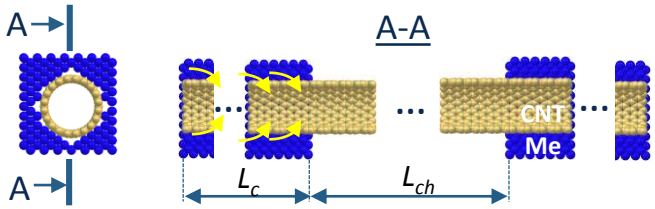
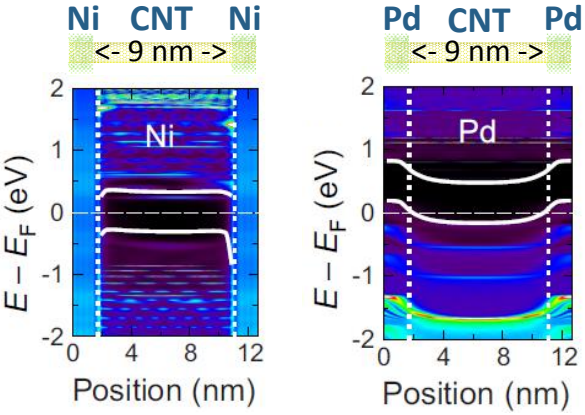
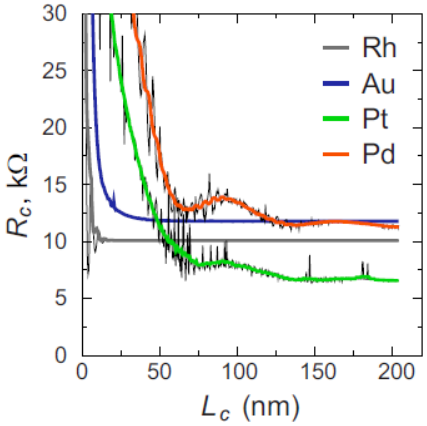
Electrical properties of extended contacts using CP2K (DFT+NEGF) / Artem Fediai, TU Dresden



↗ **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]