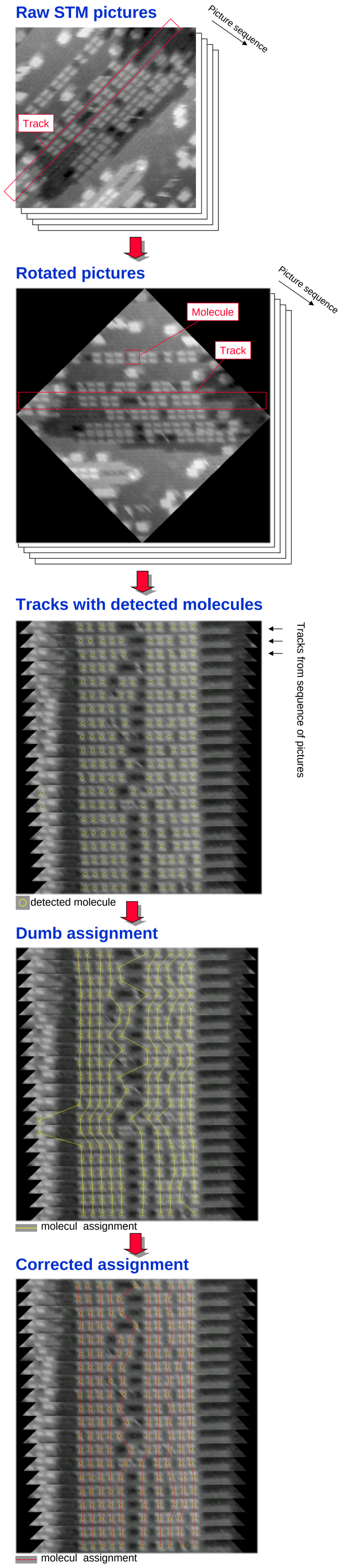
MMD&T

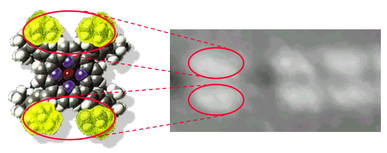
MOLECULAR MOTION DETECTOR & TRACER



Introduction and long term aim of the project

Molecular positioning of building blocks into larger supramolecular structures [1] is a key technique to construct molecular nanostructures and explore their properties. Possible applications may include **data storage**, nanoscale **optoelectronic devices** and ultrasensitive **(bio)-chemical transducer** elements responding to the recognition of a single molecule. Positioning at room temperature has been achieved for numerous molecule-substrate systems, especially of fullerenes (C60) on silicon, on Cu(111), and on bianthrone.

One of the key issues in this field, relevant to many applications, is the current limitation in speed to perform complex repositioning patterns. **This project aims at the development of techniques for optimisation of the "human-machine" interface.** Image processing and analysis have been developed to enable the automatic recognition of individual molecular units within the STM-images, and to identify the relevant molecular displacement vectors in a sequence. These procedures can then be used for performing subsequent repositioning steps and verifying the process for the formation of a predefined molecular pattern. Rigid, highly symmetrical and planar porphyrin derivatives have been chosen as a model system for such repositioning experiments.



The porphyrin molecule

The typical trace of an individual porphyrin molecule, adsorbed onto the Au(110) single-crystal surface and imaged by STM is shown above. The characteristic lobes in the STM-data correspond to the bulky di-*t*-butylphenyl substituents.

In a STM image of 20x20 nm size the individual molecular units are identifiable as pairs of bright oval spots. The molecules are aligned in rows due to their intermolecular and molecule-substrate interactions on the corrugated 2x1 reconstitution of the gold substrate.

Aim of the MMD&T project

Verify the feasibility of automated detection and tracing of molecules in a scanning probe microscopy sequence with image processing. For this study a system of porphyrin molecules on a Au(110) substrate was chosen. Due to the asymmetric corrugation of the substrate (2x1 reconstruction of the substrate) molecular motion is confined to only one dimension at room Temperature. For the algorithm it is assumed, that the majority of the molecules will not move between two frames and that the molecules within one row can not pass each other.

Solution

The whole process of recognition and assignment works as follows:

- Choose the sequence of pictures
- Mark the rotation angle of the molecule tracks in the picture
- Mark a sample molecule

User entries

- Fast approximate drift compensation using cross-correlation of several high-contrast areas in the pictures
- Cut track image out of the picture
- Search for patterns of molecules giving good correlation results (no motion detected) within the sequence of track images
- Use coordinates of the identified immobile molecules to correct drift
- Assign connections between identified molecules in two following tracks, from left to right, beginning with the first track (see figure 'Dumb assignment')
- Use plausibility algorithm to correct assignment and search for molecules with low correlation (highly mobile molecules)

Conclusions & outlook

- High accuracy correlation is possible with approximately 90% of the molecules
- Using heuristic information and plausibility tests for the behaviour of the system most of the remaining molecules can be traced (about 99%)
- Due to the numerous rules and conditions used for decision making, a Fuzzy system might further improve the probability for correct assignment of molecules
- Algorithms will be further developed to identify mobile molecules in systems where they perform two dimensional motion

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Reference

[1] T.A. Jung, R.R. Schlittler, J.K. Gimzewski, H. Tang and C. Joachim, Science 271, 181 (1996).

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