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CURRICULUM VITÆ

Born : 5th October 1966, Kraków, Poland

Professional experience :

2002- CRMC[2] (Marseille) et GPS (Paris)
Researcher, detached to CNRS

1995-2002 University of Aix–Marseille II, CRMC[2]
University teacher, Dr. Guy Tréglia's group

1994-1995 Keele University, Great Britain
Post-doctoral position, Prof. Mike Gillan's group

1991-1994 University of Paris-Sud, LPS, France
Graduate student, Dr. Claudine Noguera's group

1990-1991 Jagellonian University, IF, Kraków, Poland
Assistant, Prof. Andrzej Kisiel's group

Expertise and diplomas :

1995-2003 University of Aix–Marseille II, CRMC[2]
Habilitation in physics,
Oxide substrates : from model calculations towards realistic simulations.

1991-1994 University of Paris-Sud, LPS, France
Doctor degree in physics,
Electronic, Structural and Reactivity Properties of Oxide Surfaces.
supervisor : Dr. Claudine Noguera

1988-1990 Jagellonian University, Kraków, Poland
Magister degree in Physics,
Metamagnetism of Transition Metals.
supervisor : Dr. Marek Podgórny

1985-1988 Jagellonian University, Kraków, Poland
university studies in physics

Research experience :

1988 - 1990 MAGISTER DEGREE,
INSTITUTE OF PHYSICS, JAGELLONIAN UNIVERSITY, KRAKÓW, POLAND

Theoretical study of magnetism in transition metals and transition metal compounds. *Ab initio* LMTO simulations of the spin-polarized electronic band structure within the Fix Spin Moment method. Interpretation within the framework of the Stoner model.

1990 - 1991 ASSISTANT AT INSTITUTE OF PHYSICS,
INSTITUTE OF PHYSICS, JAGELLONIAN UNIVERSITY, KRAKÓW, POLAND

Ab initio modeling of the electronic band structure of II-VI semiconductors doped with transition metals : problematics of diluted magnetism. Theoretical evaluation of the optical transitions matrix, dielectric constant and application to interpretation of XANES spectra.

1991 - 1994 DOCTOR DEGREE,
LABORATOIRE DE PHYSIQUE DES SOLIDES,
UNIV. PARIS XI, ORSAY, FRANCE

Semi–empirical, HF study of the electronic, structural and reactivity properties of insulating oxide surfaces and the analysis of the main factors which control their evolution as a function of the iono–covalent character of material and of the surface orientation.

The electronic characteristics are principally determined by a competition between the electrostatic and covalent terms : the first fixes the separation of effective atomic levels of anions and cations, the second is related to the delocalization of electrons. Electron screening effects, which weaken the perturbations induced by the surface formation were found to be important. Surface structural distortions were found to be controlled mainly by the relative strength of electronic delocalization and short range repulsion. A new mechanism for rumpling was proposed, relying on differences in second neighbor electron delocalization on the anion and cation sublattices.

Modeling of the dissociative adsorption of water in two limiting cases (adsorption of isolated H^+ and OH^- molecules and full saturation of surface by the adsorbate) showed the importance of the local environment on the adsorption site, details of both the adsorption geometry and adsorbate coverage, as well as the role of screening effects and decohesion of the substrate.

1994 - 1995 POST-DOCTORAL POSITION,
KEELE UNIVERSITY, KEELE, GREAT BRITAIN

Ab initio (plane–wave) study of water adsorption on SnO_2 and TiO_2 (110) surfaces. Molecular and dissociative modes of adsorption were investigated along with the stabilizing effect of the surface hydrogen bonds. Finally, the dissociation path, related to proton transfer towards the surface along a hydrogen bond, was examined in order to evaluate the height of the energy barrier for water dissociation.

Standard Local Density Approximation approach tends to overestimate adsorption energies and wrongly reproduces the relative stability of different adsorption geometries. The numerical results were improved by the application of the Generalized Gradient Approximation method.

1995 - 2003 UNIVERSITY TEACHER
CENTRE DE RECHERCHE SUR LES MÉCANISMES DE LA CROISSANCE CRISTALLINE, UNIV. AIX–MARSEILLE II, MARSEILLE, FRANCE

Since the arrival to the *Centre de Recherche sur les Mécanismes de la Croissance Cristalline* my scientific interests have been principally focused on the problematics of numerical simulation of deposition and adsorption on oxide surfaces. We have used *ab initio* electronic band structure calculations for a better understanding of the basic microscopic mechanisms responsible for the observed/studied phenomena. On this basis, we have been trying to construct simple models of inter-atomic interactions that can be, by means of Molecular Dynamics and Monte Carlo methods, used directly for simulation of the growth processes.

Quite naturally, this problematics can be divided into four parts :

Oxide substrate : perfect surfaces, defects, polarity, nano-structures Characterization of perfect and defective oxide surfaces is a basis of any adsorption studies. In this field, use of *ab initio* calculations helps the verifications and extension of the existing results and concepts issued from semi-empirical or analytical models. An important example are the non-stoichiometric surfaces, where the physics related to the transition between an insulating and a locally metallic character, was treated in an extensive study of surface vacancies on the MgO (100) surface. Similarly the issue of stoichiometric surface point defects was recently treated in the study on reactivity of surface divacancies.

Transition metals on the oxide surfaces Detailed analysis of the relation between the adsorption energetics and the characteristics of the electronic structure of the deposited metal, performed systematically for a series of model metal/oxide systems has shown some general tendencies and has revealed basic microscopic mechanisms (related principally to the polarization of the metal deposit in the electrostatic field of the substrate), that can be held responsible for metal growth properties and for the morphology of the interfaces observed experimentally.

Interaction of molecules with oxide surfaces Theoretical study of water on the perfect MgO (100) surface has shown a possibility of existence of a dissociative adsorption mode. This latter, resulting principally from the interaction between the co-adsorbed molecules, has been for a long time a subject of speculations on both experimental and theoretical level, and seem necessary for the full interpretation of the existing experimental results.

Towards effective potentials The *ab initio* calculations show their great utility for the verification of hypothesis underlying the existing semi-empirical approaches (eg we were able to verify that the assumption of local neutrality in metals applies not only to atoms but also to different type of orbitals), as well as for a direct construction of new models of interactions (eg we were able to use the *ab initio* results as to fit an interaction potential on the metal/semiconductor and especially at the metal/oxide interface).

List of Publications

Full papers

1. *Magnetism of hexagonal 3d transition metals*,
M. Podgórny, J. Goniakowski, Phys. Rev. B **42**, 6683 (1990).
2. *Metamagnetism of hexagonal iron*,
M. Podgórny, J. Goniakowski, Il Nuovo Cimento, D **13**, 311 (1991).
3. *Antiferromagnetism in hexagonal chromium, manganese and iron*,
J. Goniakowski, M. Podgórny, Phys. Rev. B **44**, 12348 (1991).
4. *Acido-basic properties of simple oxide surfaces III : systematics of H^+ and OH^- adsorption*,
J. Goniakowski, S. Bouette–Russo, C. Noguera, Surf. Sci. **284**, 315 (1993).
5. *Electronic structure of clean insulating oxide surfaces I : A numerical approach*,
J. Goniakowski, C. Noguera, Surf. Sci. **319**, 68 (1994).
6. *Electronic structure of clean insulating oxide surfaces II : Modifications of the iono–covalent bonding*,
J. Goniakowski, C. Noguera, Surf. Sci. **319**, 81 (1994).
7. *Relaxation and rumpling mechanisms on oxide surfaces*,
J. Goniakowski, C. Noguera, Surf. Sci. **323**, 129 (1995).
8. *Theoretical investigation of hydroxylated oxide surfaces*,
J. Goniakowski, C. Noguera, Surf. Sci. **330**, 337 (1995).
9. *Atomic and electronic structure of steps and kinks on MgO(100) and (110)*,
J. Goniakowski, C. Noguera, Surf. Sci. **340**, 191 (1995).
10. *The structure of the stoichiometric and reduced SnO_2 (110) surface*,
I. Manassidis, J. Goniakowski, L. N. Kantorovich, M. J. Gillan, Surf. Sci. **339**, 258 (1995).
11. *The influence of gradient corrections on bulk and surface properties of TiO_2 and SnO_2*,
J. Goniakowski, J. M. Holender, L. N. Kantorovich, M. J. Gillan, J. A. White, Phys. Rev. B **53**, 957 (1996).
12. *The adsorption of H_2O on TiO_2 and SnO_2 (110) studied by first–principles calculations*,
J. Goniakowski, M. J. Gillan, Surf. Sci. **350**, 145 (1996).
13. *The concept of weak polarity : an application to the $SrTiO_3$ (001) surface*,
J. Goniakowski, C. Noguera, Surf. Sci. Lett. **365**, L657 (1996).
14. *Molecular adsorption on unrelaxed and relaxed ionic steps. Application to Ar, CO, CO_2 and NH_3 adsorbed on MgO (110)*,
S. Briquez, C. Girardet, J. Goniakowski, C. Noguera, J. Chem. Phys. **105**, 678 (1996).
15. *A Theoretical study of the stability and electronic etructure of the polar (111) face of MgO*,
A. Pojani, F. Finocchi, J. Goniakowski, C. Noguera, Surf. Sci. **387**, 354 (1997).
16. *Charge redistribution at Pd surfaces : ab initio grounds for tight-binding interatomic potentials*,
S. Sawaya, J. Goniakowski, C. Mottet, A. Saúl, G. Tréglia, Phys. Rev. B **56**, 12161 (1997).
17. *Electronic structure of MgO supported palladium films : Influence of the adsorption site*,
J. Goniakowski, Phys. Rev. B **57**, 1935 (1998).
18. *Adsorption of palladium on the MgO(100) surface : Dependence on the metal coverage*,
J. Goniakowski, Phys. Rev. B **58**, 1189 (1998).
19. *Partial dissociation of water molecules in the (3×2) water monolayer deposited on the MgO (100) surface*
L. Giordano, J. Goniakowski, J. Suzanne, Phys. Rev. Lett. **81**, 1271 (1998).
20. *Interaction between oxygen vacancies on MgO(100)*,
F. Finocchi, J. Goniakowski, C. Noguera, Phys. Rev. B **59**, 5178 (1999).
21. *Transition metals on the MgO(100) surface : Evolution of adsorption characteristics along the 4d series*,
J. Goniakowski, Phys. Rev. B **59**, 11047 (1999).

22. *LDA study of semiconductor/metal adsorption characteristics : Ge/Ag(100)* ,
S. Sawaya, J. Goniakowski, G. Tréglia, Phys. Rev. B **59**, 15337 (1999).

23. *Characteristics of Pd deposition on the MgO(111) surface*,
J. Goniakowski, C. Noguera, Phys. Rev. B **60**, 16120 (1999).

24. *Ge deposition on Ag surfaces : Dependence of the adsorption characteristics on the surface orientation*,
S. Sawaya, J. Goniakowski, G. Tréglia, Phys. Rev. B **61**, 8469 (2000).

25. *Ge/Ag(111) semiconductor on metal growth : A hidden nanoscale Ag_2Ge surface alloy*,
H. Oughaddou, S. Sawaya, J. Goniakowski, B. Aufray, G. Le Lay, J.M. Gay, G. Tréglia, J.P. Bibérian, N. Barret, C. Guillot, A. Mayne, G. Dujardin, Phys. Rev. B **62**, 16653 (2000).

26. *Reversibility of water dissociation on the MgO (100) surface*,
L. Giordano, J. Goniakowski, J. Suzanne, Phys. Rev. B **62**, 15406 (2000).

27. *Characteristics of Pd adsorption on the MgO(100) surface : role of oxygen vacancies*,
L. Giordano, J. Goniakowski, G. Pacchioni, Phys. Rev. B **64**, 075417 (2001).

28. *Interactions of a water molecule with the oxygen vacancy on the MgO(100) surface*,
F. Finocchi, J. Goniakowski, Phys. Rev. B **64**, 125426 (2001).

29. *Theoretical study of the atomic structure of Pd nanoclusters deposited on MgO(100) surface*,
W. Vervisch, C. Mottet, J. Goniakowski, Phys. Rev. B **65**, 245411 (2002).

30. *Microscopic mechanisms of stabilization of polar oxide surfaces : transition metals on the MgO(111) surface*,
J. Goniakowski, C. Noguera, Phys. Rev. B **66**, 085417 (2002).

31. *Properties of MgO(100) ultra-thin layers on Pd(100) : Influence of the metal support*,
L. Giordano, J. Goniakowski, G. Pacchioni, Phys. Rev. B **67**, 045410 (2003).

32. *Electronic states and Schottky barrier height at metal/MgO(100) interfaces*,
J. Goniakowski, C. Noguera, Interf. Sci., **12** 93 (2004).

33. *Nucleation of Pd dimers at defect sites of the MgO(100) surface*,
L. Giordano, C. Di Valentin, J. Goniakowski, G. Pacchioni, Phys. Rev. Lett. **92**, 096105 (2004) ; article selected for : Virtual Journal of Nanoscale Science & Technology **9**, March 15 (2004).

34. *Non-ractive metal-oxide interfaces : from model calculations towards realistic simulations*,
J. Goniakowski, C. Mottet, C. Noguera, Highlight in Ψ_k Newsletter **62**, 85-112 (2004).
http ://psi-k.dl.ac.uk/newsletters/News_62/Highlight_62.pdf

35. *Water dissociation on defective MgO(100) surface : Role of divacancies*,
B. Ealet, J. Goniakowski, F. Finocchi, accepted Phys. Rev.

36. *First Principles studies of complex oxide surfaces and interfaces*,
F. Finocchi, J. Goniakowski, C. Noguera, accepted J. Phys. : Cond. Matt.

37. *Formation of Pd dimers at regular and defect sites of the MgO(100) surface : Cluster model calculations*,
L. Giordano, C. Di Valentin, G. Pacchioni, J. Goniakowski, accepted Chem. Phys.

Conference papers

C 1. *The XANES K-edge spectra for HgMnSe and HgFeSe*,
A. Kisiel, J. Oleszkiewicz, J. Goniakowski, R. Markowski, E. Burattini, G. Dalba, F. Rocca, Acta Physica Polonica A **80**, 373 (1991).

C 2. *Electronic structure of clean and hydroxylated oxide surfaces*,
C. Noguera, J. Goniakowski, S. Bouette–Russo, Surf. Sci. **287/288**, 188 (1993).

C 3. *Rôle de la coordinence sur la force acide ou basique des sites de surface d'oxydes simples*,
J. Goniakowski, C. Noguera, Le Vide, les Couches Minces, **268** SS, 11 (1993).

C 4. *Critical analysis of classical acid–base approaches : A theoretical study of polar molecules on MgO surfaces*,
J. Goniakowski, C. Noguera, Le Vide, les Couches Minces, **272** SS, 74 (1994).

C 5. *Stability and electronic properties of non–stoichiometric MgO surfaces*,
E. Castanier, J. Goniakowski, A. Pojani, F. Finocchi, C.Noguera, Il Vuoto **25**, (1996).

C 6. *Electronic properties of CdSe and $Cd_{1-x}Fe_xSe$ wurzite compounds : theoretical ab-initio study*,
J. Konior, J. Goniakowski, S. Kaprzyk, J. Alloys Comp. **328**, 139 (2001).

C 7. *Effect of epitaxial strain on the atomic structure of Pd clusters on MgO (100) substrate*,
W. Vervisch, C. Mottet, J. Goniakowski, Eur. Phys. J. D **24**, 311 (2003).

C 8. *Modeling Free and Supported Metallic Nanoclusters : Structure and Dynamics*,
C. Mottet, J. Goniakowski, F. Baletto, R. Ferrando, G. Treglia, Phase Transitions, **77**, 101 (2004).

C 9. *Melting and Freezing of Pd nanoclusters : effect of the MgO(100) substrate*,
C. Mottet, J. Goniakowski, accepted Surf. Sci.

Chapters in books

L 1. *Acid–base interactions at oxide surfaces*,
J. Goniakowski, C. Noguera, dans *Electron Processes at Surfaces*, Ed. E. Ilisca et K. Makoshi, World Scientific (1996), ISBN 981-02-2012-X.

L 2. *Stability of polar oxide surfaces : oxygen vacancies and non-stoichiometric reconstructions*,
C. Noguera, A. Pojani, F. Finocchi, J. Goniakowski, dans *Chemisorption and Reactivity on Supported Clusters and Thin Films*, Ed. R.M. Lambert et G. Pacchioni, Kluwer, NATO ASI series E : Applied Sciences, (1997), ISBN 0-7923-4448-0.

L 3. *An introduction to the simulation of extended systems based on density functional and Hartree–Fock theories*,
F. Finocchi, J. Goniakowski, X. Gonze, and C. Pisani, dans *Handbook of Numerical analysis. Volume X : Computational Chemistry*, Ed. C. Le Bris, Elsevier (2003), ISBN 0-444-51248-9.