Towards a multiscale modeling framework for metal-CNT interfaces

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INTRODUCTION

Very recently, astonishing experimental results for ultra-short Carbon nanotube transistors (CNTFETs) with channel lengths below 10 nm were published in [1] disproving some theoretical claims made before regarding the scalability of CNTFETs (see [2] for a related discussion). It turned out and it has already been pointed out in e. g. [3] that the contacts need to be carefully described in order to predict the transistor characteristics correctly. Several attempts have been made to model the contact regions and to explain the experimental results in [1] (see [2] for a list of references). Here, we adopt a multi-scale simulation strategy to understand and to model the contact regions at different levels of complexity ranging from (*i*) a sophisticated atomistic simulation approach based on density functional theory (DFT) as implemented in CP2K [4], (*ii*) a tight-binding (TB) model as described in [5] to (*iii*) an effective-mass (EFM) Schrödinger-Poisson solver as used in [2].

While in DFT simulations the metal atoms of the contacts are included in the simulation of a transistor explicitly, they are considered in the TB approach only by a well-defined self-energy and properly chosen coupling parameters. In the EFM approach the extended metal coated tube region is reduced to a single point and included in the EFM simulations by means of boundary conditions comprising an effective dispersion relation and an effective injection gap (see [2] for more details). With the latter approach, the simulation of the transistor is thus reduced to the simulation of the channel region (excluding the extended contact regions) and properly defined boundary conditions.

RESULTS

From the experimental device structure described in [1], three similar structures compatible with the different simulation methods are derived.

Fig. 1 and Fig. 2 show the local zero-bias DOS for the DFT and the EFM solver, respectively. In the EFM calculations, the mean local DFT-DOS in the contact region (see Fig. 3(a)) is used to describe the EFM boundary conditions. Additionally, effective bands are shown marking the region with a negligible DOS. Both calculations are in good agreement and both predict the injection gap as well as the available states nearby the contact regions in the channel correctly.

Fig. 3(a) shows a comparison between the mean local DOS of the DFT and the TB model in the metal coated tube portion. For the relevant energies around the Fermi level a good agreement between the DFT and the TB results is reached for a medium coupling strength which justifies the TB model. The local DOS in the contact region significantly depends on the interaction strength between the metal and the C atoms. In the TB model, the interaction between them is empirically modeled with a coupling parameter. Fig. 3(b) shows the related TB results for different coupling strengths. It is obvious that the effective injection gap depends on the coupling strength. The stronger the interaction, the smaller is the injection gap.

From the DFT and the TB simulation results, effective dispersion relations are derived for the EFM approach allowing the calculation of the current voltage characteristics for different coupling strengths by means of

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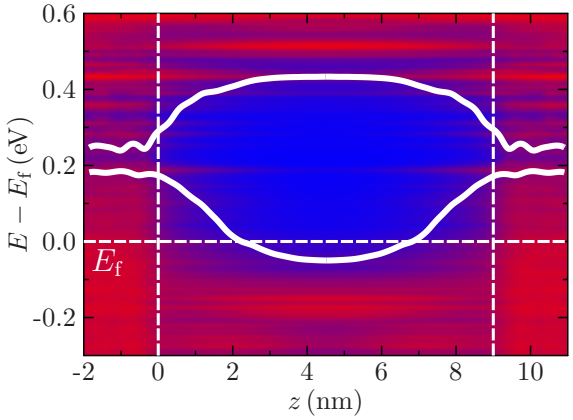

Fig. 1: DFT calculated local DOS (logarithmic scale) along the transistor (including the contact region) projected to the C atoms.

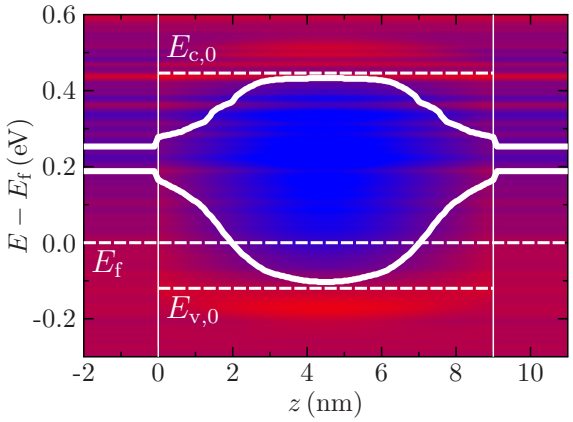

Fig. 2: EFM calculated local DOS (same logarithmic scale as in Fig. 1) along the transistor (including the contact region).

the EFM approach. The simulation results of the TB and the EFM approach are in good agreement (not shown here). A comparison of the EFM results with the experimental results published in [1] is shown in Fig. 4 for different coupling strengths. Obviously, the optimal coupling strength for a good fit should be neither very strong nor too weak.

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REFERENCES

[1] A. D. Franklin, M. Luisier, S.-J. Han, G. Tulevski, C. M. Breslin, L. Gignac, M. S. Lundstrom, and W. Haensch, "Sub-10 nm carbon nanotube transistor," *Nano Letters*, vol. 12, no. 2, pp. 758–762, 2012.

[2] M. Claus, S. Blawid, and M. Schröter, "Impact of near-contact barriers on the subthreshold slope of short-channel cntfets," in *International Conference on Simulation of Semiconductor Devices and Processes (SISPAD)*, 2013, pp. 159 – 162.

[3] J. Svensson and E. E. B. Campbell, "Schottky barriers in carbon nanotube-metal contacts," *Journal of Applied Physics*, vol. 110, no. 11, p. 111101, 2011.

[4] J. VandeVondele, M. Krack, F. Mohamed, M. Parrinello, T. Chassaing, and J. Hutter, "Quickstep: Fast and accurate density functional calculations using a mixed gaussian and plane waves approach," *Computer Physics Communications*, vol. 167, no. 2, pp. 103 – 128, 2005.

[5] J. Knoch and J. Appenzeller, "Tunneling phenomena in carbon nanotube field-effect transistors," *physica status solidi (a)*, vol. 205, no. 4, pp. 679–694, 2008.

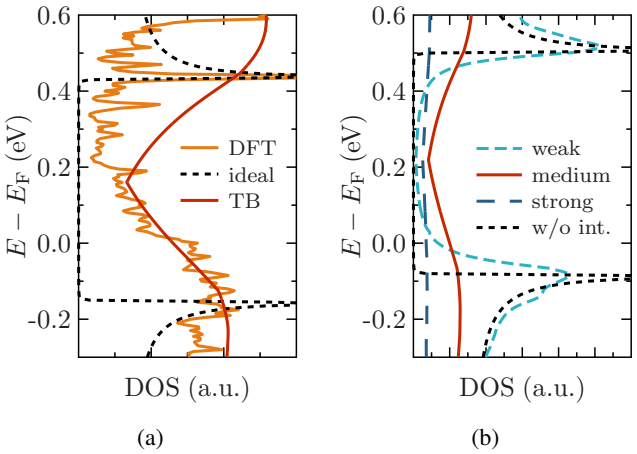

Fig. 3: (**a**) Mean values for the DOS in the contact region from the DFT and the TB approach. (**b**) TB calculated DOS in the contact region for different coupling strengths. Note that the DOS plots are partially scaled.

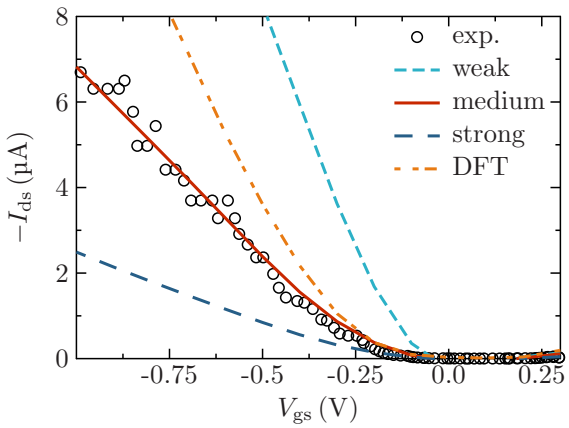

Fig. 4: Comparison between experimental [1] and EFM results for different coupling strengths ($V_{ds} = -0.4\,\text{eV}$).