Surface Structure and Reactivity
by Scanning Tunneling Microscopy

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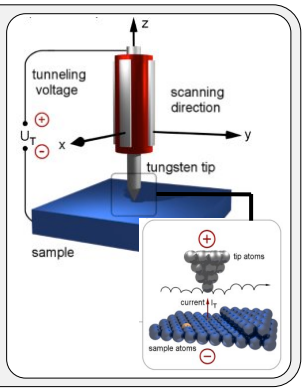
Main research interest: characterizing the geometric and electronic structure of solid surfaces, with specific interest in describing their evolution during surface processes (e.g. bond formation, segregation, growth, chemical reactions).

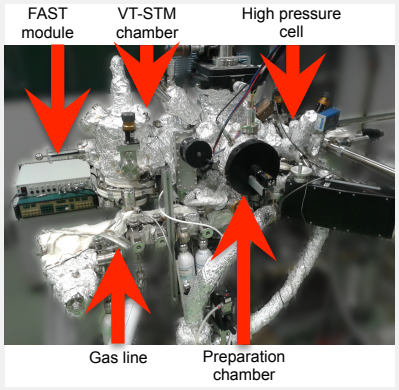
Investigated systems: epitaxial graphene, self-assembled organic monolayers, adsorbate covered surfaces.

Techniques: Mainly Scanning Tunneling Microscopy, capable of characterizing both structural and electronic modifications at the atomic scale. Complementary conventional or synchrotron radiation spectroscopic measurements are also performed. Experimental results are often compared to *ab initio* calculations performed by collaborating theoretical groups.

Instrumentation: two independent, complementary STM setups. One is dedicated to variable temperature (140-900 K) measurements, with high rate image acquisition (up to ~100 frames/s) and *in operando* conditions; a high pressure cell allows for sample preparation with heavy gas exposure. The second system is specialized in low temperature (4-77 K) measurements with sub-molecular resolution and offers the possibility to perform molecular manipulation and scanning tunneling spectroscopy.

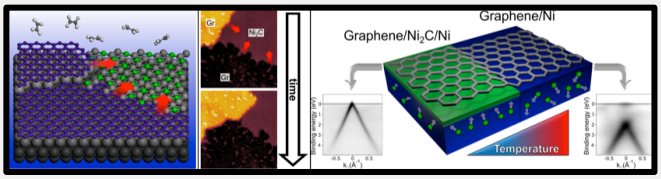


Variable Temperature STM



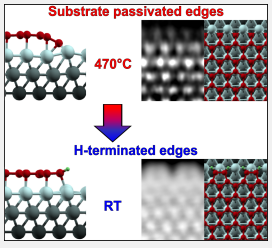
- Temperature range from 140 K to 900 K
- Gas dosing: $1x10^{-6}$ mbar in UHV, up to 20 mbar in HPC
- FAST scanning mode up to 100 frames/s
- Sputter gun, LEED optics, mass spectrometer, gas line.

Selected results



Graphene growth on Ni(111). (left) STM images and sketch of surface carbide conversion to graphene; (right) μ-ARPES plots and sketch of decoupling process by interlayer buffering.

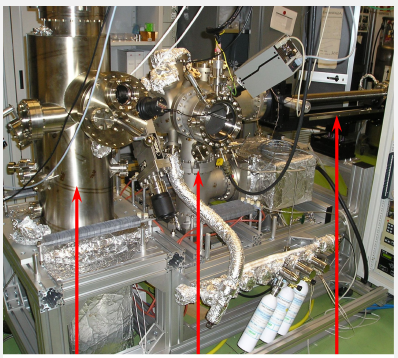
Patera et al, ACS Nano ***7****, 7901-7912 (2013); Africh et al,* Sci. Rep. ***6****, 19734 (2016)*



Coupling and detaching of graphene edges from a Ni substrate. (top) lateral sketch, Fast-STM image (acquired in 250 ms) and model of a substrate-passivated graphene edge at high temperature; (bottom) lateral sketch, Fast-STM image (acquired in 250 ms) and model of a hydrogen-passivated graphene edge at room temperature.

Patera et al, Nano Lett. ***15****, 56-62 (2015)*

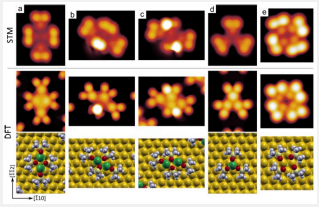
Low Temperature STM



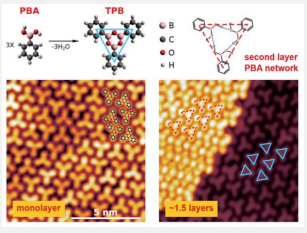
- Temperature down to 4 K (LHe) or 77 K (LN_2)
- Single-point spectroscopy measurements of *dI/dV* and d^2I/dV^2
- Preparation stage with wide temperature range (77-1100 K)
- Sputter gun, LEED optics, mass spectrometer, gas line

Selected results

STM images of various complexes formed on a gold surface by dimethyl sulfide (DMSO), a widely used solvent. Both experimental (top row) and density functional theory (DFT) calculated images (middle row) are shown.
The bottom row shows ball models of the geometries obtained by DFT calculations, where the green balls represent gold adatoms trapped by the DMSO molecules.



Z. Feng et al, ACS Nano ***9****, 8697 (2015)*



D.Toffoli et al, Chem. Sci. ***8****, 3789 (2017)*

Organic layers on Au(111). Top: Schematic representation of phenyl-boronic acid (PBA) and triphenylboroxine (TPB) molecules (left) and of the suggested hydrogen bonding network of PBA trimers forming the second molecular layer on a gold surface (right).. Bottom: STM images of the monolayer (left) and of the 1.5 layer (right). Blue and red triangles indicate the size and shape of the TPB molecule and PBA trimers forming the first and second layer, respectively

Long term collaborations

Maria Peressi	UniTS (*ab initio* calculations)
Cinzia Cepek	CNR-IOM (photoemission spectroscopy)
Albano Cossaro	CNR-IOM (synchrotron radiation spectroscopy)
Andrea Locatelli	Elettra Sincrotrone Trieste (synchrotron radiation microscopy)

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