

PROF. DR. CARMEN HERRMANN

Universität Hamburg

“Controlling and understanding conductance in molecular junctions”

Thursday, 12 February 2015

10:30

Room 205 (MÜL/ELCH/E) — Müller-Bau
TU Dresden, Bergstr. 66b, 01069 Dresden

Abstract:

Molecular conductance is measured in different experimental setups such as scanning tunneling microscopes (STMs), molecular break junctions, and nanoparticle arrays. The motivation behind these experiments is not only studying potential reproducible nanoscale building blocks for electronics or spintronics, but also learning about molecules under unusual conditions.

We show how theory can help understanding and controlling molecular conductance based on several examples from our research, ranging from a conceptual comparison of conductance and exchange spin coupling, to a study on switching conductance by protonation, to a simulation of combined STM/atomic-force microscopy experiment on platform-mounted porphyrin complexes.

[1] J. Proppe, C. Herrmann, *J. Comput. Chem.*, early view, DOI 10.1002/jcc.23781.

[2] C. Herrmann, J. Elmsz, *Chem. Commun.* 49, 2013, 10456-10458.

[3] H. Schlicke, C. Herrmann, Controlling molecular conductance: switching off π sites through protonation, *ChemPhysChem* 15, 2014, 4011-4018.

[4] N. Hauptmann, L. Groß, K. Buchmann, K. Scheil, C. Schütt, F. Otte, R. Herges, C. Herrmann, R. Berndt, *New J. Phys.*, accepted.

We are looking forward to welcoming you to this lecture and an inspiring discussion.

Prof. Gotthard Seifert

cfaed Carbon Path Co-Leader