Electrical properties of extended contacts using CP2K (DFT+NEGF) / Artem Fediai, TU Dresden

Fig. 1. Example of a local contact: side CNT/metal contact of a CNT field effect transistor (cross- and longitudinal section)

Fig. 2. Local density of states and band edges for Ni- and Pd- contacted CNTFETs

Fig. 3. CNTFET contact resistance $R_c$ as a function of the contact length $L_c$ for different contact metals

Highlights:

- Access to the electronic properties of extra-long side-contacts ($L_c > 2$ nm), which are prohibitively expensive for a standard DFT+NEGF combination. Alternative method has been developed: [Phys. Rev. B 91, 165404];

- Explanation of a contact length scaling in CNTFETs and GFETs from the first principles: [Towards optimal contact metal for CNTFETs, submitted]