Abstract Submitted
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Tuning the Thermoelectric Properties of a Single-Molecule Junction by Mechanical Stretching[1] RENATO PONTES, Federal University of Goias, ALBERTO TORRES, Federal University of Santa Catarina, ANTONIO J.R. DA SILVA, Brazilian Synchrotron Light Laboratory (LNLS), ADALBERTO FAZZIO, Sao Paulo University — We theoretically investigate, as a function of the stretching, the behaviour of the thermoelectric properties - Seebeck coefficient (S), the electronic heat conductance (κ_{el}) and the figure of merit (ZT) - of a molecule-based junction composed by benzene-1,4-dithiol molecule (BDT) coupled to Au(111) surfaces at room temperature. We show that the thermoelectric properties of a single molecule junction can be tuned by mechanic stretching. The Seebeck coefficient is positive, indicating that it is dominated by the HOMO. Furthermore, it increases as the HOMO level, which is associated to the sulphur atom, goes to energies close to the Fermi energy. By modelling the transmission coefficient of the system as a single lorentzian peak, we propose a scheme to obtain the maximum ZT of any molecular junction.

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