

Scientific Presentation

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Statement of Research

During the PhD, my research was focused on the detailed surface science study of model catalysts for energetics applications (such as the oxygen reduction reaction, ORR) and water remediation. The studied model systems were carbon-based substrates that were modified by means of ion implantation. On these substrates, active phases such as Pt, Pd, Cu, Ag, Co, Fe, Fe and Co oxides, Au, Ag-Cu, Pd-Cu, Pd-Y and Pd-Ce alloys were deposited (via PVD) and studied in-situ by surface science and synchrotron radiation techniques such as XPS, FT-IRAS, HR-PES, ResPES, XAS, UPS and STM. The catalytic activity of these model catalysts was studied ex-situ using the common tools provided by electrochemistry, such as CV, RDE and EIS.

The research interests have then moved towards the preparation of single layer graphene (SLG) on metal substrates, by CVD and UHV-assisted CVD deposition. The obtained systems, also doped with B, N or S, were investigated because of their peculiar interaction with metal/metal oxides/metal chalcogenides (such as Ni, Fe, Ti, Co, Mo and their oxides, Pt, $\text{MoS}_{x,x=2,3}$), as proved by XPS, HR-PES, ResPES, XAS, UPS and *micro*-ARPES, as well as STM. Not only surface science: during the PhD my research was also focused on the preparation of 3D hierarchical and nano-shaped graphene-derived materials (such as Graphene Papers, Graphene Foams and Graphene Quantum Dots), obtained by different approaches (electrochemical ablation or hydrothermal synthesis); the introduction of several dopants (B, N, S, and their combinations) leads to interesting optical and catalytic properties of these new materials.

As post-doc and currently as research associate, my main interest is to couple XPS and XAS with electrochemistry in a new technique, performing Ambient Pressure XPS/XAS under electrochemical conditions using both soft and tender X-rays (2.0-9.0 keV). The most important physical and chemical processes in energy material research and electrochemistry take place at interfaces between the liquid and solid phase under ambient pressure or even higher. With the previous success of soft X-ray Ambient Pressure XPS-XAS in probing the gas-solid interface, researchers have started to gain insights into the liquid-solid boundaries. This will shed new light on the understanding of the chemical changes at the electrode surfaces during realistic working conditions. Not only: these developing techniques allow to investigate *in operando* the electrical double layer (EDL) at the WE/electrolyte junction, making possible to point out the particular role played by the ionic species present in the electrolyte in the charge transfer mechanism at the electrified interphase.

In my research, synchrotron radiation techniques are widely employed in order to provide a deep insight in the chemistry/structure/properties relationships, using in particular resonant spectroscopies and angle-resolved photoelectron spectroscopies. Several beam-times were performed at the Elettra synchrotron radiation facility (TS, Italy), Diamond (OX, UK), SSRL (Menlo Park, USA), ALS (Berkeley, USA) and MaxIV (Lund, Sweden) both as user and principal investigator. Beamlines: Bach, Bear, Escamicroscopy, Material Science, Nanospectroscopy, Spectromicroscopy, (Elettra), B18 (Diamond), 7-3 and 11-2 (SSRL), 9.3.1, 9.3.2, 10.3.2, 6.3.2, 11.0.2 (ALS), HIPPIE (MaxIV).

List of Publications on Peer-Reviewed Journals

42. C. Rüdiger*, C. Valero-Vidal, **M. Favaro**, S. Agnoli, G. Granozzi, J. Kunze-Liebhäuser*, *The effect of air-aging on the electrochemical characteristics of TiO_xC_y films for electrocatalysis applications*, Chem. Electro. Chem. 2017, DOI:10.1002/celc.201700912 [\[DOI\]](#);
41. **M. Favaro***, F. F. Abdi, M. Lamers, E. J. Crumlin, Z. Liu, R. van de Krol, D. E. Starr*, *Light-Induced Surface Reactions at the Bismuth Vanadate/Potassium Phosphate Interface*, J. Phys. Chem. B 2017, DOI:10.1021/acs.jpcc.7b06942 [\[DOI\]](#);
40. **M. Favaro***, J. Yang, S. Nappini, E. Magnano, F. M. Toma, E. J. Crumlin, J. Yano, I. D. Sharp*, *Understanding the oxygen evolution reaction mechanism on CoO_x using operando ambient pressure X-ray photoelectron spectroscopy*, J. Am. Chem. Soc. 2017, 139, 8960-8970 [\[DOI\]](#);
39. **M. Favaro**#, H. Xiao#, T. Cheng, J. Yano*, W. A. Goddard*, E. J. Crumlin*, *Water and carbon dioxide interaction on copper surfaces, from experiment to theory* (#: these two authors have equally contributed to the work), Proc. Natl. Acc. Sci. 2017, 114, 6706-6711 [\[DOI\]](#);
38. D. E. Starr*, **M. Favaro**, F. F. Abdi, H. Bluhm, E. J. Crumlin, R. van de Krol, *Combining soft and hard X-ray photoelectron spectroscopy at ambient conditions for a molecular-level understanding of water splitting semiconductor/electrolyte interfaces*, J. Elect. Spectrosc. Relat. Phenom. 2017, DOI: 10.1016/j.elspec.2017.05.003 [\[DOI\]](#);
37. **M. Favaro**, C. Valero-Vidal, J. Eichhorn, F. M. Toma, P. N. Ross, J. Yano, Z. Liu, E. J. Crumlin*, *Elucidating the alkaline oxygen evolution reaction mechanism on Platinum*, J. Mater. Chem. A 2017, 5, 11634-11643 [\[DOI\]](#);
36. C. Rüdiger*, **M. Favaro**, C. Valero-Vidal, L. Calvillo, N. Bozzolo, S. Jacomet, J. Hein, L. Gregoratti, S. Agnoli, G. Granozzi, J. Kunze-Liebhäuser*, *Substrate grain-dependent chemistry of carburized planar anodic TiO₂ on polycrystalline Ti*, ACS Omega, 2017, 2, 631-640 [\[DOI\]](#);
35. **M. Favaro**#, W. S. Drisdell#, J. M. Gregoire, E. J. Crumlin*, J. Haber*, J. Yano*, *An operando investigation of (Ni-Fe-Co-Ce)O_x system as highly efficient electrocatalyst for oxygen evolution reaction*, ACS Catalysis, 2017, 7, 1248-1258 (#: these two authors have equally contributed to the work) [\[DOI\]](#);
34. A. Eilert, F. Cavalca, F. S. Roberts, J. Osterwalder, C. Liu, **M. Favaro**, E. J. Crumlin, H. Ogasawara, D. Friebe, L. G. M. Pettersson, A. Nilsson*, *Subsurface oxygen in oxide-derived copper electrocatalysts for carbon dioxide reduction*, J. Phys. Chem. Lett., 2017, 8, 285-290 [\[DOI\]](#);
33. C. Ampelli*, F. Tavella, C. Genovese, S. Perathoner, **M. Favaro**, G. Centi, *Analysis of the factors controlling performances of Au-doped TiO₂ nanotube array based photoanode in photo-electrocatalytic (PECA) cells*, J. Energy Chem. 2017, doi:10.1016/j.jechem.2016.11.004 [\[DOI\]](#);
32. J. Yang, J. K. Cooper, F. M. Toma, K. A. Walczak, **M. Favaro**, J. W. Beeman, L. H. Hess, C. Wang, C. Zhu, S. Gul, J. Yano, C. Kisielowski, A. Schwartzberg, I. D. Sharp*, *A multifunctional biphasic water splitting catalyst tailored for integration with high performance semiconductor photoanodes*, Nat. Mater. 2017, 16, 335-341 [\[DOI\]](#);
31. **M. Favaro**, B. Jeong, P. N. Ross, J. Yano, Z. Hussain, Z. Liu*, E. J. Crumlin*, *Unravelling the electrochemical double layer by direct probing of the solid/liquid interface*, Nat. Commun. 2016, 7, 12695 [\[DOI\]](#);
30. H.-J. Lewerenz*, M. F. Lichterman*, M. H. Richter, E. J. Crumlin, S. Hu, S. Axnanda, **M. Favaro**, W. S. Drisdell, Z. Hussain, B. S. Brunschwig, Z. Liu, A. Nilsson, A. T. Bell, N. S. Lewis*, D. Friebe, *Operando analyses of solar fuels light absorbers and catalysts*, Electrochim. Acta 2016, 211, 711-719 [\[DOI\]](#);
29. C. Rüdiger*, **M. Favaro**, C. Valero-Vidal, L. Calvillo, N. Bozzolo, S. Jacomet, J. Hein, L. Gregoratti, M. Amati, S. Agnoli, G. Granozzi, J. Kunze-Liebhäuser*, *Ti substrate grain dependent C/TiO₂ composites through carbothermal treatment of anodic TiO₂*, Phys. Chem. Chem. Phys. 2016, 18, 9220-9231 [\[DOI\]](#);

28. S. Agnoli*, **M. Favaro**, *Doping graphene with boron: a review of synthesis methods, physicochemical characterization, and emerging applications*, J. Mater. Chem. A 2016, 4, 5002-5025 (The paper has been marked as HOT by Journal of Materials Chemistry A in 2016 as recommended by referees. Within the top 30 most cited articles published in Journal of Materials Chemistry A in 2016) [\[DOI\]](#);
27. G. D. Nguyen, F. M. Toma, T. Cao, Z. Pedramrazi, C. Chen, D. J. Rizzo, T. Joshi, C. Bronner, Y.-C. Chen, **M. Favaro**, S. G. Louie, F. R. Fischer, M. F. Crommie*, *Bottom-up synthesis of N=13 sulfur-doped graphene nanoribbons*, J. Phys. Chem. C 2016, 120, 2684-2687 [\[DOI\]](#);
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24. **M. Favaro**, G. Rizzi, S. Nappini, E. Magnano, F. Bondino, S. Agnoli, G. Granozzi*, *A synchrotron-based spectroscopic study of the electronic structure of N-doped HOPG and PdY/N-doped HOPG*, Surf. Sci. 2016, 646, 132-139 (invited paper on a special issue in honor of R. Lambert) [\[DOI\]](#);
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 3. M.Cattelan, S. Agnoli, **M. Favaro**, D. Garoli, F. Romanato, M. Meneghetti, A. Barinov, P. Dudin, G. Granozzi, *Microscopic view on a chemical vapor deposition route to boron-doped graphene nanostructure*, *Chem. Mater.* 2013, 25, 1490-1495 [DOI];
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1. **M. Favaro**, Z. Liu, E. J. Crumlin, *Ambient-Pressure X-ray Photoelectron Spectroscopy to Characterize the Solid/Liquid Interface: Probing the Electrochemical Double Layer*, *Synchrotron Radiation News* 2017, 30, 38-40 [\[DOI\]](#).