

Preface

This book encompasses contributions of the third AtMol Workshop in Berlin, September 2012. AtMol is a 4-year research project funded by the European Commission's ICT-FET programme. It was launched on 1 January 2011 with the objective to construct the first ever complete molecular chip where common microelectronic functionalities are brought and encapsulated at the atomic scale. The core of a molecular chip will make use of the extraordinary properties of individual molecules and surface atomic wires, regarding both their chemical and quantum electronic characteristics that should be of practical use and appealing to future information technologies (IT) manufacturing.

Real space imaging of the electronic cloud of a single atom or molecule is now of prime importance in the field of quantum information transmission, manipulation and storage and in the field of single-molecule mechanics. Also, the intramolecular electronic and magnetic phenomena inside a single molecule are of fundamental scientific interest. This AtMol workshop brought for the first time research groups from all around the world together, working on the theory or experiments on the spatial extension (associated with electronic spectroscopy) of the electronic cloud of a single atom or molecule. When possible, the maps recorded or reconstructed by Fourier Transform can be interpreted on the basis of the spin-orbitals entering in the Slater determinants decomposition of the electronic quantum states of a single atom or molecule. Depending on the used experimental and calculation techniques, the relation between the obtained data and the mathematical concept of orbitals was vividly debated. Manipulation techniques to change the spatial distribution or quantum properties by interacting with single molecules were also discussed.

This workshop was open for contributors in the fields of single atom and single molecule imaging using, for example, the FEM, TEM, Photoemission, Attosecond Tomography, NC-AFM or LT- STM instruments. It was the occasion to celebrate the first recording of the image of a single molecule by E. Müller 60 years ago in Berlin-Dahlem, the precise location of this third AtMol workshop (see Fig. 1).

The topics reported in this book form one of the scientific backgrounds required for building up the future of calculators and memory as recognized at the European Commission level. We thank the ICT-FET programme and A*STAR of Singapore for the financial support in organizing this third workshop, and Springer Verlag and its staff members for the publication of this book.

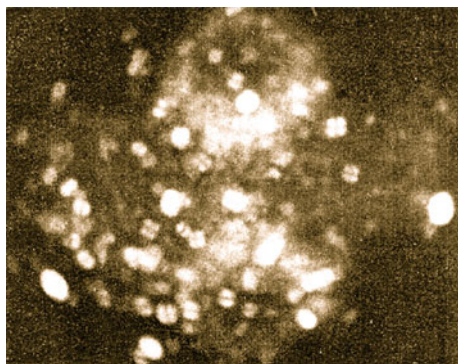


Fig. 1 The first ever recorded image of a few isolated molecules in real space by Erwin W. Müller in 1950 with a Field Emission Microscope. The imaged molecules are Cu-Phthalocyanines deposited on a broad tungsten tip with about a 200 nm radius of curvature. This image was first submitted on 7 August 1950 and published in the journal *Zeitschrift für Naturforschung* 5a, 473 (1950). At that time E. Müller was at the Kaiser-Wilhelm-Institut für Physikalische Chemie und Elektrochemie in Berlin. Before this direct space image, these molecules were only known indirectly via a Fourier analysis of the Röntgen X-Ray diffraction pattern of a crystal of Cu-Phthalocyanine molecules as obtained for the first time by J.M. Robertson in 1935 (*J. Chem. Soc.*, 615 (1935))

Imaging and Manipulating Molecular Orbitals

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