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Controlling Negative Differential Resistance in Molecular Electronic Devices by Means of Designer Transition Metal Interfaces[1] HUGH DALGLEISH, GEORGE KIRCZENOW, Department of Physics, Simon Fraser University, Burnaby, BC, Canada, V5A 1S6 — Observations of negative differential resistance (NDR) have been reported for a number of molecular junctions with potential for device applications and have helped fuel the promise of viable molecular nano-electronic technologies. Here we present predictions of non-linear transport phenomena in molecular junctions where single organic molecules bridge transition metal nanocontacts. We predict the transmission to be mediated by interface states that appear within the HOMO-LUMO gap due to hybridization between thiol-terminated ends of the molecules and the d-orbitals of the transition metal. Our calculations reveal resonant enhancement and reduction in the interface state transmission under the application of moderate bias that result in NDR in molecular junctions with Pd nanocontacts. We show that this NDR can be tailored by suitably choosing the nanocontact materials: If a Rh electrode is substituted for one Pd contact we predict the NDR of the molecular junction to be strongly enhanced.

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