Alteration of scanningtunnelling-spectroscopy images of molecular orbitals as a probe of electron correlation Massimo Rontani

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Scanning tunnelling spectroscopy (STS) allows to image single molecules decoupled from the supporting substrate. The obtained images are routinely interpreted as the square moduli of molecular orbitals, dressed by the mean-field electron-electron interaction. Here we demonstrate that the effect of electron correlation beyond mean field qualitatively alters the uncorrelated STS images. Our evidence is based on the ab-initio many-body calculation of STS images of planar molecules with metal centers. We find that many-body correlations alter significantly the image spectral weight close to the metal center of the molecules. This change is large enough to be accessed experimentally, surviving to molecule-substrate interactions.

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