Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Charge Transport in Azobenzene-Based Single-Molecule Junctions ARAN GARCIA-LEKUE, Donostia International Physics Center (DIPC) - Ikerbasque (Spain), YOUNGSANG KIM, Department of Mechanical Engineering, University of Michigan (USA), DMYTRO SYSOIEV, Department of Chemistry, University of Konstanz (Germany), THOMAS FREDERIKSEN, Donostia International Physics Center (DIPC) - Ikerbasque (Spain), ULRICH GROTH, Department of Chemistry, University of Konstanz (Germany), ELKE SCHEER, Department of Physics, University of Konstanz (Germany) — The azobenzene class of molecules has become an archetype of molecular photoswitch research, due to their simple structure and the significant difference of the electronic system between their *cis* and *trans* isomers. However, a detailed understanding of the charge transport for the two isomers, when embedded in a junction with electrodes is still lacking. In order to clarify this issue, we investigate charge transport properties through single Azobenzene-ThioMethyl (AzoTM) molecules in a mechanically controlled break junction (MCBJ) system at 4.2 K. Single-molecule conductance, I-V characteristics, and IETS spectra of molecular junctions are measured and compared with first-principles transport calculations. Our studies elucidate the origin of a slightly higher conductance of junctions with *cis* isomer and demonstrate that IETS spectra of *cis* and *trans* forms show distinct vibrational fingerprints that can be used for identifying the isomer.[1]

1. Y. Kim, A. Garcia-Lekue, D. Sysoiev, T. Frederiksen, U. Groth, E. Scheer, Phys. Rev. Lett. (accepted).

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Date submitted: 07 Nov 2012 Electronic form version 1.4