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Negative differential resistance in molecular junctions: The effect of the electrodes electronic structure[1] NATALYA ZIMBOVSKAYA, University of Puerto Rico-Humacao, MARK PEDERSON, Naval Research Laboratory — We have carried out calculations of electron transport through a metal-molecule-metal junction with metal nanoclusters taking the part of electrodes. We show that negative differential resistance peaks could appear in the current-voltage curves. The peaks arise due to narrow features in the electron density of states of the metal clusters. The proposed analysis is based on the ab initio computations of the relevant wave functions and energies within the framework of the density functional theory using NRLMOL software package.

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