming supercell periodicity, while the nodes are used to form a finite element basis describing the large-scale behavior of the system.

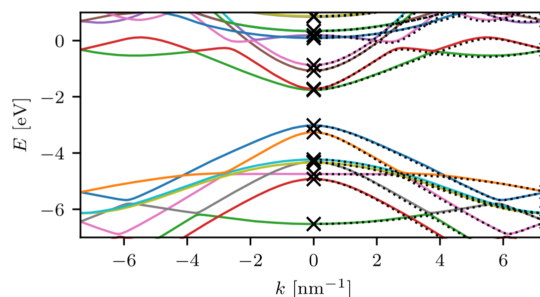

Fig. 3: The electronic band structure of the GNR ribbon shown in Fig. 2. The figure shows a comparison of the full empirical pseudopotential calculation (dashed black lines) to our method (colored lines) which uses only the Bloch waves at the indicated points (x).

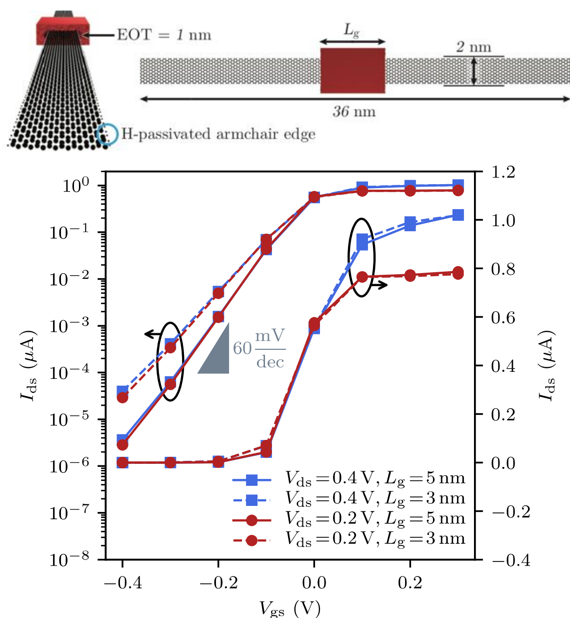

Fig. 2: *Top:* A three-dimensional depiction of the gate-all-around graphene nanoribbon field-effect transistor (GNR FET). Spheres indicate the position of carbon (black) and hydrogen (blue) atoms. *Bottom:* The transfer characteristics (I_{ds}– V_{gs}) of the GNR FET, shown above, at different drain-source bias (V_{ds}) and gate-lengths (L_g).

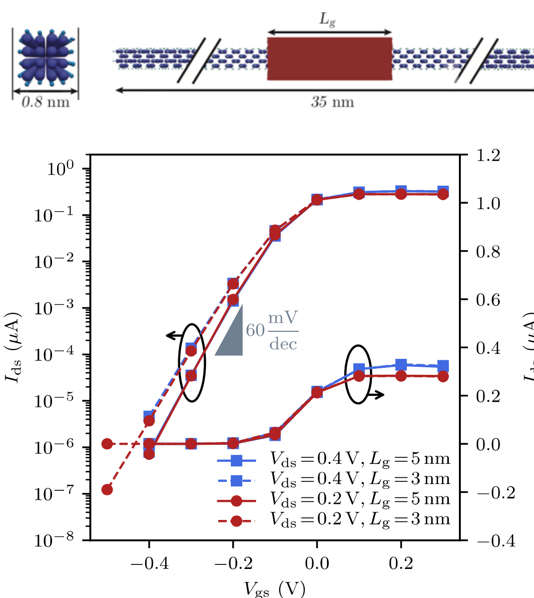

Fig. 5: *Top:* A three-dimensional depiction of the gate-all-around silicon nanowire field-effect transistor (Si-NW FET). Spheres indicate the position of silicon (dark blue) and hydrogen (light blue) atoms. *Bottom:* The transfer characteristics (I_{ds}– V_{gs}) of the Si-NW FET, shown above, at different drain-source bias (V_{ds}) and gate-lengths (L_g

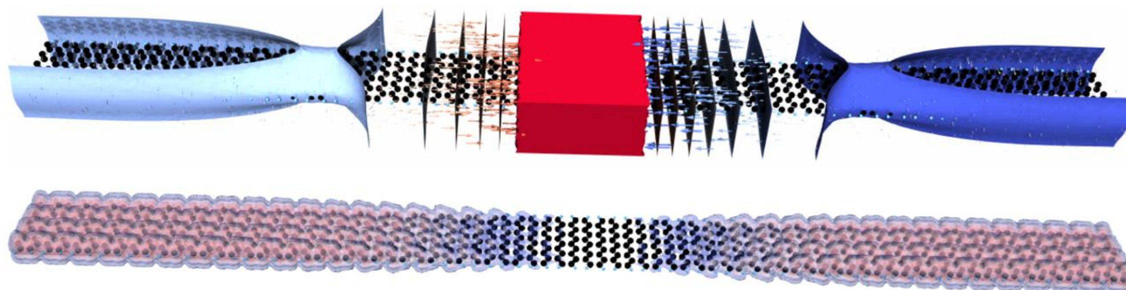

Fig.4: For the GNR FET of Fig. 2 in the off-state. *Top:* Shows the self-consistent potential and electric field, with the gate indicated in red. *Bottom:* Shows the free electron density, displaying spatial resolution well below the atomic scale. Spheres indicate the positions of the carbon (black) and hydrogen (blue) atoms.