Project No. NMP4-CT-2004-001594

Project acronym: GSOMEN

Project Title:
Growth and Supra-Organization of Transition and Noble Metal Nanoclusters

Instrument: STREP

Thematic Priority:
Nanotechnologies and nanosciences, knowledge-based multifunctional materials and new production processes and devices (NMP)

Publishable Final Activity Report

Period covered from 01/10/2004 to 30/09/2007 Date of preparation: 30/10/2007

Start date of the project: 01/10/2004 Duration: 36 months

Project coordinator name: Alessandro Fortunelli

Project coordinator organization name:
Consiglio Nazionale delle Ricerche – Istituto per i Processi Chimico-Fisici (CNR-IPCF)

Revision 1

Dissemination Level: CO

EUROPEAN COMMISSION

Community Research

GSOMEN
PUBLISHABLE EXECUTIVE SUMMARY

NMP Priority: Nanotechnologies and nanosciences, knowledge-based multifunctional materials and new production processes and devices

Self-organization and self-assembling
Expanding knowledge in site-dependent phenomena.

GSOMEN[1] is a Specific Targeted Research Project[2] funded by the EC which addresses the development of new materials (specifically, transition and noble metal nanoclusters) through a thorough understanding of the mechanism of their growth and supra-organization in 1D, 2D, 3D super-structures. The project also involves research on general features of the relationships between structure and properties of these materials. The aim is to achieve control over the size, size distribution, morphology, and hence on the properties of metal nanoparticles and supra-lattices.

Metal nanoclusters are self-assembled particles less than 10–100 nm in diameter. Two classes of metal nanoclusters have been selected as the object of GSOMEN:

- supported on oxide surfaces, as obtained by metal vapour deposition under UHV
- coated by a layer of surfactants, as obtained in solution, and subsequently deposited an oxide surfaces.

These materials possess very appealing potential applications, which however still wait to be fully exploited because of the lack of knowledge, and hence lack of control, on their synthesis (the self-assembling and supra-organization processes). The aim of GSOMEN is to produce

[1] "Growth and Supra-Organization of transition and noble MEtal Nanoclusters" (Contract Number **:** NMP4-CT-2004-001594)

[2] Specific Targeted Research Project : EU's instrument designed to generate new knowledge in a particular research topic with the aim of improving or developing new products, processes or services.

this knowledge by combining the most advanced techniques in the experimental synthesis and characterization with the theoretical simulation of the structure, growth and properties of metal nanoclusters. The recent advances in these fields, at the synthetical level (also through the use of external fields), at the characterization level (see, e.g., synchrotron-related techniques), at the simulation level (advances in computer hardware, development of accelerated techniques in the study of dynamical processes), if properly coordinated, make this goal feasible, thus allowing one to achieve control and orientation on the fabrication of these materials. Information on the basic metal-support, metal-ligand and nanoparticle-nanoparticle interactions is derived from the interplay of calibrated experiments and first-principle calculations, and is used to build up appropriate inter-particle potentials. These potentials are utilised in molecular dynamics and kinetic Monte Carlo simulations of the various growth processes under realistic conditions, from which a direct comparison with actual growth experiments is immediately possible. The concluding part of the project is also dedicated to the study of general structure/property relationships, to bridge the link with scientific and technological applications.

This three-year project had a total estimated budget of about € 3 million of which € 2 million was funded by the EU. It has been completed in September 2007.

Potential impact

The possible applications of (supra)-self-assemblies of transition and noble metal nanoclusters are diverse, and many of them are fascinating. Among these, interesting applications are:

- quantum dots, of use in the miniaturization of electronic devices: the development of nanoscale single-electron transistors would increase the storage data capacity by a factor > 10^5
- magnetism: nanoscale ferromagnets to be used in the field of spintronics
- opto-electronic materials or linear wave-guides for the transport of electromagnetic energy
- chemical reactivity (sensors and catalysts): they are widely used in the modern car exhaust systems and as extremely sensitive gas sensors, and are proposed as a viable way to produce hydrogen from water
- polymer composites containing metal clusters with unusual optical, etc. properties
- biological labeling experiments: when coated with properly chosen organic materials, metal nanoclusters are proving very useful probes, due to their extreme sensitivity and low invasiveness, the latter related to the tiny quantity of matter to be introduced, and due to the possibility to chose the most bio-compatible metal elements and coatings among the possible ones

Socio-economic and policy objectives

Transition and noble metal nanoclusters can be environmentally friendly materials. With a proper choice of the type of metal and environment, the following advantages can be at hand: (a) the raw material is available at reasonable costs and without any foreseeable shortage for a long time; (b) as in most areas of nanotechnology, the consumption of the raw material in the production process is limited to the smallest possible amounts (limit of the miniaturization threshold); (c) the production processes are clean and the use of toxic substances can be minimized. For example, according to point (b) orders of magnitude “smart materials” with the same consumption of raw material as in conventional processes can be produced. This

addresses the NMP objective of an eco-compatible and sustainable technology and production processes and development.
The EU strategies requiring efforts to promote gender equality and to provide information for and to foster dialogue with society have also been taken into account.

Work performed and results achieved
The basic processes of growth have been thoroughly investigated (both experimentally and via theoretical simulations) as a function of temperature and synthetic conditions: diffusion of single atoms or small clusters in the case of bare metal clusters vs. ligand desorbing (with the presence of ancillary species such as reducing agents) in the case of solvated clusters, aggregation, nucleation and final possible agglomeration. The structure of the resulting particles has been elucidated as a function of their size, employing proper experimental and theoretical simulation tools. In the case of bare metal clusters, the interaction with defects on the oxide surfaces that act as nucleation centers and its influence on the structural evolution of the clusters has been explored, opening the way to the creation of surface magic clusters. Reactive channels (e.g., interfacial reactivity) have also been considered as a function of the choice of the specific metal-oxide or metal-ligand system. The novel phenomena that occur when the dimension of the oxide layer shrink to the nanoscale have also been pioneered (i.e., considering ultra-thin oxide films grown on metal supports as substrates for the deposition), such as charge transfer effects between the nanoclusters and the underlying metal support. This was directly linked to the theme of surface nanopatterning, as many of these novel ultra-thin oxide films exhibit reproducible patterns at nanometer lengths, and these patterns have been exploited to obtain regular arrays of nearly monodisperse metal particles. Several nanopatterning techniques have been explored: the creation of networks of interfacial dislocations, Moiré patterns, naturally nanostructured oxide surfaces, and nanofabrication and nanosculpting tools. The organization of these particles into supra-lattices has been studied in detail, and the conditions that allow the synthesis of extremely regular arrangements have been discovered. The catalytic, optical and magnetic properties of the single metal particles and those arising from their collective behavior have finally been investigated and in many cases fully rationalized. To pursue this research, the development of novel characterization tools and protocols at both the experimental and theoretical levels has been essential. This has allowed the groups involved in GSOMEN to obtain realistic images of a variety of systems with disparate sizes, shapes and morphologies, ranging from single or few-atom species to mesoscale assemblies of particles composed of thousand of atoms. The results have been published in a number of publications on high-impact scientific journals (the complete list is included in the project Web site). The synthesis, characterization and simulation protocols are available upon request to the scientific community.

Project Partners
The GSOMEN project represents a consortium of nine research centres and universities which pool expertise to achieve its objectives:

- ✓ IPCF - Consiglio Nazionale delle Ricerche, IT
- ✓ INFM - Consiglio Nazionale delle Ricerche, IT
- ✓ Université Pierre et Marie Curie, FR
- ✓ Centre National de la Recherce Scientifique, FR
- ✓ Commissariat à l' Energie Atomique, FR
- ✓ Universität Ulm, DE
- ✓ Max Planck Gesellschaft, DE
- ✓ Universität Graz, AT
- ✓ Technische Universität Münich, TUM

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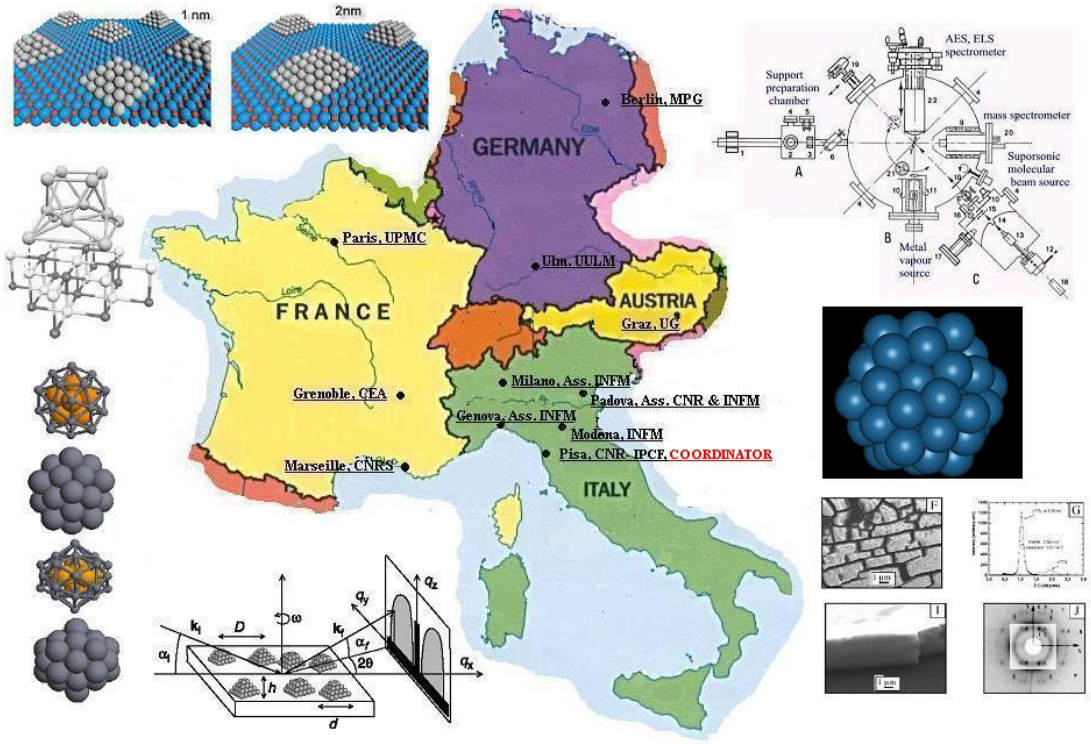
Project Web site

http://h2.ipcf.cnr.it/alex/gsomen.html



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Thematic Priority:
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Final plan for using and disseminating the knowledge

Due date of deliverable: 30/03/2007
Actual submission date: 30/10/2007

Start date of the project: 01/10/2004 Duration: 36 months

Organization name of lead contractor for this deliverable:
Consiglio Nazionale delle Ricerche – Istituto per i Processi Chimico-Fisici (CNR-IPCF)

Dissemination Level: PU

The outcome of GSOMEN research has continuously been monitored by the Dissemination and Communication Committee (DCC). Best media for dissemination has been appropriately chosen in each given case, with a strong bias toward publication on highly qualified scientific journals and presentations at international conferences – as it is natural given the basic-research, frontier-of-knowledge character of most of the activities pursued within the project. It is expected that the dissemination activity will continue in the future even after the end of the project.

Section 2 – Dissemination of knowledge

As most dissemination activities generated within GSOMEN are either publications on top-rank scientific journals or presentations at international conferences, attached is the list of publications and presentations divided according to each team leader of each research unit. The partner involved will thus be immediately apparent; the type of audience will be Research; the countries addresses will be potentially all, as international journals and conferences are invariably considered; as for the size of audience, we report the impact factor for publications. The medium (which journal or conference) where to present the research results has been chosen with the goal of achieving the largest dissemination impact, also following the suggestions of the DCC Committee.

Additionally, a European patent has been applied by CNR-ICCOM and a connected spin-off initiative is in an advanced stage, as described below under the appropriate item.

Along the direction of technological applications, it is foreseen that the partners will soon publish results or summary of the project on industry-related journals and magazines. Actions have already been taken to this effect.

List of publications and presentations

Unit 1

Publications

A. Fortunelli

Barcaro G., Fortunelli A., "The interaction of coinage metal clusters with the MgO(100) surface", *J. Chem. Theory Comput.*, 1 , 972 (2005) [IF NA]

Rapallo A., Rossi G., Ferrando R., Fortunelli A., Curley B. C., Lloyd L. D., Tarbuck G. M., Johnston R. L., "Global optimization of bimetallic cluster structures. I. Size-mismatched Ag-Cu, Ag-Ni, and Au-Cu systems", *J. Chem. Phys.*, 122, 194308 (2005) [IF 02.950]

Rossi G., Ferrando R., Rapallo A., Fortunelli A., Curley B. C., Lloyd L. D., Johnston R. L., "Global optimization of bimetallic cluster structures. II. Size-matched Ag-Pd, Ag-Au, and Pd-Pt systems", *J. Chem. Phys.*, 122, 194309 (2005) [IF 02.950]

Ferrando R., Fortunelli A., Rossi G., "Quantum effects on the structure of pure and binary metal nanoclusters", *Phys. Rev. B,* 72, 085449 (2005) [IF 02.962**]**

Ferrando R., Fortunelli A., Rossi G., "Quantum effects on the structure of pure and binary metal nanoclusters", *Virtual J. Nanosci. Nanotech.*, 12, Iss. 10 (2005) [IF NA]

Barcaro G., Fortunelli A., Nita F., Ferrando R., "Diffusion of palladium clusters on magnesium oxide", *Phys. Rev. Lett.*, 95, 246103 (2005) [IF 07.035]

Aprà E., Ferrando R., Fortunelli A., "Density-functional global optimization of gold nanoclusters", *Phys. Rev. B*, 73, 205414 (2006) [IF 03.185]

Barcaro G., Fortunelli A., "Rotational Invariance and Double Frustration in the Structures of Gold Clusters Growing around the F_s-Defected MgO (100) surface" *J. Phys. Chem. B*, 110, 21021 (2006) [IF 04.033]

Barcaro G., Fortunelli A., Rossi G., Nita F., Ferrando R., "Electronic and structural shell closure effects in AgCu and AuCu nanoclusters" *J. Phys. Chem. B*, 110, 23197 (2006) [IF 04.033]

Barcaro G., Fortunelli A., "Structure and diffusion of small Ag and Au clusters on the regular MgO (100) surface" *New J. Phys.*, 9, 22 (2007) [IF 3.585]

Paz-Borbon L. O., Johnston R. L., Barcaro G., Fortunelli A., "A Mixed Structural Motif in 34-Atom Pd-Pt Clusters" *J. Phys. Chem. C*, 111, 2937 (2007) [IF NA]

Barcaro G., Causà M., Fortunelli A., "A comparison between the Adsorption Properties of the Regular and F_s-defected MgO(100) Surface"
Theor. Chem. Acc., in press [IF 02.446]

Barcaro G., Aprà E., Fortunelli A., "Structure of Ag Clusters Grown on the F_s-defected MgO(100) Surface",
Chem. Eur. J., 13, 6408 (2007) [IF 05.015]

Barcaro G., Sedona F., Fortunelli A., Granozzi G., "The Structure of A TiO_x zigzag-like nanophase on Pt(111)"
J. Phys. Chem. C, 111, 6095 (2007) [IF NA]

Barcaro G., Fortunelli A., Rossi G., Nita F., Ferrando R., "Epitaxy, Truncations, and Overhangs in Palladium Nanoclusters Adsorbed on MgO(001)"
Phys. Rev. Lett., 98, 156101 (2007) [IF 07.072]

Barcaro G., Fortunelli A., "A study of bimetallic Cu-Ag, Au-Ag and Pd-Ag clusters adsorbed on a double-vacancy-defected MgO(100) terrace"
Faraday Discuss., in press [IF 04.731]

Barcaro G., Fortunelli A., "A Magic Pd-Ag cluster on the F_s-defected MgO(100) Surface"
J. Phys. Chem. C, 111, 11384 (2007) [IF NA]

Paz-Borbon L. O., Mortimer-Jones T. V., Johnston R. L., Posada-Amarillas A., Barcaro G., Fortunelli A., "Structure and energetics of 98-atom Pd-Pt nanoalloys: potential stability of the Leary Tetrahedron for Bimetallic Nanoparticles"
Phys. Chem. Chem. Phys., 38, 5202 (2007) [IF 02.892]

Ferrando R., Fortunelli A., Johnston R. L., "Searching for the optimum structures of alloy nanoclusters"
Phys. Chem. Chem. Phys., in press [IF 02.892]

Barcaro G., Fortunelli A., "Magic silver cluster on a MgO(100) surface with defects"
Phys. Rev. B, in press (2007) [IF 03.107]

Olivier S., Conte R., Fortunelli A., "Derivation of an empirical potential for gold with angular corrections"
Phys. Rev. B, submitted [IF 03.107]

Sedona F., Granozzi G., Barcaro G., Fortunelli A., "Defect structure and evolution in a titania nanophase"
Phys. Rev. B, submitted [IF 03.107]

Barcaro G., Fortunelli A., Barretta G., Evangelisti C., Salvadori P., "Experimental and computational studies of the diffusion of Pt complexes in C_6D_6"
Chemical Physics, in preparation [IF 01.984]

Barcaro G., Fortunelli A., "Density-functional global optimization of Pt complexes with unsaturated ligands",
Chem. Phys. Lett., in preparation [IF 02.462]

Barcaro G., Kuntova Z., Mottet C., Nita F., Rossi G., Ferrando R., Fortunelli A., "Computational study of the stable structural motifs of Ag, Au, Pd and Pt clusters on MgO(100)",
J. Chem. Phys., in preparation [IF 03.166]

G. Vitulli

F. Balzano, A. Cuzzola, P. Diversi, F. Ghiotto, G. Uccello Barretta, "Cationic Gold(I) Phosphanyl Thiolates: Aurophilic Interactions in the Solid State and in Solution", European Journal of Inorganic Chemistry, *accepted* [IF 2.704].

C. Evangelisti, P. Raffa, F. Balzano, G. Uccello Barretta, G. Vitulli, P. Salvadori, "Size-Controlled Synthesis and NMR Characterization of Mesitylene - Vinylsiloxanes Stabilized Pt Nanoparticles in Solution", Journal of Nanosci. and Nanotechnol., *in press* [IF 2.194].

Barcaro G., Fortunelli A., Barretta G., Evangelisti C., Salvadori P., "Experimental and computational studies of the diffusion of Pt complexes in C_6D_6"
Chemical Physics, in preparation [IF 01.984]

Patents:

G. Vitulli, C. Evangelisti, F. Ciardelli, P. Salvadori, F. Rocchi, "Pt-containing hydrosilylation catalyst, its preparation and use in the crosslinking of organosilicon compounds" European Patent Application, EP 1 797 949, (2007)

Spin-off:

The procedure for a spin-off initiative based on the above Patent has been initiated and is at an advanced stage.

Presentations:

A. Fortunelli

Barcaro G., Fortunelli A., "The interaction of coinage metal clusters with the MgO(100) surface", Poster,
MMD Meeting, Genova, June 22^{th} – 25^{th} 2005 .

Barcaro G., Fortunelli A., "Diffusion of palladium clusters on magnesium oxide", Poster,
Workshop on Surface Nanopatterning, Tirrenia (Pisa), June 30, July 1^{st} 2005

Barcaro G., Fortunelli A., "DFT study of the interaction of small coinage metal clusters and extended depositions with the regular and defected MgO(100) surface", Poster,
Summer School on Self-Organised Nanostructures, Cargese (Corsica), July 17^{th} – 2^{th} 2005

Barcaro G., Fortunelli A., "Metal-oxide potentials: the Pd-MgO case study", Talk,

CECAM Workshop on Ab Initio Meets Classical Simulations: The Development of Empirical Potentials for Atomistics Systems, Lion (France), October 17th – 19th 2005

Fortunelli A., "Design and growth of deposited metal nanoclusters", Invited Lecture,
Self-Organized NanoStructures (SONS) – Conference, Pisa (Italy), June 29th – July 1st 2006

Barcaro G., Aprà E., Fortunelli A., "Density-functional global optimization studies of coinage metal clusters on the regular and defected MgO(100) surface", Poster,
Self-Organized NanoStructures (SONS) – Conference, Pisa (Italy), June 29th – July 1st 2006

Fortunelli A., "First-principles and empirical approaches to metal-containing systems", Two Lectures at
Summer School on Metal Clusters and Surfaces, Pisa (Italy), July 2nd – 6th 2006

Barcaro G., Aprà E., Fortunelli A., "A study of structure and diffusion of coinage metal clusters deposited on the regular and defected MgO(100) surface", Poster,
Summer School on Metal Clusters and Surfaces, Pisa (Italy), July 2nd – 6th 2006

Paz O., Barcaro G., Johnston R. L., Fortunelli A., "DFT studies on 34-atom Pd-Pt nanoclusters",
Summer School on Metal Clusters and Surfaces, Pisa (Italy), July 2nd – 6th 2006

Fortunelli A., "Density-functional global optimization of metal clusters supported on the regular and F_s-defected MgO(100) surface: A study of their structure and growth", Talk,
V International Workshop on Oxide Surfaces (IWOX-V), Lake Tahoe, CA (USA), January 7th – 12th 2007

Fortunelli A., "Nucleation and growth of deposited metal nanoclusters", Talk,
Workshop on Self-Organised NanoStructures (SONS), Strasbourg (France), May 31st – June 1st , 2007

Barcaro G., Fortunelli A., "Metal clusters on the regular and defected MgO(100) surface: a theoretical study of their structure and growth", Poster,
Workshop on Self-Organised NanoStructures (SONS), Strasbourg (France), May 31st – June 1st , 2007

Fortunelli A., Barcaro G., Monti S., Sedona F., Granozzi G., "Nanopatterned oxide surfaces as templates for biological growth", Poster,
ESF-EMBO Symposium Conference on Biological Surfaces and Interfaces, Saint Feliu de Guixols (Spain), July 1st – 6th 2007

Conte R., Fortunelli A., Barcaro G., Monti S., Sedona F., Granozzi G., "Nanopatterned oxide surfaces as templates for biological growth", Poster,
3rd International Symposium on Theoretical Biophysics (TheoBio07), Cetraro (Italy), June 16th – 20th 2007

Fortunelli A., "A study of bimetallic Cu-Ag, Au-Ag and Pd-Ag clusters adsorbed on a double-vacancy-defected MgO(100) terrace", Invited Talk at
Faraday Discussion 138, Nanoalloys: From Theory to Applications, Birmingham (UK), September 3rd – 5th 2007

Barcaro G., Fortunelli A., "A magic Pd-Ag binary cluster adsorbed on the F_s-defected MgO(100) surface", Poster,
Faraday Discussion 138, Nanoalloys: From Theory to Applications, Birmingham (UK), September 3rd – 5th 2007, awarded the Skinner Prize

Posada-Amarillas A., Paz-Borbon L. O., Mortimer-Jones T. V., Johnston R. L., Barcaro G., Fortunelli A., "Computational Studies of the Structures and Energetics of PdPt Nanoalloy Clusters of 98 and 100 Atoms", Poster,
Faraday Discussion 138, Nanoalloys: From Theory to Applications, Birmingham (UK), September 3rd – 5th 2007

Paz-Borbon L. O., Johnston R. L., Barcaro G., Fortunelli A., "Structural motif competition and segregation effects in 38-atom binary clusters", Poster,
Faraday Discussion 138, Nanoalloys: From Theory to Applications, Birmingham (UK), September 3rd – 5th 2007

Fortunelli A., "Density-functional global optimization of pure and binary metal clusters supported on the regular and F_s-defected MgO(100) surface: A study of their structure and growth", Invited talk,
University of Leicester, September 5th 2007

Barcaro G., "DFT study of bimetallic nanoclusters on defected MgO(100) surfaces and of ultra-thin TiO_X/Pt(111) films", Invited talk,
King's College London, September 5th 2007

Fortunelli A., "Theoretical studies of metal clusters on oxide surfaces", Invited Talk,
Annual Meeting 2007 of the COST Action D41: Inorganic oxides: Surfaces and Interfaces, Berlin (Germany), October 21st – 23rd 2007

G. Vitulli

C. Evangelisti, P. Raffa, G. Vitulli, P. Pertici, F. Balzano, G. Uccello Barretta, P. Salvadori, "Metal Nanoclusters in Catalysis: Size Control of Platinum Particles"; "GIC 2007", XV National Congress of Catalysis" 10-14 June 2007, Tirrenia (Pisa), Abstract O 30.

G. Vitulli, C. Evangelisti, G. Uccello Barretta, F. Balsano, P. Salvadori, .Armelao, E. Tondello, "Size Tailored Materials: the role of organic stabilizerson the metal aggregation from atoms to clusters and colloids", SAMIC 2004: "Trends in Nanoscience", Bressanone (BZ) 5 – 7 December 2004, Abstract L6.

G. Vitulli, C. Evangelisti, M. Vitulli, A: M. Caporusso, P. Pertici, S. Bertozzi, P. Salvadori, "Nanostructured Metal Catalysts in Fine ChemicalSynthesis", "VIII Italian Seminar on Catalysis 2005", Verbania-Pallanza, 19-24June 2005, p. 207.

Unit 2

Publications:

S. Valeri

A. Ferrari, S. Casassa, C. Pisani, S. Altieri, A. Rota, S. Valeri, "Polar and non-polar domain borders in MgO ultrathin films on Ag(001)",
Surf. Sci. 588, 160-166 (2005). [IF 02.063]

P. Luches, S. Benedetti, M. Liberati, F. Boscherini, I.I. Pronin and S. Valeri, "Absence of oxide formation at the Fe/MgO(001) interface",
Surf. Sci. 583, 191-198 (2005). [IF 02.063]

S. Benedetti, P. Luches, M. Liberati, S. Valeri, “Chemical reactions and interdiffusion at the Fe/NiO(001) interface”,
Surf. Sci. Lett., 572 (2004) L348-L354. [IF 02.063]

S. Colonna, P. Luches, S. Valeri, F. Boscherini, “The Fe/NiO interface studied by polarization dependent X – ray absorption spectroscopy”,
Nuclear Instruments and Methods in Physics Research B 246 (2006) 131-135 [IF 01.041]

S. Benedetti, P. Torelli, P. Luches, A. Rota, S. Valeri, “Morphology and chemical activity at the Au/NiO interface”,
Surf. Sci, 600, 4251-4255 (2006) [IF 02.063]

A. Rota, S. F. Contri, G. C. Gazzadi, S. Cottafava, S. Valeri, “Focused Ion Beam induced swelling in MgO(001)”,
Surf. Sci. 600, 3718-3722 (2006) [IF 02.063]

P. Luches, V. Bellini, S. Colonna, L. Di Giustino, F. Manghi, S. Valeri, F. Boscherini, “Iron oxidation, interfacial expansion and buckling at the Fe/NiO(001) interface”,
Phys. Rev. Lett., 96, 106106 (2006). [IF 07.035]

S. Benedetti, H.M. Benia, N. Nilius, S. Valeri, H.J. Freund, “Morphology and optical properties of MgO thin films on Mo(001)”,
Chem. Phys. Lett. 430, 330-335 (2006) [IF 02.438]

S. Benedetti, P. Torelli, P. Luches, E. Gualtieri, A. Rota and S. Valeri, “Preparation and characterization of MgO stepped surfaces”,
Surf. Sci., 601, 2636-2640 (2007) [IF 02.063]

P. Torelli, E. A. Soares, G. Renaud, S. Valeri, X. X. Guo and P. Luches, “Nano-structuration of CoO film by misfit dislocations”,
Surf. Sci., 601, 2651-2655 (2007) [IF 02.063]

S. Valeri, S. Benedetti and P. Luches, "Metals on oxides: structure, morphology and interface chemistry",
J. Phys.: Condens. Matter 19, 225002 (2007) [IF 02.145]

P. Luches, P. Torelli, S. Benedetti, E. Ferramola, R. Gotter, S. Valeri, “Structure and electronic properties of Fe nanostructures on MgO(001)”,
Surf. Sci. 601, 3902-3906 (2007) [IF 02.063]

S. Colonna, F. Ronci, A. Cricenti, P. Luches, S. Valeri, J. Qi, Y. Xu, J.K. Miller, and N. Tolk, “Ferromagnetic-Antiferromagnetic Fe/NiO(100) interface studied by non-linear Kerr effect”, Surf. Sci. 601, 4362-4365 (2007).

P. Torelli, E. A. Soares, G. Renaud, L. Gragnaniello, S. Valeri X. Guo and P. Luches. “Self-organized growth of Ni clusters on a cobalt-oxide thin film induced by a buried misfit dislocation network”, Appl. Phys. Lett. Submitted [IF 03.977]

P. Luches, A. di Bona, S.F. Contri, G.C. Gazzadi, P. Valvassori, F. Alberini, F. Casoli, L. Nasi, S. Fabbrici, S. Valeri “Arrays of metal nanostructures produced by focussed ion beam” submitted to Acta Physica Polonica.

A. Wörz, K. Judai, S. Abbet, U. Heiz, A. Del Vitto, L. Giordano, G. Pacchioni, "Chemistry on single atoms: Key factors for the acetylene trimerization on MgO supported Rh, Pd, and Ag atoms", *Chemical Physics Letters*, 399, 266-270 (2004). [IF 02.438]

L. Giordano, G. Pacchioni, "Pd nanoclusters at the MgO(100) surface", *Surface Science*, 575, 197-209 (2005). [IF 02.063]

K. Judai, A. Wörz, S. Abbet, U. Heiz, A. Del Vitto, L. Giordano, G. Pacchioni, "Acetylene trimerization on Ag, Pd, and Rh atoms deposited on MgO thin films", *PCCP - Physical Chemistry Chemical Physics*, 7, 955-962 (2005). [IF 01.959]

A. Del Vitto, L. Giordano, G. Pacchioni, U. Heiz, "Cluster and periodic DFT calculations of MgO/Pd(CO) and MgO/Pd$(CO)_2$ surface complexes", *J. of Physical Chemistry B*, 109, 3416-3422 (2005). [IF 03.679]

A. Del Vitto, G. Pacchioni, F. Delbecq, P. Sautet, "Au atoms and dimers on the MgO(100) surface: a DFT study", *J. of Physical Chemistry B*, 109, 8040-8048 (2005). [IF 03.679]

L. Giordano, D. Ricci, G. Pacchioni, P. Ugliengo, "Structure and vibrational spectra of crystalline SiO_2 ultra-thin films on Mo(112)", *Surface Science*, 584, 225-236 (2005) [IF 02.063].

G. Pacchioni, L. Giordano, M. Baistrocchi, "Charging of metal atoms on ultra-thin MgO/Mo(100) films", *Physical Review Letters*, 94, 226104-4 (2005). [IF 07.035]

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Presentations:

S. Valeri

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S. Benedetti, et al., "Preparation pf MgO stepped surfaces for metallic nanowires growth" (poster), Fourth International Workshop on Oxide Surfaces (IWOX-4) Torino University, Torino Italy and Centre Paul Langevin, Aussois, France, 04-08 January 2005.

S. Valeri, "Metals on oxides: from epitaxy to nanofabrication" (invited), Joint Physics Colloquium, Karl-Franzens-University and Technical University of Graz, Graz, 18 January 2005.

S. Valeri, Micro-nano structures in metal-oxide systems (invited), NIS Colloquia "Nanostructured Oxide Surfaces", Torino (Italy), February 17, 2005.

S. Colonna, P. Luches, S. Valeri, and F. Boscherini, "The Fe/NiO interface studied by polarization dependent X – ray absorption spectroscopy" (poster), E-MRS 2005 Spring Meeting. May 31 – June 3, 2005, Strasbourg (France)

S. Benedetti, et al., "Interfacial reactivity and morphology at the Au/NiO(001) interface" (poster), Matter, Materials and Devices Meeting, Genova (Italy) 22-25 June 2005.

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P. Luches , “Fe local atomic environment at the Fe/NiO(001) interface studied by polarization dependent XAS” (oral), XIII Meeting of the Italian Society for Synchrotron Radiation, Modena (Italy) 7 - 9 July 2005.

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L. Gragnaniello: “Fabrication and morphological characterization of metal nanoclusters” (poster), Pisa school on Metal clusters and Surfaces, Pisa (3-6 July 2006), Italy

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Luches P.. et al. “The Fe/NiO(001) epitaxial interface” (poster), ESRF User Meeting, Nano-scale materials: growth - dynamics - magnetism at ESRF, 6-8 February 2007, Grenoble

L. Gragnaniello et al., poster presentation at "inorganic oxide surfaces and interfaces" COST 21 meeting, march 29-30, London, poster title: "Nanopatterned metal-oxide surfaces: templates for nanoparticles self assembling"

A. Rota, et al. STM and XPS study of ultra-thin epitaxial NiO(001) films grown on Ag(001) by atomic oxygen" (poster), (IVC-17) (ICSS-13) (ICN+T2007) July 2-6, 2007 Stockholm, Sweden

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G. Pacchioni

G. Pacchioni, "Charging of metal atoms on oxide surfaces and thin films: mechanisms and consequences" (invited), WATOC 2005 - 7th Congress of the World Association of Theoretically Oriented Chemists, Cape Town (Sud Africa), 17 gennaio 2005.

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G. Pacchioni, “Charge transfers at metal-oxide interfaces” (invited), Satellite Workshop Computer Simulation of Surface and Interface Phenomena, Sinctrotrone Trieste, Trieste, 16 dicembre 2005.

G. Pacchioni, “CO on MgO: the story of 20 years of interplay between theory and experiment” (invited), Workshop: A day of science dedicated to Prof. A. Zecchina, Torino, 23 giugno 2006.

G. Pacchioni, “The unusual structure of Au clusters on MgO/Mo(100) films”, Workshop on Supported Metal Clusters, Technical University of Munich, Garching (Germania), 6 luglio 2006.

G. Pacchioni, “The unusual chemical properties of Au atoms and clusters deposited on ultra-thin oxide films” (invited), Workshop Microelectronics Meets Catalysis: Innovative Oxide Materials, Hanse Institut for Advanced Studies, Delmerhost (Germania), 21 Luglio 2006.

G. Pacchioni, “Au atoms and clusters deposited on oxide surfaces or ultra-thin films: unusual properties” (invited), XIII ISSPIC - International Symposium on Small Particles and Inorganic Clusters, Gotheborg (Svezia), 27 luglio 2006.

G. Pacchioni, “Metal atoms and clusters on oxide supports: chrage transfers at metal-oxide interfaces” (invited), Institut für Angewandte Physik Sensorik, Brandemburg Technishe Universität Cottbus, Cottbus (Germania), 22 agosto 2006.

G. Pacchioni, “The nature of paramagnetic centers in oxide materials from EPR measurements and quantum chemical calculations” (invited), Darmstadt Technical University Eduard-Zintl Institute, Darmstadt (Germany), 28 agosto 2006.

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G. Pacchioni, “Metal nano-clusters on oxide surfaces from self-aggregation of deposited metal atoms: a new approach to understand catalysis by supported particle”, European Doctorate in Physics and Chemistry of Advanced Materials – Course on self-assembled materials, Università Milano-Bicocca, Milano, 19 settembre 2006.

G. Pacchioni, “Theory of oxide surfaces: from supported metals to photocatalysis” (invited), Workshop on Catalysis and Surface Science, Santa Barbara (California, USA), 14 Dicembre 2006.

G. Granozzi

Fourth International Workshop on Oxide Surfaces (IWOX-4), January 04 to January 08 2005, Torino University, Torino Italy (Tuesday) And Centre Paul Langevin, Aussois France, Oral Presentation
"Reactive deposition of NiO ultrathin films on Pd (100): an overview",
T. Orzali, S. Agnoli, M. Sambi and G. Granozzi

Invited plenary lecture of Gaetano Granozzi, X-th Symposium on Surface Physics July 10 - 15, 2005 Prague, Czech Republic
Preparation and structure of oxide nanostructures on metal single crystals

Invited lecture of Gaetano Granozzi, at the Instituto de Ciencia de Materiales de Sevilla (CSIC-Univ. Sevilla), October 14 2005,
Preparation and structure of oxide nanostructures on metal single crystals

Invited plenary lecture of Gaetano Granozzi, ASEVA Summer School – 2005, WS-17: *Structure, Characterisation and Reactivity of TiO_2,* Avila (Spain) july 24-26 , 2005
Preparation and characterization of well ordered TiOx nanostructures on Pt(111)

Lecture of Gaetano Granozzi at the Summer School on Metal Clusters and Surfaces, Tirrenia, 3-6 july 2006,
Nanostructured oxide films as possible templates for cluster growth

ECOSS 24 , 4-8 september 2006, Paris (France)
Poster presentation:
Ultrathin Wagon-Wheel-Like TiO_X Phases on Pt(111): A Leed and STM Investigation
Sedona F, Agnoli S, Granozzi G

ECOSS 24 , 4-8 september 2006, Paris (France)
Oral presentation:
Core and Valence Band Photoemission and X-Ray Absorption Sectroscopy of Ultrathin Titanium Oxide Films on Pt(111)
Finetti, Sedona F, Rizzi GA, Mick U, Schierbaum K, Sutara F, Matolin V, GranozziI G

Invited plenary talk of Prof. Granozzi : *TiO_x Nanostructures on Pt(111) and Pt(110) Substrates: a Combined LEED, Photoemission, STM and Theoretical Investigation*
at the International Workshop on OXide surfaces (IWOX V, Lake Tahoe, USA, 7-12 january 2007).

Invited talk of prof. Granozzi : *TiO_x nanostructures on Pt(111) and Pt(110) substrates: a combined experimental and theoretical investigation*
at the meeting of the COST action D41/ Inorganic oxide surfaces and interfaces (Vienna/Austria, November 2-4, 2006)

Invited talk of prof. Granozzi : *Nanolayers of TiO_x on Pt substrates: a combined LEED, Photoemission, STM and theoretical investigation*
at the Workshop on the Reactivity and Stability of Surfaces and Nano Particles at Elevated Temperatures (Kloster Irsee , Germany, 27-30 september 2006).

Invited talk of prof. Granozzi : *Ordered defects on oxide surfaces as preferential nucleation sites for metal cluster growth*
at the meeting of the COST action D41/ Inorganic oxide surfaces and interfaces (London/UK, March 29-30, 2007)

Invited talk of prof. Granozzi : *Recent advances on titania nanostructures on metals*
at the meeting of the COST action D41/ Inorganic oxide surfaces and interfaces (Barcellona/Spain, May 10-12, 2007)

VI Convegno Nazionale sulla Scienza e Tecnologia dei Materiali, Perugia, 12 - 15 Giugno 2007
Oral Contribution of Gaetano Granozzi: *TiO_x nanostructures on a monocrystalline Pt substrate*

R. Ferrando

G. Barcaro, A. Fortunelli, C. Mottet, G. Rossi, F. Nita and R. Ferrando "Structure and diffusion of small Pd clusters on the MgO(001) surface",
MMD Meeting, Genova July 22-25 2005.

F. Nita G. Rossi, R. Ferrando, C. Mottet, G. Barcaro, A. Fortunelli, "Structure and diffusion of Pd clusters on the MgO(001)",
23rd European Conference on Surface Science (ECOSS23), Berlin September 4-9 2005

F. Nita, G. Rossi, R. Ferrando, G. Barcaro, A. Fortunelli, ``Structure of Pd, Ag, Ni and Au clusters on MgO(001)", IWTF2 conference, Prague June 26-29, 2006 (invited)

G. Rossi and R. Ferrando ``Global optimization by excitable walkers", ISSPIC 13 conference, Goteborg, July 24-28 (2006).

G. Rossi, R. Ferrando, C. Mottet, G. Barcaro, A. Fortunelli, "Magic structures of binary metallic clusters", ISSPIC 13 conference, July 24-28 (2006).

Ferrando R., "Structure and growth of alloy nanoclusters", Invited Talk,
American Chemical Society Meeting, Chicago (USA), March 25th – 29th 2007

Rossi G., "Computational study of Au and Pd clusters on MgO(100)",
Workshop on Nanopatterning via Ions, Photon beam and Epitaxy, Sestri Levante (Italy), September 23th – 27th 2007

Kuntova Z., Rossi G., Ferrando R., "Study of small Ag/MgO(100) and AgPd/MgO(100) clusters",
Faraday Discussion 138, Nanoalloys: From Theory to Applications, Birmingham (UK), September 3rd – 5th 2007

Ferrando R., "Determining the structures of gas-phase and surface supported nanoclusters: a computational approach", Invited Talk,
III International Physics Congress, Hermosillo, Sonora (Mexico), October 10th – 12th 2007

Unit 3

Publications

N. Nilius, H.-M. Benia, C. Salzemann, G. Rupprechter, H.-J. Freund, A. Brioude, M.-P. Pileni "Light Emission Spectroscopy of Self-Assembly Arrays of Silver Nano-Crystals with the STM.",
Chem. Phys. Letters 413, 10 (2005)

M.P. Pileni, ""Reverse micelles used as templates: a new understanding in the nanocrystals growth of silver and copper nanocrystals by using hydrazine as reducing agent.",

Journal of Experimental Nanoscience 2006, 1, 13-27 [IF NA]

J. Wikander, C. Petit, K. Holmberg, and M.P. Pileni,"Size control and growth process of alkylamine-stabilized platinum nanocrystals: a comparison between the phase transfer and reverse micelles methods",
Langmuir (2006) on the web 29 march 2006 [IF 3.295]

M. P. Pileni, "Self organization of inorganic nanomaterials",
J. Phys. Cond. Mat., 18, S67-S84, (2006)

I. Lisiecki, D. Parker, C. Salzemann and M.P. Pileni, "A new intrinsic magnetic property due to the mesoscopic ordering of cobalt nanocrystals in supra-crystals",
The Open Physical Chemistry Journal 1, 5, 2007

I. Lisiecki, D. Parker, C. Salzemann and M.P. Pileni, "Fcc supra-crystals and disordered 3D assemblies of 7.5 nm cobalt nanocrystals: Influence of the mesoscopic ordering on the magnetic properties",
Chem. Mat., 19, 4030, 2007

I. Lisiecki, C. Salzemann, D. Parker, P.A. Albouy and M.P. Pileni, "Emergence of new collective magnetic properties of cobalt nanocrystals ordered in fcc supra-crystals: I- Structural investigation",

J. Phys. Chem. 111, 12625, 2007

D. Parker, I. Lisiecki, C. Salzemann and M.P. Pileni, "Emergence of new collective magnetic properties of cobalt nanocrystals ordered in fcc supra-crystals: II- Magnetic investigation",
J. Phys. Chem. C, 111, 12632, 2007

K. Naoe, C. Petit and M. P. Pileni
From worm-like to spherical palladium nanocrystals: Digestive ripening
J.Phys.Chem.C in press

Presentations:

Christophe Petit (invited talk), "Collective Magnetic Properties of Mesostructure made of cobalt Nanocrystals",
Workshop on surface nanopatterning Pisa , Italy, 30/6 /05-1/07/05

Christophe Petit (invited talk),""Self-organization of Inorganic Nanocrystals",
Nana-X-2, Nanoscience with Nanocrystals 7-10 January 2006 Autrans , France

Marie-Paule Pileni (invited talk) " Metal Nanoparticles from Reverse Micelles"
School on Metal Clusters and Surfaces, Pisa, Italy, 3/07/06-6/07/06

Marie-Paule Pileni (invited talk) "Self organization of inorganic nanocrystals"
The Jubilee Nanotechnology Symposium Israel

Marie-Paule Pileni (invited talk) "Self organization of organic and inorganic materials"
SIS 2006 Seoul

Marie-Paule Pileni (invited talk) "Self organization of inorganic nanocrystals"
ISSPIC 13, Goteborg July 2006

Marie-Paule Pileni (invited talk) “Self organization of inorganic nanocrystals: Fabrication and properties”
European Colloid and Interface Society Budapest (2006)

Marie-Paule Pileni (invited talk) “Self organization of inorganic nanocrystals”
Self assembly and Properties of complex Patterns Portonoz Slovenia 3-6 September 2006

A. Demortières and C. Petit “Simple chemical synthesis of CoPt magnetic alloy nanocrystals”(Poster)
School on Metal Clusters and Surfaces, Pisa, Italy, 3/07/06-6/07/06

Anne-Isabelle Henry, Alexa Courty, Pierre-Antoine Albouy and Marie-Paule Pileni “Crystal growth of self-assmbled silver nanocrystals” (Poster)
School on Metal Clusters and Surfaces, Pisa, Italy, 3/07/06-6/07/06

Anne-Isabelle Henry, Herbert Wormeester, Stefan Kooij, Bene Poelsema, Marie-Paule Pileni “Ellipsometric identification of collective optical properties of silver nanocrystals arrays”
School on Metal Clusters and Surfaces, Pisa, Italy, 3/07/06-6/07/06

Network for “Crystal growth and nucleation of complex materials : Linking experiment and theory”, Reading, Angleterre (2005)
“2D and 3D organizations of Co and Ag nanocrystals obtained either with or without an applied magnetic field”
I.Lisiecki

Nato Nanotechnology Research Forum Ankara (2006)
“Self organization of inorganic nanocrystals”
M.P. Pileni

International worshop Nanomagnets by self organization, Eisenerz, Austria
“Self organization of inorganic nanocrystals: Ordering effect on the mesoscopic structure and magnetic properties”
M.P. Pileni

International worshop on nanostructured materials Nanomat 2006, Antalya Turkey
“Self organization of inorganic nanocrystals”
M.P. Pileni

Functional Chemistry dedicate to Krister Holmberg, Chalmers, 2006
“Self assembly of nanocrystals”
M.P. Pileni

7^{th} annual surface and colloid symposium: Nanostructure from self assembly-in solution at interfaces and as synthetic tool. Sweeden (2007)
“Self ornanization of inorganic materials”
M.P. Pileni

Hamano-Kobe International Symposium on “Laser and Nano/Bio Sciences”
self organization of Inorganic Nanocrystals: Emergence of a New Physic.,
M.P. Pileni

Unit 4

Publications:

R. Henry

C. Barth, C.R. Henry;"High resolution imaging of gold clusters on KBr(100) surfaces investigated by Dynamic Scanning Force Microscopy",
Nanotechnology 15(2004)1264-1272 [IF 02.304]

S. Sao-Joao, S. Giorgio, C. Chapon, S. Bourgeois, J.M. Penisson, C.R. Henry, "Structure and deformations of Pd-Ni core-shell nanoparticles ",
J. Phys. Chem B 109(2005)342 [IF 03.679]

O. Meerson, G. Sitja, C.R. Henry; "Low temperature and low pressure CO oxidation on gold clusters supported on MgO(100)",
Eur. Phys. J. D 34(2005)119-124 [IF 01.612]

C. Barth, C. Claeys, C.R. Henry; "Surface preparation of hard ionic crystals by UHV cleavage",
Rev. Sci. Intrum. 76(2005)083907 [IF 01.343]

C.R. Henry, "Morphology of Supported Nanoparticles",
Prog. Surf. Sci. 86(2005)92-116 [IF 03.744]

O.H. Pakarinen, C. Barth, A.S. Fosters, R.M. Nieminen, C.R. Henry; "High resolution atomic force microscopy of gold nanoclusters on the KBr (001) surface",
Phys. Rev. B 73(2006)235428 [IF 02.962]

C. Barth, C.R. Henry; "Kelvin probe force microscopy on surfaces of UHV-cleaved ionic crystals",
Nanotechnology; 17(2006)S155-S161 [IF 02.304]

C. Barth, O. Pakarinen, A. Foster, C. R. Henry; "Imaging nanoclusters in the *constant height mode* of the dynamic SFM",
Nanotechnology; 17(2006)S128-S136 [IF 02.304]

G. Hamm, C. Becker, C.R. Henry, "Pd-Au nanocluster arrays grown on nanostructured alumina templates",
Nanotechnology 17(2006)1943-1947 [IF 02.304]

S. Giorgio, S. Sao-Joao, S. Nitsche, D. Chaudenson, C.R. Henry; "Environmental electron microscopy (ETEM) for catalysts with a closed E-cell with carbon windows"
Ultramicroscopy 106(2006)503-507 [IF 2.215]

S. Sao Joao, S. Giorgio, C. Mottet, J. Goniakowski, C.R. Henry; "Interface structure of Ni nanoparticles on MgO(100): a combined HRTEM and Molecular Dynamics study",
Surf. Sci. 600(2006)L86-L90 [IF 2.063]

G. Hamm, C. Barth, C. Becker, C.R. Henry; Phys. Rev. Lett. 97(2006)126106 [IF 7.035]
The surface structure of an ultrathin alumina film on Ni3Al(111): An AFM study

C. Barth, C.R. Henry; Appl. Phys. Lett. 89(2006)252119
Gold Nanoclusters on alkali halide surfaces: Charging and tunnelling

C. Barth, C.R. Henry; Phys. Rev. Lett. 98(2007)136804
Surface double layer on (001) surfaces of alkali halide crystals: A scanning force microscopy study

M.A. Röttgen, S. Abbet, K. Judai, J.M. Antonietti,A.S. Wörz, M. Arenz, C.R. Henry, U. Heiz; J.Am. Chem. Soc.129(2007)9635 [**Highlighted in Science** 317(2007)297]
Cluster chemistry: Size-dependent reactivity induced by reverse spill-over

G. Hamm, M. Marsault, A. Wörz, G. Sitja, C.R. Henry; Faraday Discussion (2007) *in print*
Preparation of regular arrays of bimetallic clusters with independent control of size and chemical composition

P.L. Gai, E.D. Boyes, S. Helveg, P.L. Hansen, S. Giorgio, C.R. Henry; MRS Bull (2007) *in print*
Atomic-Resolution Environmental Transmission Electron Microscopy (ETEM) for probing Gas-Solid Reactions in Heterogeneous Catalysis

O.H. Pakarinen, C. Barth, A.S. Foster, C.R. Henry; J. Appl. Phys (2007) *submitted*
Imaging the real shape of nano-objects in scanning force microscopy

C. Barth, C.R. Henry; Phys. Rev. Lett. (2007) *submitted*
Imaging Suzuki precipitates on NaCl:Mg^{2+} (001) by scanning force microscopy

C. Mottet

F Leroy, G Renaud, A Letoublon, R Lazzari, C Mottet, J Goniakowski, "Self-organized growth of nanoparticles on a surface patterned by a buried dislocation network",
Phys. Rev. Lett 95, 185501 (2005). [IF 07.035]

A Ouahab, C Mottet, J Goniakowski, "Atomistic simulation of Ag thin films on MgO(100) substrate: A template substrate for heterogeneous adsorption",
Phys. Rev B 72, 035421 (2005). [IF 02.962]

C Mottet, G Rossi, F Baletto, R Ferrando, "Single impurity effect on the melting of nanoclusters.",
Phys. Rev. Lett 95, 035501 (2005). [IF 07.035]

C Mottet, J Goniakowski, G Rossi, R Ferrando, F Baletto, "Melting of metallic nanoclusters: Alloying and support effects.",
Ann. Chim. Sci. Mat. 30, 303 (2005). [IF 00.480]

J Goniakowski, C Mottet, "Palladium nano-clusters on the MgO(100) surface: substrate-induced characteristics of morphology and atomic structure",
J. Cryst. Growth 275, 29 (2005). [IF 01.707]

S. Sao-Joao, S. Giorgio, C. Mottet, J. Goniakowski and C.R. Henry, "Interface structure of Ni nanoparticles on MgO (1 0 0): A combined HRTEM and molecular dynamic study.",
L86-L90, Surf. Sci. 600 (2006). [IF 02.063]

Rossi, G.; Mottet, C.; Nita, F.; Ferrando, R. "Global Optimization Study of Small (10 N 120) Pd Clusters Supported on MgO(100)",
J. Phys. Chem. B.110 (2006) 7436-7442. [IF 03.679]

J. Goniakowski, C. Mottet, C. Noguera, "Non-reactive metal/oxide interfaces: from model calculations towards realistic simulations",
Phys. Stat. Sol. (b), 243 (2006) 2516-2532. [IF 00.836]

V. Moreno, J. Creuze, F. Berthier, C. Mottet, G. Tréglia, B. Legrand, "Site segregation in size-mismatched nanoalloys: application to Cu-Ag",

Surface Science 600 (2006) 5011-5020. [IF 02.168]

D. Bazin, D. Sayers, J. Lynch, C. Mottet, G. Tréglia, "Combining solid state physics concepts and X-ray absorption spectroscopy to understand $DeNO_{(x)}$ catalysis",
Oil & Gas Science and Technology – Revue de l'IFP 61 (2006) 677-689.

P. Müller, C. Mottet," Equilibrium nanoshapes: from thermodynamics to atomistic simulations", J. of Computational and Theoretical Nanoscience 4, (2007) 316 – 325,

C. Mottet, J. Goniakowski, "Influence of epitaxial strain on supported metal cluster shapes via atomistic simulations"
J. of Computational and Theoretical Nanoscience 4 (2007) 326 – 334,

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G. Rossi, R. Ferrando, C. Mottet, "Structure and chemical ordering in CoPt nanoalloys", Faraday Discussions, in press

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C. Langlois, D. Alloyeau, Y. Le Bouar, A. Loiseau, T. Oikawa, C. Mottet, C. Ricolleau, "Growth and structural properties of CuAg and CoPt bimetallic nanoparticles", Faraday Discussions, in press

Presentations:

C. R. Henry

NC-AFM conference, Seattle (USA), October 2004,
Oral: O.H. PAKARINEN, C. Barth, A.S. Foster, R.M. Nieminen, C.R. Henry, "NC-AFM imaging of Au clusters on the KBR surface",

IWOX-4, Aussois (France), January 2005,
Invited talk : C. BARTH, C.R. Henry, "The clean (001) surface of UHV-cleaved MgO and KBr : An investigation by Dynamic Scanning Force Microscopy and Spectroscopy",
Oral : G. HAMM, C. Becker, C.R. Henry, „Monometallic Au, Pd and bimetallic Au-Pd cluster arrays on thin alumina film on Ni_3Al (111)"
Poster : C.R. HENRY, S. Ferrero, O. Meerson, C. Barth, K. Hoejrup-Hansen, "Gold on MgO(100): Nucleation, Structure and Reactivity

JSI (Journées Surface-Interface, Lyon (France) January 2005
Poster: S. Sao Joao, S. GIORGIO, C. Mottet, L. Piccolo, J. Goniakowski, C.R. Henry, "Interface Ni/MgO – Agrégats « Cœur-coquille » Pd-Ni/MgO : structure et réactivité",
Poster : J. Prunier, B. Domenichini, S. Sao-Joao, S. GIORGIO, C.R. Henry, S. Bourgeois ; "Premiers instants de la croissance du nickel sur MgO(100) »

Ecole de Sciences des Surfaces de Porquerolles "OXYSOL", Porquerolles island (France) June 2005
Invited Talk: C. R. HENRY, "Etude par microscopie en champ proche des surfaces d'oxydes et de la croissance de nanoparticules métalliques sur ces surfaces"

ESF-SONS, (Pisa, Italy) June 2005
Invited talk: C. R. HENRY, "Self-Organised Growth of Metal Clusters on Oxide Surfaces",
Poster: G. Hamm, C. Becker, C.R. Henry
Growth of highly ordered metal nanocluster arrays on a thin alumina film

EUROPACAT-7 (Sofia, Bulgaria) August-Septembre 2005

Oral: G. Hamm, G. Sitja, J.C. Dupin, C.R. HENRY; “Arrays of bimetallic clusters supported on alumina used as model catalysts”,
Oral: S. Sao-Joao, S. Giorgio, C. Mottet, L. Piccolo, C.R. HENRY; “Core-shell nanoparticles of Pd-Ni/Mg: structure and reactivity”

ECOSS 23 (Berlin, Germany) Sept. 2005
Invited talk: C. R. HENRY, “Bimetallic clusters arrays grown on nanostructured alumina surfaces : a new type of supported model catalysts”,
Poster : C. Barth, C.R. HENRY, “Imaging clusters with the dynamic scanning force microscope: techniques and solutions”,
Poster: C. BARTH, C.R. Henry, “Kelvin probe force microscopy on surfaces of UHV cleaved ionic crystals”

NC-AFM 8, Bad Essen (Germany) August 2005
Oral : C. BARTH, C.R. Henry “Imaging nanometer sized metal clusters in the constant height mode”,
Poster: C. BARTH, C.R. Henry, “Kelvin probe force microscopy on surfaces of UHV cleaved ionic crystals”,

GSOMEN meeting, Modena (Italie) Novembre 2005
Oral: C. HENRY, “Nucleation, Growth and Morphology of supported gold nanoparticles”,

Research Advances in Rational Design of Catalysts and Sorbents, IFP-Lyon, Decembre 2005
Oral: C.R. HENRY, G. Hamm, J.C. Dupin , “Arrays of metal clusters grown on nanostructured alumina surfaces: toward ideal supported model catalysts”,

JSI-2005, February 2006 (Marseille)
Oral : G. HAMM, C. Barth,, C.R. Henry, “Nano-agrégats métalliques (Au-Pd) supportés sur des couches minces d’alumine : Croissance auto-organisée et réactivité”,
Posters : S. Giorgio, S. Sao-Joao, S. Nitsche, D. Chaudanson, G. Sitja, C.R. Henry, “Microscopie environnementale appliquée àl’étude des catalyseurs modèles“
C. Barth, C.R. Henry; ”L’imagerie AFM non-contact des annao-agrégats métalliques en mode *hauteur constante*”,

APS –March Meeting, Baltimore (USA) March 2006
Oral : G. Hamm, C. Becker, C.R. HENRY, “Self organized growth of regular arrays of Pd-Au bimetallic nanoclusters on nanostructured alumina films”,
Oral : C. Barth, G. Hamm, C. Becker, C.R. HENRY, ” Surface structure of alumina ultrathin films grown on Ni3Al (111) studied by nc-AFM”,

NANO SEA 2006, Aix en Provence, July 2006
Invited Talk : C. Barth, G. Hamm, C.R. HENRY, “Surface structure of nanostructured ultrathin alumina films”,
Oral: G. Hamm, G. Sitja, C.R. HENRY, “Self organized growth of bimetallic clusters on a nanostructured alumina surface”

Self-Organized Nanostructures, SONS2006, Pisa (Italy), July 2006
Oral : G. Hamm, C. Barth, C.R. HENRY, Surface structure of Al2O3 films on Ni3Al(111) and their use as templates to grow arrays of bimettalic clusters
Poster : C. BARTH, C.R. Henry, Imaging clusters in the constant height mode of the Dynamic Scanning Force Microscopy

Summer School on Metal Clusters and Surfaces Pisa (Italy), July 2006
Invited Talk : C. R. HENRY, Metal deposition on Oxide Surfaces

ISSPIC XIII, Göteborg ; July 2006
Poster : A.S. WOERZ, G. Hamm, C.R. Henry, Small gold particles on thin nanostructured alumina films: influence of the deposition rate, surface coverage and surface temperature

JMC10, Toulouse, August 2006
Oral: A. WÖRZ, G. Hamm, C. Barth, G. Sitja, C.R. Henry, Nano-agrégats métalliques (Au, Pd) supportés sur des couches minces d'alumine : Croissance auto-organisée et réactivité

IMC 16 (Sapporo) Sept. 2006
Oral: S. GIORGIO, S. Sao Joao, S. Nitsche, D. Chaudenson, G. Sitja, C.R. Henry, Environmental Electron Microscopy for Model catalysts with closed Ecell

Workshop on the reactivity of surfaces and nanoparticles at elevated pressures, Kloster Irsee (Allemagne) Septembre 2006
Invited Talk : C. R. HENRY, S. Giorgio, Bridging the material gap and the pressure gap in heterogeneous catalysis: HRTEM on supported nanoparticules during reaction conditions up to 10 mbar

ECOSS 24 (Paris) Sept. 2006
Orals: - G. Hamm, C. Barth, C. Becker, C.R. HENRY, Surface Structure of Ultrathin Alumina film on Ni3Al(111)
- C. BARTH, C.R. Henry, Gold Nanoclusters on clean alkali halide surfaces: Tunnelling phenomena between clusters
Posters: - C. BARTH, C.R. Henry, UHV-cleavage induced charges on (001) surfaces of alkali halide crystals: a Kelvin probe force microscopy study
- A. WÖRZ, G. Hamm, G. Sitja, J.C. Dupin, C.R. Henry
Growth and reactivity of regular arrays of metallic clusters on alumina

COST Meeting D41: Inorganic oxide surfaces and interfaces, Vienna, Novembre 2006
Oral: G. Hamm, C. Barth, C.R. HENRY
Nanostructured alumina ultrathin films used as templates to grow arrays of bimetallic clusters.

IWOX 5, Lake Tahoe (USA), Janvier 2007
Oral: C. Barth, G. Hamm, A. Wörz, G. Sitja and C. R. Henry
From the atomic structure to the deposition of metallic nanocluster: Ultrathin Al_2O_3 films grown on $Ni_3Al(111)$

Poster: C. BARTH, C.R. Henry
Imaging nanoclusters in the constant height mode of the Dynamic Scanning Force Microscope

ACS meeting, Chicago (USA), Mars 2007
Invited Talk : C. R. HENRY
Elaboration of supported model catalysts : controlling shape, size, spatial distribution and chemical composition of metal nnaoparticles on oxide surfaces

Oral: S. Giorgio, M. Cabié, C.R. HENRY
Bridging material and pressure gaps in heterogeneous catalysis using environmental-HRTEM

School: NANOCATALYSIS, Les Houches (France), Mai-Juin 2007

Invited Talks : C.R. HENRY
- Supported nanoparticles: what is different at the nanoscale
- Nucleation, growth, morphology and organisation of metal nanoparticles on oxide surfaces

NC-AFM international Conference, (Turquie), septembre 2007
Oral: C. BARTH, O. H. Pakarinen, A. S. Foster and C. R. Henry
Imaging nanoclusters with their correct size and shape:The *constant height mode*

Poster: C. BARTH, C. R. Henry
The charge state of (001) surfaces of ionic crystals: A force microscopy study

Faraday Discussion 138 'Nanoalloys', Birminmgham (UK), Septempbre 2007
Oral: G. Hamm, M. MARSAULT, A. Wörz, G. Sitja, C.R. Henry
Preparation of regular arrays of bimetallic clusters with independent control of size and chemical composition

Europacat, Turku (Finland) Aout 2007
Oral: S. GIORGIO, M. Cabié, G. Sitja, C.R. Henry; Environmental high resolution electron microscopy with a closed Ecell: Application to gold catalysts

General Meeting of the COST D41(Inorganic Oxides: Surfaces and Interfaces), Berlin (Germany) October 2007.
Oral: A. Foster, O.H. Pakarinen, C. Barth, C.R. Henry
Imaging the real shape of nano-objects: scanning force microscopy study of Pd nnaoparticles on MgO

Poster: U. Heiz, Ch. Harding, M.A. Röttgen, M. Arenz, C.R. Henry
Cluster Chemistry: Size-dependent reactivity induced by reverse-spillover.

C. Mottet

C Mottet, J Goniakowski, R Ferrando, "Structure and dynamics of model metallic clusters",
in The American Chemical Society National Meeting in San Diego, march 2005.
American Chemical Society National Meeting in San Diego, march 2005.
Invited Talk : C Mottet, J Goniakowski, R Ferrando

OXYSOL, Surface Science School in Porquerolles: "Oxides in solution, at the interface between surface physics and chemistry and earth science, Porquerolles island (France), June 2005.
Invited talk: C. Mottet, "Atomistic description of crystal growth on surfaces"

JMC10, National Condensed Matter meeting, Toulouse (France), August 2006.
Oral: C. Mottet, J. Goniakowski, "Structure and morphology of supported metallic clusters: a numerical simulation study".

Faraday Discussion 138 « Nanoalloys : From Theory to Applications », University of Birmingham, United Kindom, 3-5 septembre 2007
Oral: C. Mottet, G. Rossi, R. Ferrando, "Structure and chemical ordering in CoPt nanoalloys."

Unit 5

Publications:

Torelli, P. ; Soares E. A. ; Renaud G. : Valeri S. ; Guo X. X. ; Luches P.
Nano-structuration of CoO film by misfit dislocations
Surf. Sci, 601, 2651 (2007) [IF 02.063]

C. Tusche, H.L. Meyerheim, N. Jedrecy, G. Renaud, J. Kirschner
Growth sequence and interface formation in the Fe/MgO/Fe(001) tunnel junction analyzed by surface x-ray diffraction
Phys. Rev. B, 74, 195422 (2006) [IF 02.962]

Revenant, C; Renaud, G; Lazzari, R; Jupille, J
Growth of Ag on MgO(001) studied in situ by grazing incidence small angle X-ray scattering
NUCLEAR INSTRUMENTS & METHODS IN PHYSICS RESEARCH SECTION B-BEAM INTERACTIONS WITH MATERIALS AND ATOMS, 246 (1): 112-117 MAY 2006

Tusche, C; Meyerheim, HL; Jedrecy, N; Renaud, G; Ernst, A; Henk, J; Bruno, P; Kirschner, J
Comment on "Destructive effect of disorder and bias voltage on interface resonance transmission in symmetric tunnel junctions" - Tusche et al. reply
PHYSICAL REVIEW LETTERS, 96 (11): Art. No. 119602 MAR 24 2006 [IF 7.035]

Jedrecy, N; Renaud, G; Lazzari, R; Jupille, J
Unstrained islands with interface coincidence sites versus strained islands: X-ray measurements on Ag/ZnO
PHYSICAL REVIEW B, 72 (19): Art. No. 195404 NOV 2005 [IF 02.962]

F Leroy, G Renaud, A Letoublon, R Lazzari, C Mottet, J Goniakowski, “Self-organized growth of nanoparticles on a surface patterned by a buried dislocation network”,
Phys. Rev. Lett 95, 185501 (2005). [IF 7.035]

Tusche, C; Meyerheim, HL; Jedrecy, N; Renaud, G; Ernst, A; Henk, J; Bruno, P; Kirschner, J
Oxygen-induced symmetrization and structural coherency in Fe/MgO/Fe(001) magnetic tunnel junctions
PHYSICAL REVIEW LETTERS, 95 (17): Art. No. 176101 OCT 21 2005 [IF 7.035]

Jedrecy, N; Renaud, G; Lazzari, R; Jupille, J
Flat-top silver nanocrystals on the two polar faces of ZnO: An all angle x-ray scattering investigation
PHYSICAL REVIEW B, 72 (4): Art. No. 045430 JUL 2005 [IF 02.962]

Presentations:

G. Renaud, “Surface Nanopatterning through GISAXS”,
Workshop on Surface Nanopatterning, Tirrenia (Pisa), June 30, July 1st 2005

F. Leroy, “GISAXS studies of surface growth and patterning”,
Summer School on Metal Clusters and Surfaces, Tirrenia (Pisa), July 2-7 2006

Unit 6,9

Publications:

A. Del Vitto, L. Giordano, G. Pacchioni, U. Heiz, “Cluster and periodic DFT calculations of MgO(Pd(CO) and MgO/Pd(CO)$_2$ surface complexes”,
J. Phys. Chem. B., *109 (8)*, 3416-3422 (2005). [IF 3.679]

A.S. Wörz, U. Heiz, F. Cinquini, G. Pacchioni, “Charging of Au atoms on TiO_2 thin films from CO vibrational spectroscopy and DFT calculations”,
J. Phys. Chem. B, 109, 18418-18426 (2005). [IF 03.679]

A. Del Vitto, G. Pacchioni, K.H. Lim, N. Rösch, J.-M. Antonietti, M. Michalski, U. Heiz, H. Jones, “Gold atoms and dimers on amorphous SiO_2: Calculation of optical properties and cavity ringdown spectroscopy measurements”,
J. Phys. Chem. B, *109*, 19876 (2005). [IF 3.679]

K. Judai, S. Abbet, A. S. Wörz, U. Heiz, L. Giordano, G. Pacchioni, “Mechanisms of the acetylene trimerization on MgO supported Rh, Pd, and Ag atoms”,
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