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Effects of electron-phonon coupling in the Kondo regime of a two-orbital single-molecule junction[1] EDSON VERNEK, GISELE IORIO, Universidade Federal de Uberlândia, LILI DENG, KEVIN INGERSENT, University of Florida - USA, ENRIQUE ANDA, Pontificia Universidade Catolica do Rio de Janeiro - Brazil — Single-molecule junctions (SMJs) are electronic devices formed by a molecule bridging the gap between two metallic contacts. Despite their apparent simplicity, such systems have attracted much attention for the rich variety of experimentally accessible physics that they display. The spatial confinement of electrons in molecules can lead to collective phenomena such as Coulomb blockade and the Kondo effect, as well as to strong coupling of electrons to molecular vibrations. We explore the interesting interplay of electron-electron and electron-phonon interactions in a model of an SMJ in which the central molecule has two active orbitals. The nonperturbative numerical renormalization group method is used to treat the many-body Kondo physics and electron-phonon coupling on equal footing. Electron-phonon coupling renormalizes the energies and Coulomb interactions of the molecular orbitals. The effects are most pronounced in cases where both molecular orbitals lie close to the Fermi energy of the contacts. Here, a sufficiently strong phonon-assisted inter-orbital tunneling can suppress the Kondo effect and cause a crossover to a phonon-dominated regime having very different electrical transport properties.

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