# Alberto Andrés Saúl

**Senior Research Associate (Directeur de Recherche)**
Centre Interdisciplinaire de Nanoscience de Marseille (CINaM)
Centre National de la Recherche Scienctifique (CNRS)
Marseille (France) | +33 6 62 92 28 88 | andres.saul@cnrs.fr
8 décembre 2025

## Degrees

**Habilitation à Diriger des Recherches**
Université de la Méditerranée (Marseille, France) — December 2002

**PhD in Physics**
Universidad de Buenos Aires (Argentina). — September 1990

**M.Sc in Physics (Licenciatura)**
Universidad de Buenos Aires (Argentina). — March 1987

## Appointments

**Senior Research Associate (Directeur de Recherche 1re, CNRS)**
CINaM (Marseille, France). — Oct-2017 to present

**Senior Research Associate (Directeur de Recherche 2e, CNRS)**
CRMCN and CINaM (Marseille, France). — Oct-2004 to Sep-2017

**Research Affiliate**
Civil and Environmental Engineering, MIT (Cambridge, USA). — Sep-2015 to Aug-2016

**Senior Research Scientist**
Civil and Environmental Engineering, MIT (Cambridge, USA). — Sep-2013 to Aug-2015

**Research Associate (Chargé de Recherche, CNRS)**
CRMC2 and CRMCN (Marseille, France). — Apr-1994 to Sep-2004

**Collaborateur Temporaire Étranger**
Service de Recherche en Métallurgie Physique, CEA (Saclay, France). — Oct-1992 to Mar-1994

**Visiting researcher**
IBM T. J. Watson Research Center, (Yorktown Heights, USA) — Jan-1992 to Mar-1992

**Research Fellow (Investigador Residente)**
Computer Research and Advanced Application Group, IBM Argentina. — Mar-1991 to Sep-1992

**Technical Assistant**
Low Temperatures Laboratory FCEN-UBA. (Buenos Aires, Argentina) — Jul-1983 to Mar-1987

**Teaching Assistant**
Physics Laboratory. Escuela Tecnica ORT. (Buenos Aires, Argentina) — Mar-1981 to Jul-1983

**Technical Assistant**
Instrumentation Laboratory FI-UBA. (Buenos Aires, Argentina) — Mar-1980 to Dec-1980

## Responsabilities

**Invited Member of the Advisory Board**
Centre Interdisciplinaire de Nanoscience de Marseille — 2017 to present

**Member of the Executive Committee**
Centre Interdisciplinaire de Nanoscience de Marseille — 2017 to present

**Head of the Theory and Computer Simulations Department**
Centre Interdisciplinaire de Nanoscience de Marseille — 2017 to present

**Head of the Theory and Computer Simulations Department**
Centre Interdisciplinaire de Nanoscience de Marseille — 2012 to 2013

**Member of the Scientific Committee**
Centre Interdisciplinaire de Nanoscience de Marseille — 2012 to 2013

**Invited Member of the Advisory Board**
Centre Interdisciplinaire de Nanoscience de Marseille — 2012 to 2013

**Member of the Advisory Committee**
ModMat (GDR) research network — 2012 to 2015

**Member of the Advisory Committee**
NanoAlliages (GDR) research network — 2012 to 2015

**Member of the Advisory Committee**
CoDFT (GDR) research network — 2010 to 2013

**Member of the Advisory Committee**
DFT++ (GDR) research network — 2006 to 2009

**Head of the Theory and Computer Simulations Group**
Centre de Recherche sur la Matière Condensée et les Nanosciences — 2004 to 2006

**Elected Member of the Advisory Board**
Centre de Recherche sur la Matière Condensée et les Nanosciences — 2004 to 2006

**Elected Member of the Advisory Board**
Centre de Recherche sur les Mecanismes de Croissance Cristalline — 2000 to 2004

## Expertise and principal research interests

**Topics**

Magnetic and electronic properties of low dimensional systems. Magnetic (magnons) and vibrational (phonons) excitations and their coupling. Magneto-elastic interactions. Quantum magnetism of low dimensional systems. Quantum transport. Metallic nanowires. Surface stress and surface energy. Elastic properties. Surface physics. Reconstruction and phase transitions. Surface segregation, kinetics and equilibrium properties. Surface alloys and alloy surfaces.

**Methods**

Quantum and classical computer simulation in statistical mechanics. Electronic structure calculations in condensed matter. Density functional theory and semi-empirical (tight-binding) electronic structure methods. All electron linearized augmented planewave method. Semi-empirical interatomic potentials. Classical molecular dynamics and Monte Carlo methods. Computational and numerical methods in general.

## Publications

**More than 100 refereed research papers in international journals**

7 invited papers or chapters.

Full list of publications below

**Five selected publications**

— "Piezomagnetism and magnetoelastic memory in uranium dioxide" ; M. Jaime, A. Saúl, M. Salamon, V. Zapf, N. Harrison, T. Durakiewicz, J. Lashley, D. Andersson, Ch. Stanek, J. Smith, and K. Gofryk ; Nature. Communications **8**, 99 (2017).

— "Magnetic nanopantograph in the $SrCu_2(BO_3)_2$ Shastry-Sutherland lattice" ; G. Radtke, A. Saúl, H. A. Dabkowska, M. B. Salomon, M. Jaime ; Proc. Natl. Acad. of Sci. USA **112**, 1971, (2015).
— "Magnetic couplings in $CsV_2O_5$ : a new picture". A. Saúl and G. Radtke ; Phys. Rev. Lett **106**, 177203 (2011).
— "Measuring the surface stress polar dependence". J. J. Métois, A. Saúl, and P. Müller ; Nature Materials **4**, 238 (2005).
— "Different wavelength oscillations in the conductance of $5d$ metal atomic chains". L. de la Vega, A. Martín-Rodero, A. Levy Yeyati, A. Saúl ; Phys. Rev. B, **70**, 113107 (2004).

## Grants

— *Ferroelectric Rashba semiconductors for spin orbitronics.* Initiative d'excellence Aix-Marseille (AMIDEX). F. Cheynis (PI). 2023 - 2027 (∼ 535000€).
— *Orbitronics in non-centrosymmetric magnets.* French National Research Agency (ANR). A. Manchon (PI). 2021 - 2024 (∼ 152000€).
— *High Polarization High Temperature Cuprate Multiferroics.* French National Research Agency (ANR). X. Rocquefelte (PI). 2020 - 2024 (∼ 152000€).
— *Cement Radiolysis : reaction mechanisms.* Projet NEEDS (Nucléaire, Energie, Environnement, Déchets et Société). S. Le Caer (PI). 2017 (∼ 10000€).
— *Cement Radiolysis : reaction mechanisms.* Projet NEEDS (Nucléaire, Energie, Environnement, Déchets et Société). S. Le Caer (PI). 2016 (∼ 14000€).
— *Spintronics in one dimension.* French National Research Agency (ANR). M. Viret (PI). 2009 - 2011 (∼ 125000€).
— *Dewetting of solid films.* French National Research Agency (ANR). F. Leroy (PI). 2009 - 2011 (∼ 40000€).
— *Strain dependence of the diffusion.* GDR MATINEX with CEA Cadarache. P. Ganster (PI). 2009 (∼ 4000€).
— *Atomistic simulation of the SiGe system.* French National Research Agency (ANR). P. Pochet (PI). 2006 - 2008 (∼ 40000€).
— *Self ordering of epitaxial films.* French National Research Agency (ANR). O. Pierre-Louis (PI). 2006 - 2008.
— *Structure, morphology and magnetism of low dimensional systems.* Université de la Méditerranée (Axe Amérique-Europe). Andrés Saúl (PI). 2004 - 2007 (∼ 2000€).
— *Structure, morphology and magnetism of low dimensional systems.* PICS with Argentine Atomic Energy Commission. Hugues Dreysse (PI). 2004 - 2006 (∼ 10000€).
— *Structure, magnetic and electronic properties of bimetallic nanostructures.* ECOS-SECYT with Argentine Atomic Energy Commission. Andrés Saúl (PI). 2004 -2006 (∼ 20000€).
— *Fabrication of SiGe based memorys.* European Program FORUM-FIB. I. Berbezier (PI), Antonie Ronda, Andrés Saúl. 2001 - 2003 (∼ 100000€).
— *Study of the morphology and electronic structure of metallic and semiconducting surfaces.* ECOS-SECYT with Instituto Balseiro (Bariloche, Argentina). Guy Tréglia (PI) and Andrés Saúl. 1998 - 2001 (∼ 20000€).
— *Structure, magnetic and electronic properties of transition metals and their oxides.* PICS with Universidad de San Martin (Argentina). Andrés Saúl (PI). 2009 - 2011 (∼ 22000€).
— *Simulation in Solid Physics.* Université de la Méditerranée (BQR). 2001 (∼ 7000 €).
— *Self-diffusion on the Si(100) surface.* CNRS-CONICET with the Argentine Atomic Energy Commission. Guy Tréglia (PI) and Andrés Saúl. 1998 - 2000 (∼ 20000€).

## Fellowships

— *Honors Degree* Awarded by the University of Buenos Aires to graduates with a GPA greater than 9 over 10.

— *PhD fellowship* Physics Department of the Argentine Atomic Energy Commission at Buenos Aires, Argentina. (declined).
— *PhD fellowship "Iniciación"* of CONICET Buenos Aires, Argentina. for the period 1987-1988.
— *PhD fellowship "Perfectionamiento"* of CONICET Buenos Aires, Argentina, for the period 1989-1991.
— *Visiting Scientist Program* of the National High Magnetic Field Laboratory (USA) to collaborate with Los Alamos National Laboratory (June-July 2018).

## Teaching experience and lectures

**Graduate level**

— *Numerical simulation in material science :* Département de Physique. Université de la Méditerranée.
— *Numerical methods in solid state physics : electronic properties :* Département de Physique. Université Aix-Marseille.
— *Solid state physics :* Département de Physique. Université Aix-Marseille.
— *Density functional theory :* Département de Physique. Université Aix-Marseille.
— *Phonons :* Département de Physique. Université Aix-Marseille.
— *Magnetism :* Département de Physique. Université Aix-Marseille.

**Undergraduate level**

— *Electricity and magnetism :* Departamento de Física. FCEyN, Universidad de Buenos Aires.
— *Fluid mechanics :* Departamento de Física. FCEyN, Universidad de Buenos Aires.
— *Quantum mechanics :* Departamento de Física. FCEyN, Universidad de Buenos Aires.
— *Solid state physics :* Departamento de Física. FCEyN, Universidad de Buenos Aires.

**High School level**

— *Physics laboratory experiments :* Escuela Técnica O.R.T (Buenos Aires, Argentina)).

**Other**

— *Monte Carlo methods in materials science :* Ecole d'Été d'Analyse Numérique organized by EDF-CEA-INRIA (Le Bréau, France).
— *Electronic structure :* III-ème Ecole d'Été Modélisation des Matériaux organized by Réseau ModMat (Banyuls, France).

## Student and Post-doc supervising

**Post-doc**

— *Dr. Chu-Chun Fu.* From June 2001 to November 2002.
— *Dr. Javier Fuhr.* From 2001 to 2004.
— *Dr. Patrick Ganster.* From September 2006 to March 2010.
— *Dr. Robinson Cortes-Huerto.* From May 2010 to December 2011.
— *Dr. Lucile Dezerald.* From October 2014 to August 2015.
— *Dr. Khaoula Boukari.* From February 2016 to March 2017.
— *Dr. Julien Lévêque* From November 2023 to February 2024.

**PhD Level**

— *Jean Marc Roussel.* "Modélisation de la dissolution d'un dépôt métallique lors d'une hétéroépitaxie". Université de la Méditerranée. January 1999.
— *Chu-Chun Fu.* "Etude par dynamique moléculaire de la diffusion de Si et dépôt de C sur la surface (001) du Si". Universidad de Buenos Aires. Co-directed with M. Weissmann. May 2001.
— *Stephane Olivier.* "Rôle des contraintes dans les reconstructions de surfaces métalliques" Université d'Aix-Marseille II. June 2004.
— *Tristana Sondon.* "Structure et propriétés électroniques et magnétiques de nano-structures bimétalliques : étude théorique et par simulation numérique". Université de San Martin (Argentina) et Université de la Méditerranée, Co-directed with J. Guevara. July 2008.

— *Rémi Zoubkoff.* “Structure et propriétés électroniques de nanofils de métaux 5d”. Université de la Méditerranée. February 2010.

— *Julien Lévêque* “Etude théorique des propriétés électroniques et magnétiques de matériaux multiferroïques utilisant des méthodes de simulation numérique”. Université d’Aix Marseille. Co-directed with Marie-Bernadette Lepetit.

— *Florian Petot* “Magnetism of 2D van der Waals systems : a theoretical study”. Université d’Aix Marseille. Co-directed with Benoit Gremaud.

**Master level**

— *Pablo A. Dmitruk.* “Estudio del transporte de carga en semiconductores”. Licenciatura degree. Facultad de Ciencias Exactas y Naturales - Universidad de Buenos Aires. Co-directed with L. Reyna. September 1991.

— *Thierry Bigault.* “Effet Surfactant dans le systeme Ni/Ag(100)”. Ecole Nationale Superieure de Physique - Marseille. Co-directed with G. Treglia. December 1994.

— *Jean Marc Roussel.* “Effet surfactant lors d’un depot de Ni/Ag(100) : influence de la vitesse du depot”. DEA Science des Materiaux. Université de la Méditerranée. Co-directed with G. Treglia. June 1995.

— *Fabrice Ficalora.* “FeSi phase diagram”. Ecole Nationale Superieure de Physique. Marseille. Co-directed with G. Treglia. December 1995.

— *Stephane Olivier.* “Du rôle des efforts de surface dans les reconstructions”. DEA Science des Materiaux. Université de la Méditerranée. June 2000.

— *Rémi Zoubkoff.* “Structure et propriétés électroniques de nanofils de métaux 5d” Master 2 Matériaux Nanosciences - Université de la Méditerranée. June 2006.

— *Yann Maupu.* “Parallélisation de codes de dynamique moléculaire”. Institut Universitaire de Technologie site Luminy. April 2007.

— *Yann Maupu.* “Administration d’un cluster de machines pour le calcul scientifique”. Ecole supérieure d’ingénieurs de Luminy (ESIL). April 2008.

— *Sébastien Taupin.* “Behavior of cementitious materials under electron irradiation”. Chimie-Paris ParisTech. June - August 2015.

— *Adrian Macquet.* “Calculation of the ground state properties of quantum magnets”. Université Aix-Marseille. February - March 2018.

— *Quentin Gibaru.* “Quadrupole-Quadrupole interactions in uranium dioxide”. Polytech - Université Aix-Marseille. November 2018 - January 2019.

— *Sofien Boyanov Angelov.* “Calculation of the Ewald sum for dipoles”. Université Aix-Marseille. February - March 2020.

— *Hugo Careil.* “Electronic and magnetic properties of cuprate multiferroics”. Université Aix-Marseille. April - June 2020.

— *Lucien Salmon.* “Physical origin of the magnetic interactions in solids”. Université Aix-Marseille. May - June 2020.

— *Ugo Friscano, Gabriel Flores-Alfaro, Bastien Giraud, Alexis Maillard* “Physical origin of the magnetic interactions in solids”. Université Aix-Marseille. October - December 2020.

— *Florian Petot* “Magnetism of 2D van der Waals systems : a theoretical study”. Université Aix-Marseille. March - June 2023.

— *Guillaume Jacquet* “Magnetic excitations of 2D van der Waals systems : a theoretical study”. Université Aix-Marseille. March - June 2025.

**Undergraduate level**

— *Thomas Sartori.* Travaux d’Initiative Personnelle Encadrés. Classe Préparatoire, Lycée Thiers. 2011 - 2012.

— *Damir Vodericanevic.* “Simulation numérique du Modèle d’Ising par la méthode Monte Carlo”. Licence degree. Université d’Aix Marseille. (February 2012).

— *Jeffrey Mohan.* “Basis of Quantum Magnetism and Thermodynamics” Bachelor of Engineering. McGill University (Montréal, Canada). June-July 2013

— *Sebastien Aynaud, Joshua Esteves, Vadim Becquet, Gabriel Fina, Mickael Lorenzini.* “Etude des propriétés magnétiques de systémes de spins dans des matériaux”. Université Aix-Marseille. February - May 2016.

— *Robin Jaeger, Alexandre Mouret, Sophie Lunadier, Emma Simon.* "Etude des modes de vibration du cristal d'Oxyde d'Uranium" Université Aix-Marseille. February - May 2017.
— *Alexandre Mouret, Emma Simon.* "Piezomagnéetisme et magnétolélasticité dans l'oxide d'uranium". Université Aix-Marseille. June - July 2017.

## Participation in the organization of scientific activities

— *At the Frontiers of Condensed Matter I.* Dedicated to Mariana Weissmann, Buenos Aires, Argentina, December 2002.
— *Journées Surfaces et Interfaces.* Villeneuve d'Ascq, France, January 2003.
— *Symposium on Surface Science 3S03.* La Plagne, France, April 2003.
— *Journées Surfaces et Interfaces.* Mulhouse, France, January 2004.
— *Réunion générale du GDR-DFT.* La Londe les Maures, Var, France. February 2004.
— *Réunion de Simulateurs et Théoriciens de Marseille.* Luminy, Marseille, September 2004.
— *At the Frontiers of Condensed Matter II.* Buenos Aires, Argentina, December 2004.
— *Symposium on Surface Science 3S05.* Les Arcs, France, March 2005.
— *Réunion Thématique Transport Electronique - GDR-DFT++.* Luminy, Marseille, November 2006.
— *At the Frontiers of Condensed Matter III.* Buenos Aires, Argentina, December 2006.
— *Symposium on Surface Science 3S07.* Les Arcs, France, March 2007.
— *At the Frontiers of Condensed Matter IV.* Buenos Aires, Argentina, December 2008.
— *Atelier Magnétisme - GDR-CoDFT.* ENS, Lyon, November 2010.
— *At the Frontiers of Condensed Matter V.* Buenos Aires, Argentina, December 2010.
— *Réunion Thématique Nanofils d'alliages - GDR-Nanoalliages.* Université Paris Diderot, Paris, November 2013.
— *Réunion Thématique Liaisons Fortes - GDR-ModMat.* Luminy, Marseille, April 2014.
— *Marseille Condensed Matter 2016 : Optics and Magnetism* Luminy, Marseille, September 2016.
— *Cost Action Towards Understanding and Modelling Intense Electronic Excitation* Luminy, Marseille, September 2021.

## Thesis examiner

**Habilitation à Diriger des Recherches**

— *Adeline Crépieux.* (Reviewer) May 2005, Université de la Méditerranée.
— *Alexandre N. Kholod.* July 2005, Université de la Méditerranée.
— *Geoffroy Prévot.* April 2007, Université Pierre et Marie Curie.
— *Hubert Klein.* September 2009, Université de la Méditerranée.
— *Jérôme Creuze.* (Reviewer) May 2011, Université Paris XI.
— *Alexandre Gloter* (Reviewer) September 2016, Université Paris Sud.
— *Michel Freyss* (Reviewer) September 2020, Université Aix-Marseille.
— *Sylvain Latil* (Reviewer) April 2021, Université Paris-Saclay.

**PhD**

— *Coralie Gallis.* November 1997, Université Paris 6.
— *Emmanuel Clouet.* (Reviewer) February 2004, Ecole Centrale des Arts et Manufactures.
— *Stanislas Rohart.* September 2005, Université Paris 6.
— *Laura de la Vega Velázquez.* November 2006, Universidad Autónoma de Madrid.
— *Thomas Chanier.* (Reviewer) August 2008, Université de Provence.
— *Gabriel Autés.* (Reviewer) December 2008, Université Paris VI - Pierre et Marie Curie.
— *Shruti Mehendale.* (Reviewer) November 2010, Université Paris VII - Denis Diderot.
— *Christophe Taillan.* (Reviewer) September 2012, Université de Toulouse.
— *Parwana Habibi.* October 2012, Université Pierre et Marie Curie.

— *Emile Maras.* November 2012, Université Paris Sud.
— *Dongzhe Li.* September 2015, Université Paris Sud.
— *Burak Ozdamar* October 2016, Université de Strasbourg.
— *Shi Lei.* November 2016, Université d'Aix Marseille.
— *William Lafargue-dit-hauret.* September 2018, Université de Rennes.
— *Grégoire David.* November 2018, Université d'Aix Marseille.
— *Thibaud Dreher.* December 2018, Université de Clermont Auvergne.
— *Martin S. Talla Noutack.* October 2019, Université d'Aix Marseille.
— *Simon Thebaud.* October 2019, Université Claude Bernard.
— *Ludovic Le Laurent* December 2020, Université Paris-Saclay.

# Full list of publications

Researcher ID : C-1282-2012
ORCID : 0000-0003-0540-703X
Google Scholar : here

1. "Wave functions of one-dimensional incommensurate Hamiltonians ; the fractal dimension and its relationship with localization" ;
   A. Saúl, A. M. Llois and M. Weissmann ;
   Journal of Physics C**21**, 2137 (1988). doi
2. "Electronic structure of copper oxide clusters in the high Tc Superconductors : relation to some recent experimental data" ;
   A. Saúl, A. M. Llois, A. Levy Yeyati and M. Weissmann ;
   Solid State Comm. **66**, 491 (1988). doi
3. "Electronic structure of copper oxide and fluorine substituted clusters by the iterative extended Huckel method" ;
   M. Weissmann, A. Saúl, A. Levy Yeyati and A. M. Llois ;
   Progress in High Temperature Superconductivity by World Scientific Publishing Co, 290 (1988).
4. "Calculation of the nuclear quadrupole splitting in high Tc Superconductors" ;
   A. Saúl and M. Weissmann ;
   Phys. Rev. B **42**, 4196 (1990). doi
5. "Calculation of the angular correlation of the positron annihilation radiation in $YBa_2Cu_3O_7$" ;
   A. Saúl and M. Weissmann ;
   J. of Physics : Condensed Matter **2**, 9603 (1990). doi
6. "Alloy model and high temperature Superconductors" ;
   M. Weissmann and A. Saúl ;
   Physica C **180**, 381 (1991). doi
7. "On the treatment of the collision operator for hydrodynamic models" ;
   L. G. Reyna and A. Saúl ;
   The IMA Volumes in Mathematics and its Applications Volume 59, Semiconductors Part II, p321, ed. W. M. Coughran, J. Cole, P. Lloyd and J. White, Springer-Verlag New York (1994). doi
8. "On the treatment of the collision operator for hydrodynamic models" ;
   L. G. Reyna and A. Saúl ;
   IBM Research Report RC 17296 (76511) 10/17/91.
9. "High electric field approximation to charge transport in semiconductor devices" ;
   P. Dmitruk, A. Saúl and L. G. Reyna ;
   Applied Mathematics Letters, **5**, 99-102 (1992). doi
10. "High electric field approximation to charge transport in semiconductor devices" ;
    P. Dmitruk, A. Saúl and L. G. Reyna ;
    IBM Research Report RC 17818 (78382) 3/13/92.
11. "High elastic scattering rate approximation to charge transport in semiconductor devices" ;
    P. Dmitruk, L. G. Reyna, and A. Saúl ;
    IBM Research Report RC 19021 (83037) 7/16/93.
12. "Layer by layer dissolution of $Ag$ deposited on $Cu(111)$" ;
    A. Saúl ;
    Mat. Science Forum **155-156**, 233, Ed : Y. Limoge and J. L. Boquet, Trans. Tech. Pub. (Switzerland) (1994). doi
13. "Chemical and topological structure of alloy surfaces : from equilibrium to kinetics" ;
    B. Legrand, A. Saúl and G. Tréglia ;
    Mat. Science Forum **155-156**, 165, Ed : Y. Limoge and J. L. Boquet, Trans. Tech. Pub. (Switzerland) (1994). doi
14. "Kinetics of segregation and dissolution in $Cu_{1-c}Ag_c$ and surface phase transitions : comparison between Mean Field and Monte Carlo calculations" ;
    A. Saúl., B. Legrand and G. Tréglia ;
    Surf. Sci. **307-309**, 804 (1994). doi

15. "Equilibrium and kinetics in the (111) surface of Cu(Ag) alloys, comparison between Mean Field and Monte Carlo calculations" ;
A. Saúl., B. Legrand and G. Tréglia ;
Phys. Rev. B **50**, 1912 (1994). doi
16. "Link between the surface wetting in Cu(Ag) and the layer by layer dissolution mode of a thick Ag deposit on a Cu substrate" ;
A. Saúl., B. Legrand and G. Tréglia ;
Surf. Sci. **331-333**, 805 (1995). doi
17. "Flux dependence of the surfactant effect in Ni/Ag (100) : a theoretical study" ;
J-M. Roussel, A. Saúl, G. Tréglia and B. Legrand ;
Surf. Sci. **352-354**, 562 (1996). doi
18. "Competition or synergy between surface segregation and bulk ordering : the Cu-Pd system" ;
C. Gallis, B. Legrand, A. Saúl, G. Tréglia, P. Hecquet and B. Salanon ;
Surf. Sci. **352-354**, 588 (1996). doi
19. "Theoretical study of surface alloy formation through generation and annihilation of vacancies" ;
G. Tréglia, B. Legrand, A. Saúl, T. Flores and M. Wuttig ;
Surf. Sci. **352-354**, 552 (1996). doi
20. "Influence of bulk phase transitions on the behaviour of alloy surfaces and surface alloys" ;
G. Tréglia, B. Legrand and A. Saúl ;
Il Vuoto, Scienza e Tecnologia, Vol XXV, N°4, 32 (1996).
21. "Calculation of the electronic structure of Si-based nanocrystalline material" ;
L. Vervoort, A. Saúl and F. Arnaud d'Avitaya ;
Il Vuoto, Scienza e Tecnologia, Vol XXV, N°4, 53 (1996).
22. "Cinétique de dissolution d'un dépôt Fe/Cu" ;
S. Delage, B. Legrand, F. Soisson, T. Bigault, A. Saúl, and G. Tréglia ;
Journal de Physique IV, Colloque C7, 151 (1996). doi
23. "Grain interaction effect in electronic properties of silicon nanosize films" ;
A.B. Filonov, A.N. Kholod, V.A. Novikov, V.E. Borisenko, L. Vervoort, F. Bassani, A. Saúl, and F. Arnaud d'Avitaya ;
Applied Physics Letters, **70**, 774 (1997). doi
24. "Microstructure of the "surfactant-like" effect in Ni/Ag(100) and (111)" ;
J. M. Roussel, A. Saúl, G. Tréglia, and B. Legrand ;
Phys. Rev. B **55**, 10931 (1997). doi
25. "The electronic energy levels of Si-based nanocrystalline materials : Theory compared to experiment" ;
L. Vervoort, A. Saúl, F. Bassani, and F. Arnaud d'Avitaya ;
Thin Solid Films **297**, 163 (1997). doi
26. "Charge redistribution at Pd surfaces : *ab initio* grounds for *tight-binding* interatomic potentials" ;
S. Sawaya, J. Goniakowski, C. Mottet, A. Saúl, and G. Tréglia ;
Phys. Rev. B **56**, 12161 (1997). doi
27. "Grain effect in electronic properties of silicon epitaxial nanostructures" ;
A.B. Filonov, A.N. Kholod, V.E. Borisenko, A. Saúl, F. Bassani, and F. Arnaud d'Avitaya ;
Computational Materials Science, **10**, 148 (1998).doi
28. "The effects of prewetting and wetting transitions on the surface energy of liquid binary alloys" ;
P. Wynblatt, A. Saúl, and D. Chatain ;
Acta Mater. **46**, 2337 (1998). doi
29. "Dissolution modes of Fe/Cu and Cu/Fe deposits" ;
S. Delage, B. Legrand, F. Soisson, and A. Saúl ;
Phys. Rev. B **58**, 15810 (1998). doi
30. "Cobalt impurities on noble metal surfaces" ;
M. Weissmann, A. Saúl, Ana Maria Llois, and Javier Guevara ;
Phys. Rev. B **59**, 8405 (1999). doi
31. "Theoretical prediction of new dissolution modes during metal heteroepitaxy" ;
J-M. Roussel, A. Saúl, G. Tréglia, and B. Legrand ;
Journal of Crystal Growth **198-199**, 83 (1999). doi

32. "Alloy surfaces : segregation, reconstruction and phase transitions" ;
G. Tréglia, B. Legrand, F. Ducastelle, A. Saúl, C. Gallis, I. Meunier, C. Mottet, and A. Senhaji ;
Computational Materials Science, **15**, 196 (1999).doi
33. "Structure of high temperature fluid selenium" ;
J-Y. Raty, A. Saúl, J-P. Gaspard, and C. Bichara ;
Phys. Rev. B **60**, 2441 (1999). doi
34. "Magnetic contribution to the segregation energies in magnetic-nonmagnetic systems" ;
A. Saúl and M. Weissmann ;
Phys. Rev. B **60**, 4982 (1999). doi
35. "Adsorption of Pd on $MoS_2(0001)$ : *ab initio* electronic structure calculations" ;
J. D. Fuhr, J. O. Sofo, and A. Saúl ;
Phys. Rev. B **60**, 8343 (1999). doi
36. "Layer-by-layer versus surfactant dissolution modes in heteroepitaxy" ;
J-M Roussel, A. Saúl, G. Tréglia, and B. Legrand ;
Phys. Rev. B **60**, 13890 (1999). doi
37. "Disorder effects on the gap of thin Si nanocrystalline films" ;
S. Menard, A. Saúl, F. Bassani, and F. Arnaud d'Avitaya ;
Phys. Stat. Sol. (b), **216**, 955 (1999). doi
38. "On the estimation of SRO effects on surface segregation" ;
J. M. Roussel, A. Saúl, M. Polak, and L. Rubinovich ;
J. Phys. : Condens. Matter **11**, 9901 (1999). doi
39. "Atomistic modeling of bimetallic surfaces" ;
G. Tréglia, I. Meunier, C. Mottet, J. M. Roussel, A. Saúl, A. Senhaji, B. Legrand, F. Ducastelle, and R. Ferrando ;
"Quasicrystals : current topics", World Sci. Publishing Co, Singapore (2000), 240. doi
40. "Electronic Properties of Germanium Quantum Films" ;
A.N. Kholod, A. Saúl, J. Fuhr, V.E. Borisenko, and F. Arnaud d'Avitaya ;
Phys. Rev. B **62**, 12949 (2000). doi
41. "Structural and electronic properties of high-temperature fluid selenium" ;
J-Y. Raty, A. Saúl, J-P. Gaspard, and C. Bichara ;
Computational Materials Science. **17**, 239 (2000).doi
42. "Finite temperature simulation of ad-dimer diffusion between dimer row and trough on Si(001)" ;
Chu-Chun Fu, M. Weissmann, and A. Saúl ;
Appl. Surf. Sci. **175-176**, 36 (2001). doi
43. "Femtosecond structural dynamics of the prototypical Si(100) surface" ;
G. Le Lay, Chu-Chun Fu, M. Weissmann, and A. Saúl ;
Scientific Case of the X-ray Free Electron Laser (XFEL) at DESY, Hamburg. (2001)
44. "Appeareance of direct gap in silicon and germanium nanosize slabs" ;
A.N. Kholod, V.E. Borisenko, A. Saúl, F. Arnaud d'Avitaya, and J. Fuhr ;
Optical Materials, **17**, 61 (2001). doi
45. "Diffusion pathways for Si ad-dimers on Si(001) : A high temperature molecular dynamics study" ;
Chu-Chun Fu, M. Weissmann, and A. Saúl ;
Surf. Sci. **481**, 97 (2001). doi
46. "Molecular dynamics study of dimer flipping on perfect and defective Si(001) surfaces" ;
Chu-Chun Fu, M. Weissmann, and A. Saúl ;
Surf. Sci. **494**, 119 (2001). doi
47. "Experimental evidence for an Erlich-Schwoebel effect on Si(111)" ;
A. Saúl, J. J. Métois, and A. Ranguis ;
Phys. Rev. **B**, **65**, 075409 (2002). doi
48. "Coverage dependence study of the adsorption of Pd on $MoS_2(0001)$" ;
J. D. Fuhr, J. O. Sofo, and A. Saúl ;
Surf. Sci. **506**, 161 (2002). doi
49. "Relation between surface stress and $(1 \times 2)$ missing row reconstruction for (110) surface of fcc transition metals" ;

Stephane Olivier, A. Saúl, and Guy Tréglia
Appl. Surf. Sci. **212-213**, 866 (2003). doi

50. "Theoretical study of the role of surface defects on the dimer dynamics on Si(001)" ;
Chu-Chun Fu and A. Saúl ;
Surf. Sci. **527**, 113 (2003). doi
51. "Dimer flipping on the Si(001) surfaces : the role of surface defects" ;
Chu-Chun Fu, M. Weissmann, and A. Saúl ;
Proceedings of "En las Fronteras de la Materia Condensada : Workshop dedicado a M. Weissmann", Buenos Aires (Decembre 2002).
52. "Surface stress and epitaxial growth" ;
Stéphane Olivier, P. Müller, and A. Saúl ;
Current Topics in Crystal Growth Research **7** (2004).
53. "Scanning tunneling microscopy chemical signature of point defects on the $MoS_2(0001)$ surface" :
J. D. Fuhr, A. Saúl, and J. O. Sofo ;
Phys. Rev. Lett. **92**, 026802 (2004). doi
54. "Linear time dependence of the surfactant effect : A local equilibrium under flux" ;
J. M. Roussel, A. Saúl, G. Tréglia, and B. Legrand ;
Phys. Rev. **B**, **69**, 115406 (2004). doi
55. "Elastic effects on surface physics" ;
P. Müller and A. Saúl ;
Surf. Sci. Rep., **54**, 157 (2004). doi
56. "Catalytic effect of C on shaping Si surfaces " ;
Chu-Chun Fu, J. J. Métois, J. P. Astier, A. Saúl, and M. Weissmann ;
Surf. Sci., **563**, 48 (2004). doi
57. "Different wavelength oscillations in the conductance of $5d$ metal atomic chains" ;
L. de la Vega, A. Martín-Rodero, A. Levy Yeyati, A. Saúl ;
Phys. Rev. B, **70**, 113107 (2004). doi
58. "Measuring the surface stress polar dependence" ;
J. J. Métois, A. Saúl, and P. Müller ;
Nature Materials **4**, 238 (2005). doi
59. "Description élastique d'une surface et de ses défauts",
A. Saúl and P. Müller ;
"Contraintes mécaniques en micro, nano et optoéléctronique",Ed. : Marie José Casanove, Anne Ponchet et André Rocher (Lavoisier, 2006).
60. "Influence of surface stress in the missing row reconstruction of fcc transition metals",
Stephane Olivier, Guy Treglia, Andrés Saúl, F. Willaime ;
Surf. Sci., **600**, 5131 (2006). doi
61. "Magnetic Properties of Pt-Ir Nanowires" ;
T. Sondón, A. Saúl, J. Guevara ;
Surf. Sci. **601**, 4297 (2007). doi
62. "Magnetic Properties of CoRh and NiRh Nanowires" ;
T. Sondón, A. Saúl, J. Guevara ;
Physica B **398**, 352 (2007). doi
63. "Study of the structure, segregation and magnetic properties of Ni-Rh clusters" ;
T. Sondón, J. Guevara, and A. Saúl ;
Phys. Rev. **B 75**, 104426 (2007). doi
64. "Structure of gold monotamic wires connected to two electrodes" ;
Rémi Zoubkoff, L. de la Vega, A. Martín-Rodero, A. Levy Yeyati, and Andrés Saúl ;
Physica B **398**, 309 (2007). doi
65. "Momentum dependent energy loss near edge fine structure in $SrCu_2(BO_3)_2$" ;
G. Radtke and A. Saúl ;
Microsc. and Microanal. **13**, 146 (2007). doi
66. "Electronic structure of the quasi 2D spin gap system $SrCu_2(BO_3)_2$" ;
G. Radtke, A. Saúl, H. A. Dabkowska, B. D. Gaulin, and G. A. Botton ;
Phys. Rev. **B 77**, 125130 (2008). doi

67. "Are conductance independent events in atopoint contact measurements ? A statistical approach" ;
T. Leoni, R. Zoubkoff, S. Homri, N. Canyoni, P. Vidakovic, A. Ranguis, H. Klein, A. Saúl, P. Dumas ;
Nanotechnology. **19**, 355401 (2008). doi
68. "Strain effect on self diffusion in Silicon : numerical study" ;
P. Ganster, A. Saúl, and G. Tréglia ;
Phys. Rev. **B 79**, 115205 (2009). doi
69. "Atomistic modeling of strain and diffusion at the $Si/SiO_2$ interface" ;
P. Ganster, A. Saúl, and G. Tréglia ;
Phys. Rev. **B 81**, 045315 (2010). doi
70. "Ab initio study of magnetism at the $TiO_2/LaAlO_3$ interface" ;
Mariana Weissmann, Valeria Ferrari, and Andrés Saúl ;
Journal of Material Science **45**, 4945 (2010). doi
71. "Electronic structure and stability of hexagonal $Ba_3Ti_2RuO_9$" ;
G. Radtke, C. Maunders, A. Saúl, S. Lazar, H. J. Whitfield, J. Etheridge, and G. A. Botton ;
Phys. Rev. **B 81**, 085112 (2010). doi
72. "Interplay between structural, electronic, and magnetic degrees of freedom in $Sr_3Cr_2O_8$" ;
G. Radtke, A. Saúl, H. A. Dabkowska, G. M. Luke, G. A. Botton ;
Phys. Rev. Lett **105**, 036401 (2010). doi
73. "Uphill diffusion, zero flux planes and transient chemical solitary waves in garnet" ;
D. Vielzeuf and A. Saúl ;
Contributions to Mineralogy and Petrology **161**, 683 (2011). doi
74. "Magnetic couplings in $CsV_2O_5$ : a new picture" ;
A. Saúl and G. Radtke ;
Phys. Rev. Lett **106**, 177203 (2011). doi
75. "Electronic and magnetic properties of spin gap systems" ;
A. Saúl and G. Radtke ;
Proceedings of the International Conference Nanomeeting 2011. World Scientific Publishing Company (2011).
76. "Structure and properties of nanoscale materials : theory and atomistic computer simulation" ;
C. Bichara, P. Marsal, C. Mottet, R. Pellenq, F. Ribeiro, A. Saúl, G. Tréglia, and H-Ch Weissker ;
Int. J. Nanotechnol. **8**, 10-12 (2011). doi
77. "Conductance fluctuations in gold point contacts : an atomistic picture" ;
Huber Klein, Thomas Leoni, Remi Zoubkoff, Philippe Dumas, and Andres Saúl ;
Nanotechnology **23**, 235707 (2012). doi
78. "Theoretical study of the magnetic order in $\alpha$-$CoV_2O_6$" ;
A. Saúl, D. Vodenicarevic, G. Radtke ;
Phys. Rev. **B 87**, 024403 (2013). doi
79. "Magnetism of $Ba_4Ru_3O_{10}$ revealed by density functional calculations : structural trimers behaving as coupled dimers" ;
G. Radtke, A. Saúl, Y. Klein, and G. Rousse ;
Phys. Rev. **B 87**, 054436 (2013). doi
80. "Role of temperature in the formation and growth of gold mono-atomic chains : a molecular dynamics study" ;
R. Cortes Huerto, Andres Saúl, and T. Sondon ;
Phys. Rev. **B 88**, 235438 (2013). doi
81. "Simple views on surface stress and surface energy concepts" ;
P. Müller, A. Saúl, and F. Leroy ;
Adv. Nat. Sci. : Nanosci. Nanotechnol. 5, 013002 (2014). doi
82. "Density functional approach for the magnetism of $\beta$-$TeVO_4$" ;
A. Saúl and G. Radtke ;
Phys. Rev. **B 89**, 104414 (2014). doi
83. "Multiphase equation of state for carbon addressing high pressures and temperatures" ;
Lorin X. Benedict, Kevin P. Driver, Sebastien Hamel, Burkhard Militzer, Tingting Qi, Alfredo A.

Correa, A. Saul, and Eric Schwegler ;
Phys. Rev. **B 89**, 224109 (2014). doi

84. "Molecular Dynamics simulations of the formation of 1D spin-valves from stretched Au-Co and Pt-Co nanowires" ;
R. Cortes-Huerto, T. Sondon, A. Saúl ;
J. of Physics : Condensed Matter. 24, 474206 (2014). Editor selection (included in IOPselect). doi
85. "Magnetic interactions in supported and unsupported $3d$ transition metal chains" ;
M. C. Urdaniz, M. A. Barral, A. M. Llois, A. Saúl ;
Phys. Rev. **B 90**, 195423 (2014). doi
86. "Model for Ge condensation during oxidation of $Si_{1-x}Ge_x$" ;
P. Ganster, A. Saúl, and G. Tréglia ;
Defect and Diffusion Forum **363**, 210 (2015).
87. "Magnetic nanopantograph in the $SrCu_2(BO_3)_2$ Shastry-Sutherland lattice" ;
G. Radtke, A. Saúl, H. A. Dabkowska, M. B. Salomon, M. Jaime ;
Proc. Natl. Acad. of Sci. USA **112**, 1971, (2015). doi
88. "Antiferromagnetic phase of the gapless semiconductor $V_3Al$" ;
M. E. Jamer, B. A. Assaf, G. E. Sterbinsky, D. Arena, L. H. Lewis, A. Saúl, G. Radtke and D. Heiman ;
Phys. Rev. **B 91** , 094409 (2015). doi
89. "Cement as a waste form for nuclear fission products : the case of 90Sr and its daughters" ;
L. Dezerald, J. J. Kohanoff, A. A. Correa, A. Caro, R. J.-M. Pellenq, F. J. Ulm, and A. Saúl ;
Environmental Science and Technology **49**, 13676 (2015). doi
90. "Quasi-two-dimensional Bose-Einstein condensation of spin triplets in the dimerized quantum magnet $Ba_2CuSi_2O_6Cl_2$" ;
Makiko Okada, Hidekazu Tanaka, Nobuyuki Kurita, Kohei Johmoto, Hidehiro Uekusa, Atsushi Miyake, Masashi Tokunaga, Satoshi Nishimoto, Masaaki Nakamura, Marcelo Jaime, Guillaume Radtke, Andrés Saúl ;
Phys. Rev. **B 94**, 094421 (2016). doi
91. "Production of $H_2$ by water radiolysis in cement paste by electron irradiation : A joint experimental and theoretical study" ;
Sophie Le Caer, Lucile Dezerald, Khaoula Boukari, Maxime Lainé, Sébastien Taupin, Ryan M. Kavanagh6, Conrad S. N. Johnston, Eddy Foy, Thibault Charpentier, Konrad J. Krakowiak, Roland J.-M. Pellenq, Franz J. Ulm, Gareth A. Tribello, Jorge Kohanoff, and Aandrés Saúl.
Cement and Concrete Reserach **100**, 110 (2017). doi
92. "Piezomagnetism and magnetoelastic memory in uranium dioxide" ;
Marcelo Jaime, Andrés Saúl, Myron Salamon, Vivien Zapf, Neil Harrison, Tomasz Durakiewicz, Jason Lashley, David Andersson, Christopher Stanek, James Smith, and Krzysztof Gofryk ;
Nature. Communications **8**, 99 (2017) doi
93. "Magnetic dimerization in the frustrated spin ladder $Li_2O(CuSO_4)_2$" ;
O. Vaccarelli, G. Rousse, A. Saúl, and G. Radtke.
Phys. Rev. B **96**, 180406 (2017). doi
94. "Unconventional field induced phases in a quantum magnet formed by free radical tetramers" ;
Andrés Saúl. Gauthier, R. M. Askari, Michel Côté, T. Maris, C. Reber, A. Lannes, D. Luneau, M. Nicklas, E. Lauren Green, J. Wosnitza, A. D. Bianchi, and A. Feiguin.
Phys. Rev. B **97**, 064414 (2018). doi
95. "Influence of halogen substitution on aggregation-induced near infrared emission of borondifluoride complexes of 2'-hydroxychalcones" ;
Anthony D'Aléo, Andres Saul, Claudio Attaccalite, and Frédéric Fages.
Mater. Chem. Front. **3**, 86 (2019). doi
96. "Influence of confinement in layered nanostructures on free radical chemistry : Single atoms catalysis under confinement" ;
Khashayar Ghandi, Tait Du, Maxime Lainé, Cody Landry, Andrés Saúl, Sophie Le Caër.
Sci Rep 9, 17165 (2019). doi
97. "Magnetoelastic interaction in the two-dimensional magnetic material $MnPS_3$ studied by first principles calculations and Raman experiments" ;

Diana Vaclavkova, Alex Delhomme, Clément Faugeras, Marek Potemski, Aleksander Bogucki, Jan Suffczyński, Piotr Kossacki, Andrew Wildes, Benoit Gremaud and Andrés Saúl.
2D Mater. 7, 035030 (2020). doi

98. "Piezomagnetic switching and complex phase equilibria in uranium dioxide : X-ray diffraction in pulsed magnetic fields" ;
D. Antonio, J. T. Weiss, K. S. Shanks, J. P. C. Ruff, M. Jaime, A. Saul, T. Swinburne, M. Salamon, K. Shrestha, B. Lavina, D. Koury, S.M. Gruner, D.A. Andersson, C. R. Stanek, T. Durakiewicz, J. L. Smith, Z. Islam, and K. Gofryk.
Commun Mater 2, 17 (2021) doi
99. "Age, duration and mineral marking of magma interactions in the deep crust : an example from the Pyrenees" ;
Daniel Vielzeuf, J-L. Paquette, J. D. Clemens, G. Stevens, A. Gannoun, K. Suchorski, and A. Saúl.
Contributions to Mineralogy and Petrology 176, 39 (2021). doi
100. "Potential room temperature multiferroicity in cupric oxide under high pressure" ;
William Lafargue-Dit-Hauret, Daniel Braithwaite, Andrew D. Huxley, Tsuyoshi Kimura, Andres Saúl, Mirta Herak, Xavier Rocquefelte.
Phys. Rev. B. **103**, 214432 (2021). doi
101. "Radioactive decay of $^{90}$Sr in cement : a non-equilibrium first-principles investigation" ;
Jorge Kohanoff, Alfredo A. Correa, Gleb Gribakin, Conrad Johnston, Andrés Saúl.
Eur. Phys. J. D. 75, 248 (2021). doi
102. "Theoretical study of the magnetic properties of $BaNiF_4$" ;
J. Lévêque, E. Ribolini, A. Saúl, M. B. Lepetit.
Eur. Phys. J. B. 94, 214 (2021). doi
103. "Ab initio investigation of the magnetic and ferroelectric properties of $BaCuF_4$ under hydrostatic pressure" ;
David Vincent, Xavier Rocquefelte, Andrés Saúl.
Phys. Rev. B. **106**, 064421 (2022). doi
104. "Theoretical study of the magnetic properties of pseudo spin ladder $CoCu_2O_3$" ;
J. Lévêque, E. Ribolini, M. B. Lepetit, A. Saúl.
Phys. Rev. B. **106**, 224402 (2022). doi
105. "Magnetoelastic interactions in $SrCu_2(BO_3)_2$ studied by Raman scattering experiments and first principles calculations" ;
K. Thirunavukkuarasu, G. Radtke, Z. Lu, M. Lazzeri, P. C. M. Christianen, M. V. Ballottin, H. A. Dabkowska, B. D. Gaulin, D. Smirnov, M. Jaime, A. Saúl.
Phys. Rev. B. **107**, 064410 (2023). doi
106. "Coherent description of the magnetic properties of $SeCuO_3$ versus temperature and magnetic field" ;
Xavier Rocquefelte, Mirta Herak, Atsushi Miyake, William Lafargue-Dit-Hauret, Helmuth Berger, Masashi Tokunaga, A. Saúl.
Phys. Rev. B. **107**, 054407 (2023). doi
107. "Van der Waals epitaxy of Weyl-semimetal Td-$WTe_2$" ;
A. Llopez, F. Leroy, C. Tagne-Kaegom, B. Croes, A. Michon, C. Mastropasqua, M. Al Khalfioui, S. Curiotto, P. Müller, A. Saúl, B. Kierren, G. Kremer, P. Le Fèvre, F. Bertran, Y. Fagot-Revurat, F. Cheynis.
ACS Appl. Mater. Interfaces **16**, 20878 (2024). doi
108. "Why the pyrochlore-like antiferromagnet $NaCu_3F_7$ is magnetically non-frustrated" ;
J. Lévêque, E. Ribolini, A. Saúl, M. B. Lepetit.
J. Phys. : Condens. Matter **36**, 415803 (2024). doi
109. "Magnetic structure of a multiferroic compound : $Cu_2OCl_2$" ;
J. Lévêque, E. Ribolini, A. Saúl, M. B. Lepetit.
Faraday Discuss. **254**, 612-627 (2024). doi
110. "Pushing the thickness limit of the giant Rashba effect in ferroelectric semiconductor GeTe" ;
Boris Croes, Alexandre Llopez, Calvin Tagne-Kaegom, Bodry Tegomo-Chiogo, Bertrand Kierren, Pierre Müller, Stefano Curiotto, Patrick Le Fèvre, Fabien Bertran, Andrés Saúl, Yannick Fagot-Revurat, Frédéric Leroy, Fabien Cheynis.
Nano Lett. 24, 13224 (2024). doi

111. "Ferroelectric control of spin and orbital Rashba effects at the Ni/$HfO_2$ interface" ;
Armando Pezo, Andrés Saúl, Aurélien Manchon, Rémi Arras.
Phys. Rev. B. **111**, L140405 (2025). doi

112. "Magnetic phases and zone-folded phonons in a frustrated van der Waals magnet" ;
Amit Pawbake, Florian Petot, Florian Le Mardelé, Tristan Riccardi, Julien Lévêque, Benjamin A. Piot, Milan Orlita, Johann Coraux, Michal Hubert, Jan Dzian, Martin Veis, Yurii Skourski, Bing Wu, Zdenek Sofer, Benoît Grémaud, Andrés Saúl, and Clément Faugeras.
ACS Nano 19, 23693 (2025). doi

113. "Spin texture of $\alpha$-GeTe in the ultrathin regime" ;
Calvin Tagne-Kaegom, Alexandre Llopez, Boris Croes, Geoffroy Kremer, Bertrand Kierren, Daniel Malterre, Luc Moreau, Jaurès Fotié Ngoufo, Stefano Curiotto, Pierre Müller, Patrick Le Fèvre, Julien Rault, François Bertran, Andrés Saúl, Frédéric Leroy, Fabien Cheynis, and Yannick Fagot-Revurat.
Submitted for publication.

# Invited conferences

1. "Alloy Surfaces and Thin metallic Films". Network on Surface Crystallography. Grenoble. October 1993.
"Surface layering transitions and a layer-by-layer dissolution mode" ; A. Saúl (oral), G. Tréglia and B. Legrand.
2. "$4^{emes}$ Journées de la Matière Condensée". Société Française de Physique. Rennes. September 1994.
"Cinétiques de ségrégation et de dissolution dans Cu-Ag : Influence des transitions de phase de surface" ; A. Saúl (oral), G. Tréglia and B. Legrand.
3. "Fifth International Conference on Atomically Controlled Surfaces, Interfaces and Nanostructures (ACSIN 5)", Aix en Provence (France). July 1999.
"Kinetic and local equilibrium grounds for surface alloys formation" ; A. Saúl (oral), J. M. Roussel, G. Tréglia, B. Legrand, B. Aufray.
4. "Second French-German Crystal Growth Meeting (FGCGM2003)", Nancy (France). March 2003.
"Atomistic processes involved in semiconductors growth" ; A. Saúl (oral).
5. "Atelier sur les mécanismes intervenant dans la croissance et la relaxation des couches épitaxiées", Aussois (France), March 2003.
"Aspects thermodynamiques" ; A. Saúl (oral), Pierre Muller.
6. "Ecole thématique CNRS Contraintes Internes : de leurs origines à leur utilisation dans les matériaux à propriétés électroniques", Nant (France). September 2005.
"Description élastique d'une surface et de ses défauts" ; Pierre Müller, A. Saúl (oral).
7. "WIEN2007 - Hands on Workshop on the WIEN2k package", Penn State University, University Park, PA (USA), June 2007.
"Calculation of surface energies and surface stresses" ; A. Saúl (oral).
8. "A day in honor of Paul Wynblatt", Carnegie Mellon University, Pittsburgh, PA (USA), June 2007.
"Surface stress : definition, numerical calculation and experimental determination of its anisotropy" ; A. Saúl (oral).
9. "At the Frontiers of Condensed Matter V", Buenos Aires (Argentina), December 2010.
"Magnetic structure and superexchange pathways in $CsV_2O_5$" ; A. Saúl (oral) and G. Radtke.
10. "Sòlidos 2011", San Miguel de Tucumán (Argentina), November 2011.
"Interacciones magnéticas en un sistema con gap de spin $CsV_2O_5$. Quienes son los dimeros ?" A. Saúl (oral), G. Radtke.
11. "At the Frontiers of Condensed Matter VI", Buenos Aires (Argentina), December 2012.
"Frustration and magnetic order in $\alpha$-$CoV_2O_6$" ; A. Saúl (oral), D. Vodenicarevic and G. Radtke.
12. "Seminario *Pensando Argentina 2030*. Organisé par la Société d'Estudiants Argentins de l'Université de Harvard et le Club Argentin du MIT", May 2015.
"Désafíos Científico Tecnológicos". A. Saúl (oral).

13. "The 9th International Conference on Advanced Materials and Devices", Jeju (Korea), December 2015.
"Calculation of the effective exchange interactions of Model Hamiltonians using Density Functional based Methods" ; A. Saúl (oral).
14. "APS March Meeting", Baltimore (USA). March 2016.
"Magnetic nanopantograph in the in $SrCu_2(BO_3)_2$ Shastry-Sutherland lattice" A. Saúl (oral).
15. "Korean Physical Society" Daejeon (Korea). April 2016.
"Pionner Session : Optical and magnetic properties of low-dimensional materials : first-principles calculation approach" "Effective exchange interactions and magnetoelastic effects in the spin dimer compound $SrCu_2(BO_3)_2$." A. Saúl (oral).
16. "2016 Computer Simulation of Radiation Effects in Solids (COSIRES)" Loughborough University (UK), June 2016.
"Radiation damage in cement" A. Saúl (oral).
17. "Recent Progress on Low-Dimensional Quantum Magnetism" Ecole Polytechnique Federale de Laussane, September 2016.
"Electronic structure and magnetoelastic interactions in $SrCu_2(BO_3)_2$" A. Saúl (oral).
18. "Theory days 2016 : irradiation of nanodevices" Université Paul Sabatier, December 2016. "Cement as a nuclear waste form : the case of medium lived fission products" A. Saúl (oral).
19. "Euro-Mediterranean Conference on Materials and Renewable energies", Marrakech (Morocco). May 2017.
"Magnetoelastic interactions in $SrCu_2(BO_3)_2$ : orthogonal Cu dimers behaving as magnetic nanopantographs" A. Saúl (oral).
20. "Nanomeeting 2017", Minsk (Biellorussie). May 2017.
"Magnetoelastic interactions in $SrCu_2(BO_3)_2$ : orthogonal Cu dimers behaving as magnetic nanopantographs" A. Saúl (oral).
21. "Joint Workshop : CNRS - McMaster University", Hamilton (Canada). February 2018.
"Electronic and magnetic properties of low dimensional systems" A. Saúl (oral).
22. "Research in High Magnetic Fields", Sante Fe (USA). June 2018.
"Magneto elastic interactions in two antiferromagnetic systems under high magnetic field." M. Jaime, G. Radtke, H. A. Dabkowska, M. B. Salomon, V. Zapf, N. Harrison, T. Durakiewicz, J. Lashley, D. Andersson, C. Stanek, J. Smith, K. Gofryk, and A. Saúl (oral).
23. "International Workshop on Quantum Magnets in Extreme Conditions", Online - Organized by The University of Tokio (Japan), March 2021.
"Magnetoelastic interaction in the two-dimensional magnetic material $MnPS_3$ studied by first principles calculations and Raman experiments". A. Saúl (oral).
24. "Workshop on 2D-Materials", Warsaw (Poland), October 2022.
"Magnetoelastic interaction in the two-dimensional magnetic material $MnPS_3$ studied by first principles calculations and Raman experiments". A. Saúl (oral).
25. "X Workshop on Novel Methods for Electronic Structure Calculations", La Plata (Argentina), December 2023.
"Magnetic order, magnetic excitations and magnetoelastic interactions in a two-dimensional van-der Waals system" A. Saúl (oral).
26. "Bariloche workshop on condensed matter physics", Bariloche (Argentina), December 2023.
"Magnetic order, magnetic excitations and magnetoelastic interactions in a two-dimensional van-der Waals system" A. Saúl (oral).
27. "At the Frontiers of Condensed Matter VII", Buenos Aires (Argentina), December 2024.
"Magnetoelastic interactions in CrOCl, a frustrated van-der Waals system" A. Saúl (oral).

## Conferences, Workshops, Seminars

1. $71^{st.}$ Meeting of the Argentine Physical Association, La Cumber. October 1986.
"Dimensión fractal de las funciones de onda de sistemas inconmensurados unidimensionales y su relación con la localización". A. Saúl, A. M. Llois y M. Weissmann (Poster).

2. $72^{nd.}$ Meeting of the Argentine Physical Association, Bariloche (Rio Negro). October 1987.
   "Control de temperatura por computadora para un calorímetro diferencial". C. Alcober, J. Talpe and A. Saúl (Poster).
   "Un poco mas sobre funciones de onda de hamiltonianos inconmensurados unidimensionales : dimensión fractal y su relación con la localización". A. Saúl, A. M. Llois y M. Weissmann (Poster).
   "Oxigeno vs. fluor en propiedades electrónicas de clusters $Cu_nX_m$ (X=O, F)". M. Weissmann, A. Saúl and A. M. Llois (Poster).
3. $73^{rd.}$ Meeting of the Argentine Physical Association, Mar del Plata (Buenos Aires). October 1988.
   "Estructura electrónica de planos y cadenas Cu-O, en el superconductor $YBa_2Cu_3O_7$". A. Saúl and M. Weissmann (Poster).
4. $74^{th.}$ Meeting of the Argentine Physical Association, San Luis (San Luis). October 1989.
   "Cálculo de la correlación angular de radiación en la aniquilación de positrones (2D-ACPAR) en $YBa_2Cu_3O_7$". A. Saúl y M. Weissmann (Poster).
5. $2^{nd.}$ Latin American Conference on the Application of the Mössbauer Effect, La Habana (Cuba). November 1990.
   "Calculation of the nuclear quadrupole splitting in the high Tc Superconductors". A. Saúl and M. Weissmann (Poster).
6. $76^{th.}$ Meeting of the Argentine Physical Association, San Miguel de Tucuman. October 1991.
   "Cargas locales y superconductores de alta temperatura crítica".M. Weissmann and A. Saúl (Poster).
   "Transporte de carga en dispositivos semiconductores pequeños". P. Dmitruk, L. Reyna and A. Saúl (Poster).
7. Journées Surfaces Interfaces, Strasbourg (France), 28-29 January 1993.
   "L'équilibre local à l'épreuve des transitions de phase de surface : une illustration dans les alliages Cu(Ag)". A. Saúl, J. Eugène, A. Jouaiti, A. Mosser, B. Legrand, G. Tréglia, B. Aufray et H. Giordano (Poster).
8. "Workshop on Reactive Formation of Phases at Interfaces and Diffusion Processes", Aussois (France). May 1993.
   "Layer by layer dissolution of $Ag$ deposited on $Cu(111)$". A. Saúl (Poster).
9. "$13^{th}$ European Conference on Surface Science", University of Warwick (England). August 1993.
   "Kinetics of segregation and dissolution in $Cu_{1-c}Ag_c$ and surface phase transition : comparison between Mean Field and Monte Carlo calculations". A. Saúl, G. Tréglia and B. Legrand (Poster).
10. "$14^{th}$ European Conference on Surface Science", Leipzig (Germany). September 1994.
    "Link between the surface wetting in Cu(Ag) and the layer by layer dissolution mode of a thick Ag deposit on a Cu substrate". A. Saúl, B. Legrand and G. Tréglia (Poster).
11. "$15^{th}$ European Conference on Surface Science", Lille (France). September 1995.
    "Flux dependence of the surfactant effect in Ni/Ag (100) : a theoretical study". J.M. Roussel, A. Saúl, G. Tréglia and B. Legrand (Poster).
    "Competition or synergy between surface segregation and bulk ordering : the Cu-Pd system". C. Gallis, B. Legrand, A. Saúl, G. Tréglia, P. Hecquet and B. Salanon (Poster).
12. "NATO Advance Study Institute. Surface Diffusion : Atomistic and Collective Processes", Rhodes (grece) Août 1996.
    "Dissolution kinetics of a thin metal deposit on a metallic substrate : Ag/Cu and Ni/Ag". A. Saúl, J. M. Roussel, G. Tréglia, and B. Legrand (Poster).
13. "SEMAT'97. Structure Electronique dans les Matériaux : théorie et calculs", Orsay (France) May 1997.
    "Propriétés électroniques et structurales de l'alliage de surface $SbCu_2$" ; J. Goniakowski, G. Tréglia, and A. Saúl (Poster).
14. "Fifth International Conference on Atomically Controlled Surfaces, Interfaces and Nanostructures (ACSIN 5)", Aix en Provence (France). July 1999.
    "On the adsorption of Pd on MoS2(0001) : *ab-initio* electronic structure calculations" ; J. D. Fuhr, J. O. Sofo, and A. Saúl (Poster).
15. "Réunion générale du GDR-DFT", Cap d'Agde (France). May 2005.
    "Conductance de fils monoatomiques de métaux 5d" ; L. de la Vega, A. Martín-Rodero, A. Levy Yeyati, J. Fuhr, A. Saúl (oral).

16. "APS March Meeting", Pittsburgh (USA), March 2009.
"Electronic Structure of the quasi-two-dimensional spin gap system $SrCu_2(BO_3)_2$" ; A. Saúl (oral), G. Radtke, H. Dabkowska, B. Gaulin, and G. Botton.
17. "Departamento de Fisica - CNEA", Buenos Aires (Argentina), May 2009.
"Electronic and magnetic properties of spin gap systems" ; G. Radtke, A. Saúl (oral).
18. "Journée du Laboratoire CINaM", Marseille, October 2009.
"Propriétés électroniques et magnétiques de systèmes à gap de spin" ; A. Saúl (oral).
19. "Journée du département théorie et simulation numérique", Marseille, November 2010.
"Calculation of magnetic interactions in spin gap systems" ; A. Saúl (oral) and G. Radtke.
20. "Modélisation multi-échelle en science des matériaux", Marseille, December 2010.
"Magnetic structure and superexchange pathways in $CsV_2O_5$" ; A. Saúl (oral) and G. Radtke.
21. "Service de Recherche en Metallurgie Physique", Saclay, March 2011.
"Magnetic interactions in $CsV_2O_5$ : where are the dimers ?" ; A. Saúl (oral) and G. Radtke.
22. "APS March Meeting", Dallas (USA), March 2011.
"Magnetic structure and super-exchange pathways in $CsV_2O_5$" ; A. Saúl (oral), G. Radtke.
23. "Departement of Material Science", University of California Berkeley (USA), April 2011.
"Magnetic interactions in $CsV_2O_5$ : where are the dimers ?" ; A. Saúl (oral) and G. Radtke.
24. "MIT Concrete Sustainability Hub", Cambridge, March 2012.
"Calculation of surface energies and surface stresses" ; A. Saúl (oral).
25. "APS March Meeting", Boston (USA), March 2012.
"Density fonctional calculation of the electronic and magnetic properties of $\alpha$-$CoV_2O_6$" ; A. Saúl (oral), G. Radtke.
26. "Journée du Laboratoire CINaM", Marseille, July 2012.
"Rapide introduction au Magnétisme et propriétés du $CoV_2O_6$" ; A. Saúl (oral).
27. "Département Théorie et Simulation Numérique - CINaM", Marseille, September 2012.
"Rapide introduction au Magnétismes" ; A. Saúl (oral).
28. "Service de Physique et Chimie des Surfaces et Interfaces", Saclay, October 2012.
"Frustration and magnetic order in $\alpha$-$CoV_2O_6$" ; A. Saúl (oral), D. Vodenicarevic and G. Radtke.
29. "Département de Physique. Université de Montréal", Montréal, October 2012.
"Frustration and magnetic order in $\alpha$-$CoV_2O_6$" ; A. Saúl (oral), D. Vodenicarevic and G. Radtke.
30. "Réunion générale du GDR ModMat", Marseille (France), February 2013.
"Méthode de liaisons fortes" ; A. Saúl (oral).
31. "Département Théorie et Simulation Numérique - CINaM", Marseille, February 2012.
"Magnetism of $Ba_4Ru_3O_{10}$ : structural trimers behaving as magnetic dimers" ; A. Saúl (oral).
32. "APS March Meeting", Baltimore (USA), March 2013.
"Magnetism of $Ba_4Ru_3O_{10}$ : structural trimers behaving as magnetic dimers" ; A. Saúl (oral), G. Radtke, Y. Klein, G. Rousse.
33. "Institut Lumière Matière", Lyon, June 2013.
"Quelques surprises concernant les interactions effectives d'échange dans les oxydes" ; A. Saúl (oral).
34. "Departamento de Fisica - CNEA", Buenos Aires (Argentina), July 2013.
"Magnetism of $Ba_4Ru_3O_{10}$ : structural trimers behaving as magnetic dimers" ; A. Saúl (oral), G. Radtke, Y. Klein, G. Rousse.
35. "APS March Meeting", Denver (USA), March 2014.
"Theoretical study of the electronic and magnetic properties of $\beta$-$TeVO_4$" ; A. Saúl (oral), G. Radtke.
36. "Unité Mixte Internationale - MIT/CNRS" Cambridge (USA), March 2014.
"Radiation damage of materials (concrete)" ; A. Saúl (oral).
37. "Department of Physics - Northeastearn University", Boston (USA), March 2014,
"Surprises in the effective exchange interactions of some oxides" ; A. Saúl (oral), G. Radtke.
38. "Unité Mixte Internationale - MIT/CNRS" Cambridge (USA), April 2014.
"Density Functional Study of Radiation Damage in Cement" ; A. Saúl (oral).
39. "Departamento de Fisica - CNEA", Buenos Aires (Argentina), December 2014.
"Magnetic nanopantograph in the $SrCu_2(BO_3)_2$ Shastry-Sutherland lattice" ; A. Saúl (oral), G. Radtke, M. Jaime, H. Dabkowska, and M. Salamon

40. "Département Théorie et Simulation Numérique - CINaM", Marseille, December 2014.
"Ab-initio study of radiation damage in cement" ; A. Saúl (oral).
41. "Unité Mixte Internationale - MIT/CNRS" Cambridge (USA), January 2015.
"Radiation Damage in Cement" ; A. Saúl (oral).
42. "APS March Meeting", San Antonio (USA), March 2015.
"Theory of lattice response to external magnetic field in $SrCu_2(BO_3)_2$ magnetostriction driven by panthograph effect" ; A. Saúl (oral), G. Radtke, M. Jaime, H. Dabkowska, and M. Salamon
43. "CINaM", Marseille, March 2015.
"Etudes de la déformation d'un système de dimères magnétiques par l'application d'un champ magnétique extérieur" ; A. Saúl (oral), G. Radtke, M. Jaime, H. Dabkowska, and M. Salamon.
44. "Service de Recherche en Metalurgie Physique - CEA", Saclay (France), March 2015.
"Etudes de la déformation d'un système de dimères magnétiques par l'application d'un champ magnétique extérieur" ; A. Saúl (oral), G. Radtke, M. Jaime, H. Dabkowska, and M. Salamon.
45. "Département de Physique - Université de Montréal", Montréal (Canada), April 2015.
"Etudes de la déformation d'un système de dimères magnétiques par l'application d'un champ magnétique extérieur" ; A. Saúl (oral), G. Radtke, M. Jaime, H. Dabkowska, and M. Salamon.
46. "CECAM", Dublin (Ireland), June 2015.
"First-principles investigation of $^{90}$Sr $\beta-$ decay in cement" ; L. Dezerald, J. J. Kohanoff, A. A. Correa, A. Caro, R. J. M. Pellenq, F. J. Ulm, and A Saúl (poster).
47. "Journée du Laboratoire CINaM", Marseille, October 2015.
"Domage d'irradiation dans le ciment" ; A. Saúl (oral).
48. "Département Théorie et Simulation Numérique - CINaM", Marseille, December 2015.
"Propriétés magnétiques d'un crystal molćulaire" ; A. Saúl (oral).
49. "Département Théorie et Simulation Numérique - CINaM", Marseille, March 2016.
"Interactions magnéto-élastiques dans $SrCu_2(BO_3)_2$ révélés par spectroscopie Raman et calcul de phonons" A. Saúl (oral).
50. "CNRS-EWHA International Reserach Center", Seoul (Korea), April 2016.
"On some surprising magnetic effective exchange interactions of some oxides", A. Saúl (oral).
51. "Korea Advanced Institute of Science and Technology (KAIST)", Daejeon (Korea). April 2016.
"On some surprising magnetic effective exchange interactions of some oxides", A. Saúl (oral).
52. "Interactions effectives d'échange et effets magnéto-élastiques dans les composes à base de dimères de spin" Institut de Chimie Radicalaire (Marseille). June 2016
A. Saúl (oral).
53. "Réunion générale du GDR ModMat", Rouen (France), January 2017.
"Interactions magnetoélastiques dans $SrCu_2(BO_3)_2$ : un système de dimères de Cu orthogonaux agissant comme un pantographe" A. Saúl (oral).
54. "Département Théorie et Simulation Numérique - CINaM", Marseille, February 2017.
"Linear piezomagnetism in $UO_2$" ; A. Saúl (oral).
55. "International Center for Advanced Studies", San Martin (Argentina). June 2017.
"Bose-Einstein condensation in a quantum magnet formed by free radical tetramers" A. Saúl (oral).
56. "Physik Institut - University of Zurich", Zurich (Swistzerland). September 2017.
"Magnetoelastic interactions in a system of orthogonal Cu dimers : magnetostriction experiments and density functional calculations" A. Saúl (oral).
57. "Institut de Sciences Chimiques de Rennes", Rennes (France). October 2017.
"Interactions magnétoélastiques dans deux systèmes anti-ferromagnétiques" A. Saúl (oral).
58. "CEA - Cadarache", Cadarache (France). October 2017.
"Interactions magnétoélastiques dans deux systèmes anti-ferromagnétiques" A. Saúl (oral).
59. "Département de Physique. Université de Montréal", Montréal, February 2018.
"Interactions magnétoélastiques et piezo-magnétisme dans le dioxyde d'uranium" A. Saúl (oral).
60. "APS March Meeting", Los Angeles (USA). March 2018.
"Evidence of Bose-Einstein condensation in a quantum magnet formed by free radical tetramers."
A. Saúl (oral).
61. "Latin American Symposium on Solid State Physics", Bariloche (Argentina). April 2018.
"Evidence of Bose-Einstein condensation in a quantum magnet formed by free radical tetramers."
A. Saúl (oral).

62. "Réunion générale du GDR Meeticc", Dunkerque (France). January 2019.
"Evidence of Bose-Einstein condensation in a quantum magnet formed by free radical tetramers." A. Saúl (oral).
63. "Atomistic Simulation Center", Queen's University Belfast (UK) February 2019.
"Magneto elastic interactions in two antiferromagnetic systems under high magnetic field." A. Saúl (oral).
64. "Réunion thématique Magnétisme du GDR Meeticc", Caen (France). October 2019.
"Theoretical and experimental study of magnetoelastic interactions in two antiferromagnetic systems" A. Saúl (oral).
65. "Departamento de Física. Universidad de Buenos Aires", Buenos Aires (Argentina), October 2019.
"Evidence of Bose-Einstein condensation in a quantum magnet formed by free radical tetramers". A. Saúl (oral).
66. "Kick-off Meeting GDR Low-dimensional van der Waals Hetero-structures", Online - Organized by GDR Howdi, March 2021.
"Magnetoelastic interaction in the two-dimensional magnetic material $MnPS_3$ studied by first principles calculations and Raman experiments". A. Saúl (oral).

# Others Activities

**Reviewer**

— *Journals.* Physica Status Solidi (B). Journal of the American Chemical Society. Chemical Physics Letters. Faraday Transactions. Physical Review B. Materials Science and Engineering B. Physical Review Letters. Surface Science. Applied Surface Science. Computational Materials Science. Physica B. Physics Letters A.

— *Agencies.* ECOS-Sud. Conseil Régional Bourgogne. Secretaría de Ciencia, Tecnología e Innovación Productiva (Argentina). French National Research Agency.

— *Promotions and tenure.* Université Paul Cézanne. Université de la Méditerranée. Université de Toulon-Var.

**Languages**

Spanish, French, and English.