

Roberta Totani, Ph.D. - Curriculum vitae

Personal information

- Address: _____
- Mail: _____
- Mobile phone: _____
- Place and date of birth: _____
- + _____
- Citizenship: Italian

Experience

- **Post-doc** 01.2018 - 12.2019
Department of Physics, University of Zürich
Growth and characterization of MoS₂ monolayers on Sb₂Se₃ single crystals for photocatalysis.
[LightChEC](#) (Light to Chemical Energy Conversion) Project
- **Post-doc** 11.2015 - 12.2017
Laboratoire de Réactivité de Surface - UMR CNRS 7197
Université Pierre et Marie Curie - UPMC Paris 6,
Co-adsorption of peptides and water on metallic surfaces
[MATISSE](#) (MATERIALS, InterfaceS, Surfaces, Environment) Project

Education

- **PhD in Physics** 10.2012 - 03.2016. Degree awarded: 23.03.2016
University of L'Aquila (Italy)
Experimental Thesis in Surface Science: "*Organic molecules for molecular and organic electronics: structural properties and characterization*"
Investigated systems: CuPc and fullerene C₆₀ thin films on graphene for organic solar cells, MnPc, FePc, H₂Pc, Lu₂Pc, biphenylene as thin films and in gas phase for molecular electronics, spintronics, light-harvesting.
 - **Erasmus Placement** 05.2015 - 07.2015, Uppsala University, Sweden. "*Characterization of molecular materials by means of photoemission spectroscopies*"
 - **Visiting Ph.D. student**, Uppsala University, Sweden (02.2014 - 04-2014) and Université Pierre et Marie Curie, Paris, France (06.2014)
- **MSc. in Physics** 10.2009 - 03.2012
University of L'Aquila (Italy). Experimental Thesis in Surface Science. Supervisor: Prof. Luca Lozzi. Mark: 108/110.
- **BSc. in Physics** 10.2005 - 12.2009
University of L'Aquila (Italy). Theoretical Thesis in Quantum Optics. Supervisor: Dr. Alessandro Ciattoni. Mark: 101/110.

Experimental competences

- UHV environment and instrumentation
- Experimental preparation techniques: CVD, PVD, Electrospray, Spin-coating, Drop-casting
- Experimental characterization techniques: XPS, AR-XPS, UPS, NAP-XPS, IPES, LEED, NEXAFS, ResPES, STM, AFM, PM-RAIRS, XPD, ARPES
- Use of synchrotron radiation
ELETTRA: GasPhase, CiPo, SuperESCA, Aloisa
MAX-IV: I311
SOLEIL: Tempo
SLS: NanoXAS

Data treatment, analysis and presentation

- Windows and Mac OS platform
- Office suites (Microsoft Office, Open Office, iWork) and LaTeX
- Igor Pro, Origin, Matlab, Gwyddion, Vesta
- Programming Languages: Python, Matlab, C++
- Simulations: EDAC (Electron Diffraction in Atomic Clusters)

Languages

- Italian - native speaker
- English - C2
- Spanish - C1
- French - B1
- German - A1

Publications

1. R. Totani, C. Méthivier, D. Costa, T. J. Inizan, C. -M. Pradier, V. Humblot, "Binding and 2D organization of Arginine on Cu(110)". *App. Surf. Sci.* 509, 144865 (2020).
2. R. Totani, F. O. von Rohr, J. -Z. Zhao, Z. Novotny, W. D. Zabka, A. Soluyanov, J. Osterwalder. *Sb₂Se₃: A strongly anisotropic surface.* *Phys. Rev. Materials* 3, 125404 (2019).
3. W. D. Zabka, T. Musso, M. Mosberger, Z. Novotny, R. Totani, M. Iannuzzi, B. Probst, R. Alberto, J. Osterwalder. *Comparative Study of the Different Anchoring of Organometallic Dyes on Ultrathin Alumina.* *J. Phys. Chem. C* 123, 22250 (2019).
4. R. Totani, C. Méthivier, H. Cruguel, C. M. Pradier, V. Humblot. *Deciphering the adsorption mechanisms of RGD subunits: L-Aspartic Acid on Cu(110).* *J. Phys. Chem. C*, 121, 15842 (2017).

5. R. Totani J. Lüder, M. de Simone, I. Bidermane, T. Zhang, C. Grazioli, M. Coreno, B. Brena, L. Lozzi, C. Puglia. *Electronic structure investigation of biphenylene films*. J. Chem. Phys., 146, 054705 (2017).
6. J. Lüder, M. de Simone, R. Totani, M. Coreno, C. Grazioli, B. Sanyal, O. Eriksson, B. Brena, C. Puglia. *The electronic characterization of biphenylene - Experimental and theoretical insights from core and valence level spectroscopy*. J. Chem. Phys., 142, 074305 (2015).
7. I. Bidermane, I.E. Brumboiu, R. Totani, C. Grazioli, M. N. Shariati- Nilsson, H. C. Herper, O. Eriksson, B. Sanyal, B. Ressel, M. de Simone, L. Lozzi, B. Brena and C. Puglia. *Atomic Contributions to the Valence Band Photoelectron Spectra of Metal-free, Iron and Manganese Phthalocyanines*. J. Electron. Spectrosc. Relat. Phenom. 205, 92 (2015).
8. I. Bidermane, J. Lüder, R. Totani, C. Grazioli, M. de Simone, M. Coreno, A. Kivimäki, J. Åhlund, L. Lozzi, B. Brena, C. Puglia. *Characterization of gas phase iron phthalocyanine with X-ray photoelectron and absorption spectroscopies*. Phys. Status Solidi B, 252, 6, 1259 (2015).
9. I.E. Brumboiu, R. Totani, M. de Simone, M. Coreno, C. Grazioli, L. Lozzi, H. C. Herper, B. Sanyal, O. Eriksson, C. Puglia and B. Brena *Elucidating the 3d electronic configuration in Manganese Phthalocyanine*. J. Phys. Chem. A 118, 927 (2014).
10. A. Kivimäki, P. Norman, M. Coreno, M. de Simone, C. Grazioli, R. Totani, B. Ressel, H. Ottosson and C. Puglia. *Use of two-dimensional photoelectron spectroscopy in the decomposition of an inner-shell excitation spectrum broadened by super-Coster-Kronig decay*. Phys. Rev. A 88, 062502 (2013).

Research activity

My main research topic is the development and the characterization of the fundamental properties of innovative materials, with applications in the field of molecular electronics, renewable energies, bio/nano-technologies. A prominent part of the research work has been carried out at several European synchrotron facilities.

- During my Ph.D. at the STN (Surfaces, Thin films and Nanostructures) Laboratory of the University of L'Aquila, I studied a blend film of copper phthalocyanine (CuPc) and fullerene (C₆₀), the active layer in organic solar cell and how it interfaces with graphene as an innovative transparent electrode. A ResPES (Resonant Photoemission) investigation (beamtime at SuperESCA, Elettra, main investigator) allowed characterizing the system photovoltaic behavior, simulating its condition immediately following photon absorption. Meanwhile, the collaboration with the Department of Physics and Astronomy of the Uppsala University led me to the research in molecular electronics, with several beamtimes realized at Max-Lab (now MAX-IV, the Swedish synchrotron) on the I311 beamline and Elettra (GasPhase and CiPo beamlines). Thus, I investigated biphenylene [5,6], several transition metal phthalocyanines (TMPcs) [7,8,9] and n-butylgermane [10]. Biphenylene is considered the building block of a covalently bonded graphene-like but gap provided molecular materials. TMPcs find implementation in spintronics, quantum computing and biomimetic catalysis, while the study of the partially resolved Ge 3p core excitation spectrum of n-butylgermane belongs to a more fundamental physics context.
- At the Laboratoire de Réactivité de Surface of the Université Pierre et Marie Curie (Paris VI), I started investigating the adsorption and the organization of amino acids and small peptides on metallic surfaces. Molecular films of amino acids and peptides were obtained in UHV by means of an electrospray ionization device, from an aqueous solution [1, 4]. This allowed avoiding the high temperatures needed for sublimation, which could damage such delicate biomolecules. A NEXAFS experiment has been performed to determine arginine geometry adsorption on a Cu(110) surface [1] (beamtime at ALOISA, Elettra, main investigator). A Near-Ambient Pressure XPS experiment has been realized at the TEMPO beamline of Soleil, the French synchrotron, to investigate the interaction with water.
- Finally, while moving to the Department of Physics of the University of Zürich, I started studying the realization and the characterization of efficient, earth-abundant and cheap catalysts for photocatalytic water splitting. Their electronic and chemical properties, their structure and their stability in UHV and in more realistic in-operando conditions were investigated in the perspective of a possible implementation for solar-to-hydrogen conversion [2, 3]. Experiments were performed at the ESCA (Electron Spectroscopy for Chemical Analysis) Laboratory of the University of Zürich and at the NanoXAS beamline of SLS, the Swiss synchrotron facility.

Presentations

- FisMat 2019, Catania (Italy). Oral: $\text{Sb}_2\text{Se}_3(100)$: a strongly anisotropic surface for photocatalysis.
- Joint Annual meeting Swiss Physical Society - Austrian Physical Society 2019, Zürich (Switzerland). Oral: Characterization of Sb_2Se_3 single crystal surfaces for photocatalysis.
- ECOSS 2018, Aarhus (Denmark), August 26 - 31. Poster: Characterization of Sb_2Se_3 single crystal surfaces for photocatalysis.
- Journées Scientifiques du Comité Spectroscopies d'Electron 2017, Paris, May 17-18. Oral: *Arginine on Cu(110): different adsorption mechanisms for a single molecule;*
- LiXS 2017 Satellite Workshop, Soleil Synchrotron, Saint-Aubin (France), January 17-18. Oral: *Arginine and Aspartic Acid on Cu(110): from the liquid solution to the molecular film;*
- ECOSS 2016, Grenoble (France), August 28 - September 2. Oral: *Arginine and aspartic acid on Cu(110): unraveling the different adsorption mechanisms of peptides structural units;*
- FisMat 2015, Palermo (Italy), September 28 – October 2. Oral: *Biphenylene: building block for 2D graphene like (but gap-provided) molecular networks;*
- ECOSS 2014, Antalya (Turkey), 31 August - 5 September. Poster: *Metal-free, Iron and Manganese Phthalocyanine: a comparison between Valence Band Photoemission Spectra.*
- FisMat 2013, Milan (Italy), September 9-13. Oral: *Interface properties between CuPc:C₆₀ blend films and graphene*

Schools

- Solar Light to Chemical Energy Conversion: Symposium and Summer School, August 19 - 23, 2018, Eurotel Victoria, Les Diablerets, Switzerland.
- International School of Solid State Physics, Foundation and Centre for Scientific Culture Ettore Majorana: Materials for Renewable Energy, Erice 2014.
- XII School on Synchrotron Radiation: Fundamentals, Methods and Applications, Grado (Go), Italy, September 2013.

Zurigo, 12.08.2020