

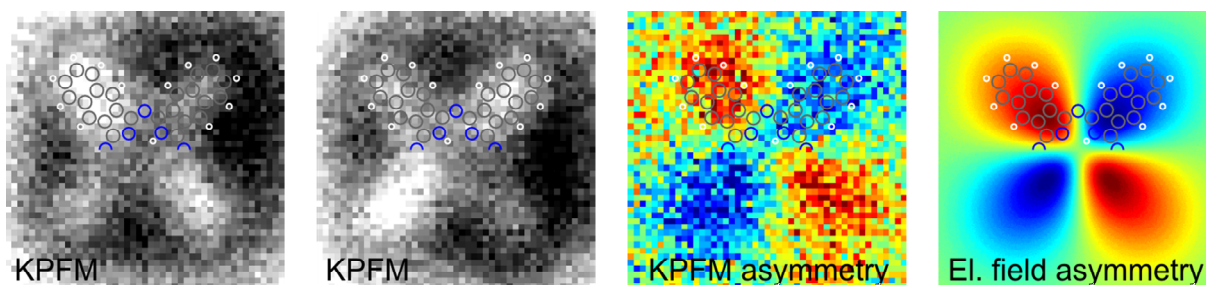
# Imaging the charge distribution within a single molecule

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It has been shown that the frontier orbitals of single organic molecules on thin insulating films can be imaged with STM [1], and their chemical structure can be imaged with noncontact-AFM with functionalized tips [2]. However, the intramolecular charge distribution is not directly accessible with these techniques. Kelvin probe force microscopy (KPFM), on the other hand, has been used to distinguish different charge states of single metal atoms [3], atomic point defects [4], and molecules [5], but no submolecular resolution has been reported until now. This suggests the possibility of combining the charge sensitivity of KPFM with the high resolution of STM and AFM to measure the charge distribution within a single molecule.

Here we present a combined STM, AFM, and KPFM study of the single-molecule hydrogen-tautomerization switch naphthalocyanine [6] on two monolayers of NaCl on Cu(111). In particular, we show that a pronounced charge asymmetry between the different lobes of the naphthalocyanine molecule exists, which manifests itself in submolecularly resolved KPFM images [7]. Furthermore, we show that – as in the case of noncontact-AFM – a tip functionalization with a single carbon monoxide molecule greatly enhances the resolution in KPFM imaging.

Our results are corroborated by density functional theory calculations, which lend support to our interpretation that the KPFM images reflect the electric field generated by the inhomogeneous charge distribution within the molecule.



## References

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