Multiscale modelling of nanoscale materials and electronic transport

Ivan Kondov[(1)] & Wolfgang Wenzel[(2)]

Karlsruhe Institute of Technology,
(1) Steinbuch Center for Computing and (2) Institute of Nanotechnology,
PO Box 3640, D-76021 Karlsruhe, Germany

To support accelerating materials development cycles we have developed simulation approaches for de-novo characterization and optimization of materials and device properties with nanoscale constituents. A unified multi-disciplinary approach that integrates materials science simulation and high performance computing is required to transform isolated solutions for specific problems into comprehensive, industry-ready platforms, which are capable of predicting the properties of complex materials on the basis of their constitutive elements.

In recent years we have therefore developed simulation methods that describe the conformation and electronic properties of materials built on the basis of well-defined nanoscale constituents. Here we discuss results on single-molecule electronics[1, 2] with application to molecular wires (metallic and organic), on the development of the atomic transistor[3, 4] and organic light emitting diodes[5].

We also discuss the integration of these methods, in close collaboration with colleagues at the CEA into a European framework for multiscale materials modelling in the EU project MMM@HPC.

1. Heurich, J., et al., *Electrical transport through single-molecule junctions: From molecular orbitals to conduction channels.* Physical Review Letters, 2002. **88**(25): p. 256803.
2. Maul, R. and W. Wenzel, *Influence of structural disorder and large-scale geometric fluctuations on the coherent transport of metallic junctions and molecular wires.* Physical Review B, 2009. **80**(4): p. 045424
3. Xie, F.Q., et al., *Independently Switchable Atomic Quantum Transistors by Reversible Contact Reconstruction.* Nano Letters, 2008. **8**(12): p. 4493-4497.
4. Xie, F., et al., *Multilevel Atomic-Scale Transistors Based on Metallic Quantum Point Contacts.* Advanced Materials, 2010. **22**(18): p. 2033-2036.
5. Kwiatkowski, J.J., et al., *Simulating charge transport in tris(8-hydroxyquinoline) aluminium (Alq3).* Physical Chemistry Chemical Physics, 2008. **10**(14): p. 1852-1858.