Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Rigidity of the conductance of an anchored dithioazobenzene optomechanical switch MARTINA ZEMANOVA DIESKOVA, Dept. of Physics, Slovak University of Technology, Bratislava, IVAN STICH, Inst. of Physics, Slovak Academy of Sciences, Bratislava, PETER BOKES, Dept. of Physics, Slovak University of Technology, Bratislava — We have investigated a reversible optomechanical molecular switch based on a single azobenzene molecule suspended via thiolate links between realistic models of gold tips [1]. Using a combination of the transfer-matrix technique and density functional theory, we focus on the conductance of the nanodevice in the two (meta)stable *cis* and *trans*-junction conformations. We find the conductance of both conformations to be broadly similar. In qualitative agreement with related experiments, we find that the same nanodevice with one/two methylene linker group(s) inserted on one/both ends of the azobenzene molecule is driven into the tunneling regime and reduces the conductances by up to 2 orders of magnitude, again, almost uniformly for both conformations. These results clarify the huge differences in switching ratios found previously and indicate that this nanodevice is not particularly suited for use as a molecular switch based on conductance change.

[1] M. Zemanová Dieśková, I. Štich, and P. Bokes, Phys. Rev. B **87**, 245418 (2013).

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Date submitted: 12 Nov 2013 Electronic form version 1.4