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Imaging the wave functions of adsorbed molecules using angle-resolved photoemmision data DANIEL LÜFTNER, THOMAS ULES, EVA MARIA REINISCH, GEORG KOLLER, University of Graz, Institute of Physics, Austria, SERGUEI SOUBATCH, F. STEFAN TAUTZ, Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich and Jülich Aachen Research Alliance (JARA), Germany, MICHAEL G. RAMSEY, PETER PUSCHNIG, University of Graz, Institute of Physics, Austria — The frontier electronic orbitals of molecules are the prime determinants of the respective compounds' chemical, electronic, and optical properties. Although orbitals are very powerful concepts, experimentally only the electron densities and energy levels are directly observable. As has been shown in recent publications, angle-resolved photoemission (ARPES) intensity maps of organic molecular layers are related to the absolute value of the Fourier transform of the initial state molecular orbital. However, the lost phase information impedes the back-transformation of the orbital into real space. Here, we show how molecular orbital images as well as the absent phase information can be retrieved by applying an iterative procedure which takes experimental ARPES maps as input and only assumes spatial confinement of the orbital. The method is demonstrated for several molecular orbitals of two proto-typical pi-conjugated molecules: the LUMO, HOMO, and HOMO-1 of pentacene, and the LUMO and HOMO of PTCDA [1]. The technique is simple and robust and further emphasizes the capabilities of ARPES looking at spatial distributions of wave functions of adsorbed molecules thereby complementing data obtained from scanning probe methods. [1] D.Lüftner et al., PNAS (accepted)

Daniel Lueftner
University of Graz, Institute of Physics, Austria

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