Single-molecule quantum thermopower

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We developed a new device platform and measurement protocol to simultaneously measure the conductance and thermoelectric properties of single molecules [Applied Physics Letters **115** (2019) 073103]. The technique allows the study of thermoelectric effects in the non-linear regime both in temperature and bias voltage. The differential conductance maps and thermocurrent maps as a function of bias and gate voltage show the characteristic Coulomb blockade diamond-like features of quantum transport through a (molecular) quantum dot [Nature Nanotechnology **16** (2021) 426 – 430]. With this method, we study how vibrational excitations, Kondo correlations and spin entropy influence the thermocurrent generated by a single molecule. We find that this current recorded as a function of gate voltage can be used to determine the spin-ground state of single molecules and that it can be used to identify the universal hallmark of the Kondo effect in a magnetic field. The full characterization of thermoelectric properties makes detailed comparison with models possible and can be further used to develop strategies to improve the power factor of single-molecule energy harvesters.

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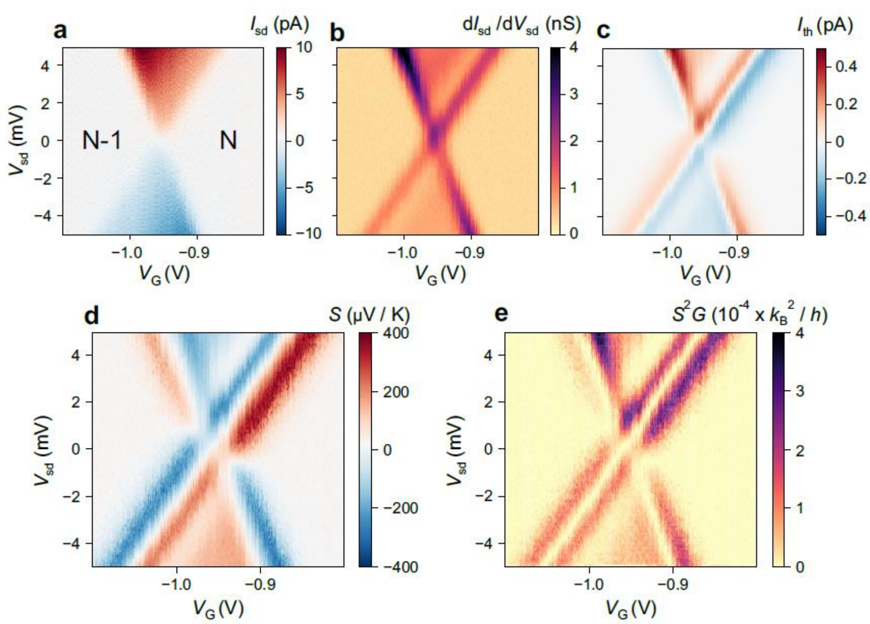

Maps of electronic and thermoelectric properties: (a) DC current, (b) differential conductance and (c) thermocurrent of a single molecule junction measured simultaneously as a function of bias and gate voltage. The data in (b) and (c) is used to calculate the Seebeck coefficient (d) and power factor as a function of bias and gate voltage (e).