Theory of transport through molecular and atomic contacts

Fabian Pauly,[1] Janne K. Viljas,[1,2] Marius Bürkle,[1] Juan Carlos Cuevas,[3] and Gerd Schön[1,2]

[1] *Institut für Theoretische Festkörperphysik and DFG-Center for Functional Nanostructures, Universität Karlsruhe, 76128 Karlsruhe, Germany*
[2] *Forschungszentrum Karlsruhe, Institut für Nanotechnologie, 76021 Karlsruhe, Germany*
[3] *Departamento de Física Teórica de la Materia Condensada, Universidad Autónoma de Madrid, 28049 Madrid, Spain*

(Dated: October 4, 2007)

We present an overview of the activities of our group on the theoretical description of transport properties of atomic-sized contacts. The systems we investigate range from metallic atomic contacts consisting of hundreds of atoms to single-molecule junctions. In our work we employ both *ab-initio* methods (density-functional theory) and semiempirical tight-binding approaches. Using these methods we describe dc conductance in the elastic-transport regime [1–3], effects due electron-vibration coupling [4], photoassisted transport [5, 6], and thermoelectric phenomena [7].

---

[1] F. Pauly, M. Dreher, J.K. Viljas, M. Häfner, J.C. Cuevas. and P. Nielaba, *Theoretical analysis of the conductance histograms and structural properties of Ag, Pt, and Ni nanocontacts*, Phys. Rev. B **74**, 235106 (2006).

[2] S. Wohlthat, F. Pauly, J.K. Viljas, J.C. Cuevas, and G. Schön, *Ab initio study of charge transport through single oxygen molecules in atomic aluminum contacts*, Phys. Rev. B **76**, 075413 (2007).

[3] F. Pauly, J.K. Viljas, J.C. Cuevas, and G. Schön, *Tilt-angle landscapes of the conductance in biphenyl-dithiol single-molecule junctions*, arXiv:0705.3285, submitted to Phys. Rev. B (2007).

[4] J.K. Viljas, J.C. Cuevas, F. Pauly, and M. Häfner, *Electron-vibration interaction in transport through atomic gold wires*, Phys. Rev. B **72**, 245415 (2006).

[5] J.K. Viljas and J.C. Cuevas, *Role of electronic structure in photoassisted transport through atomic-sized contacts*, Phys. Rev. B **75**, 075406 (2007).

[6] J.K. Viljas, F. Pauly, and J.C. Cuevas, *Photoconductance of organic single-molecule contacts*, Phys. Rev. B **76**, 033403 (2007).

[7] F. Pauly, J.K. Viljas, and J.C. Cuevas, *Length-dependent conductance and thermopower in single-molecule junctions of dithiolated oligophenylene derivatives*, in preparation (2007).