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Effect of electron-vibron coupling on electron transport via a single-molecule magnet Fe4 ALEXANDER MCCASKEY, YOH YAMAMOTO, MICHAEL WARNOCK, XIAOLIANG ZHONG, KYUNGWHA PARK, Virginia Tech, VIRGINIA TECH COMPUTATIONAL CONDENSED MATTER TEAM — Recently, single-molecule junctions consisting of individual single-molecule magnets (SMMs) bridged between electrodes have been fabricated in three-terminal devices, and magnetic anisotropy of SMMs has been shown to be affected by electron transport through the SMMs. In such junctions, vibrational modes of the SMM can couple to electronic charge and/or spin degrees of freedom, and the coupling influences magnetic and transport properties of the SMM. An effect of the electron-vibron coupling on transport has been extensively studied in 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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