Heat Dissipation in Molecular Junctions: linking Molecules to Macroscopic Contacts

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Multiscale and hierarchical methods are becoming a paradigm for the understanding of complex physical phenomena. I will present the development of a new tool for simulations of transport in nano-systems that can cope with atomistic and finite-elements descriptions and provides the platform for intercommunications between different scales and physical models.
At the microscopic scale the system is described using empirical or density-functional based tight-binding descriptions (DFTB) [1,2]. Transport calculations are obtained using non-equilibrium Green's functions methods that allow for calculations of coherent and incoherent transport and heat dissipation. At larger scales effective medium equations are represented on finite-elements meshes (FEM) to describe electronic and heat transport phenomena with drift-diffusion or Fourier equations [3]. Atomistic/FEM models are coupled imposing energy/current flux continuity at the boundaries. I will show an application of this scheme for the calculation of heat dissipation in molecular junctions.

References

[1] A Pecchia, G Penazzi, L Salvucci, A Di Carlo, New Journal of Physics 10 (2010), 065022
[2] A Pecchia, G Romano, A Di Carlo, Physical Review B 75 (3), (2007), 035401
[3] M Auf der Maur, G Penazzi, G Romano, F Sacconi, A Pecchia, A Di Carlo, IEEE Transactions on Electron Devices 99 (2011), 1-8

Figures

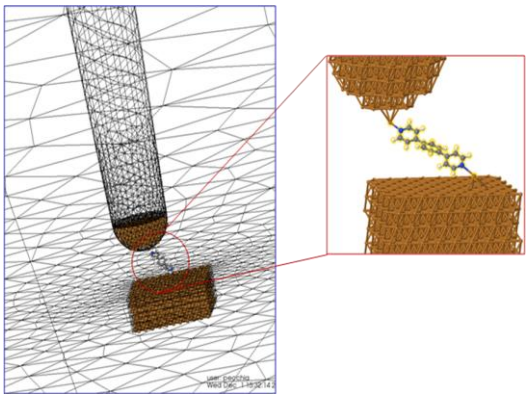

Figure 1. Atomistic/FEM coupling.

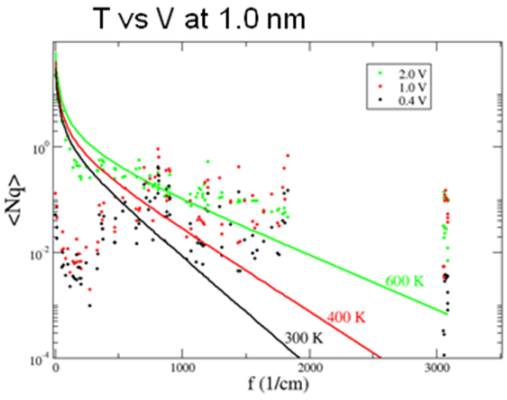

Figure 2. Molecular Temperature vs tip bias for a tip-substrate distance of 1.0 nm.