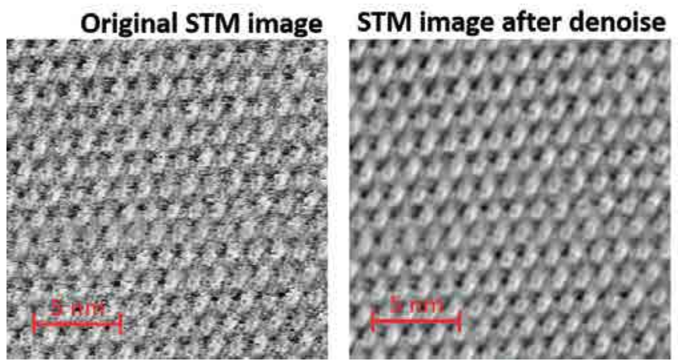
STMImage

Scanning Tunneling Microscopy Image Processing Tools

Scanning tunnelling microscopy (STM) is a powerful technique to characterize and manipulate materials at atomic/molecular scale. Since its invention, scientists have improved the technique and used it to play with matter, moving and adding atoms and molecules. The STMImage project aims to develop the first computational tools specifically designed to denoise the images obtained from STM..



Main Project Team	
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Indicators	
Funding	33k €
Journal Papers	6

Two Main Publications

Q. Ferreira, A. Bragança, L. Alcácer, J. Morgado, Conductance of Well-Defined Porphyrin Self-Assembled Molecular Wires up to 14 nm in Length, Journal of Physical Chemistry C, Vol. 118, No. 3, pp. 7229 - 7234, March, 2014

PROJECT WEBPAGE URL
http://www.lx.it.pt/~jpaos/stm/

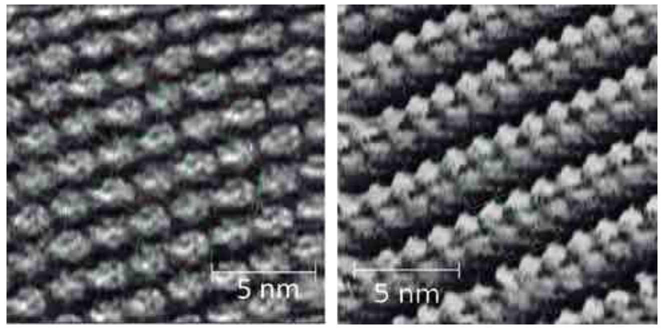

Fig. 1 Detection of unit cells of STM images of a porphyrin monolayer: a) hexagonal and b) rectangular.

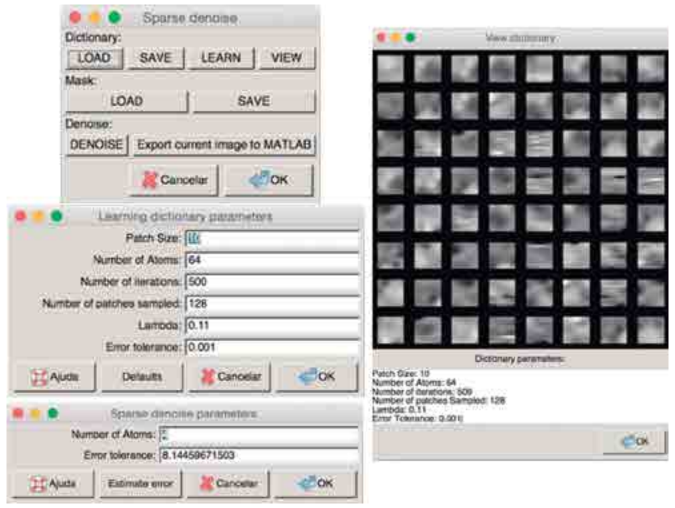

Fig. 2 Screenshots of the denoise computational tools available in the freeware Gwyddion software.

GENERAL MOTIVATION AND OBJECTIVES

The progress in advanced functional materials has demanded a deep research of their properties, including their characteristics at atomic scale. The knowledge of materials at fundamental level has allowed an outstanding progress of semiconductor technology, energy storage and conversion devices, quantum computers and also the creation of smart biomaterials able to mimic biological tissues. The optimization of materials properties at atomic scale is due to the powerful ability of high-resolution imaging techniques such as the stm. This technique allows the visualization of materials at atomic resolution providing images of the surfaces composition and quantitative information of its constituent parts (atoms and/or molecules). The stm images are more than an illustration, they give chemical identification of individual atoms including, for instance electronic, magnetic and spectroscopy information at atomic level. For this reason, the STM is the technique of choice of researchers to design and develop new nanomaterials. However, this technique is very sensitive to the vibrational and electronic noise of environment that influences the quality of images. The accurate interpretation of images with atomic and molecular resolution is a very challenging task, due to the number and the dimensions of details that have to be quantified. This process is strongly affected by noise and by the drift caused due to the relative motion of the sample and the probe, that occurs during stm measurements. In an effort to solve this problem, we developed a computational tool where the STM denoising is reformulated as sparse regression problem, often termed sparse coding. The image is partitioned into small overlapping square patches and the vector corresponding to each patch is modeled as a sparse linear combination of vectors, termed atoms, taken from a set called dictionary. the dictionary is learned from the data and it represents via matrix factorization, with sparsity constraints on the code. The sparsity of a representation on a dictionary is strongly linked with the level of self-similarity of the images under study. It happens that STM images have a high level of self-similarity and, therefore, they are natural candidates to be denoised via sparse regression on learned dictionaries. The denoise algorithm works as follows: (i) the noisy STM image is decomposed in small patches; (ii) a dictionary is learned from the data; (iii) the patches are sparsely coded using just a few atoms from the learned dictionary; and (iv) the denoised/restored image is obtained by composition of the coded patches.

CHALLENGE

The main challenge of this project is to develop the first computational tools to improve the quality of STM images, removing the noise in order to perform a correct image analysis..

WORK DESCRIPTION AND ACHIEVEMENTS

During this project was developed a toolbox of algorithms that denoise the STM images and automatically detect their unitary cells of crystal lattices.

The denoising algorithm is based on state-of-art algorithms but it was optimized for periodic images such as the STM images. Since these images have plenty of outliers, the existing techniques were adapted in order to deal with these missing information. The cover figure shows the comparison between an original image and with a denoised image. The small dots represent porphyrins molecules which are very well detailed after the processing with the denoise algorithm.

The denoised STM images were analysed in order to obtain their smallest pattern that contains the whole molecular information – the unitary cell. A robust algorithm was developed based on the analysis of local peaks of the autocorrelation function of the STM image. Figure 1 shows two STM images with an hexagonal and rectangular geometries identified by the developed algorithm.

To facilitate the use of the denoise algorithm by the STM community, a module for Gwyddion freeware software was developed. Figure 2 shows some screenshots of the resulting tool.