Electronic transport properties of nanostructured materials

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This talk will highlight some of the unique features of Atomistix ToolKit and Virtual NanoLab [1] software relevant for simulation of nanostructured materials in general, and for nano-carbon composite materials in particular. Non-equilibrium Green's function formalism is used to describe the electronic transport properties of such structures. This methods includes all the relevant ingredients required to model realistic metal-semiconductor interfaces and allows for a direct comparison between theory and experiments via I–V bias curve simulations [2], for exmaple.
Finally, the new one-probe configuration for reliable simulations of surfaces is also introduced. The central difference to traditional slab calculations is that the surface electronic structure is coupled to the bulk electronic structure through the non-equilibrium Green's function (NEGF) method with physically correct boundary conditions.

References

[1] Atomistix ToolKit version 2016.0, QuantumWise A/S (www.quantumwise.com).
[2] Stradi D., Martinez U., Blom A., Brandbyge M., and Stokbro K. Phys. Rev. B 93, 155302 (2016)