Effect of electron-vibron coupling on electron transport via a single-molecule magnet Fe4

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Recently, single-molecule junctions consisting of individual single-molecule magnets (SMMs) bridged between electrodes, have been fabricated in three-terminal devices, and electron transport through SMMs was shown to be affected by magnetic anisotropy of the SMMs. In such junctions, vibrational modes of SMMs can couple to electronic charge and/or spin degrees of freedom, and the coupling influences magnetic and transport properties of the SMMs. An effect of the electron-vibron coupling on transport, has been extensively studied in single-molecule junctions and scanning tunneling microscopy/spectroscopy of small molecules, but not yet for junctions of SMMs. In this talk, we present our calculations of the electron-vibron coupling in a SMM Fe4 based on density-functional theory, and an effect of the coupling on electron transport. In addition, we compare our results with experimental data.

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