Dr. Souraya Goumri-Said

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Personal

Citizenship: French

Gender : Female

Education

1. Ph.D. Physics, University of Bourgogne (France), 2004. Mention : Nano-Optic. Title : "Contribution to study of the optical images formation in Near-field Microscopy: two-dimensional study of the probe".

2. Master of Physics (validation), University of Bourgogne (Dijon, France), (2000). Mention : Quantum mechanics in conjugated polymers.

Academic Awards

1. CERUNA project Award, from University of Namur (Belgium) , Solid state physics Laboratory (2008-2009).

2. "Bourse Regional de Pays de la loire" award from Maine University (France) (2006-2007)

3. EU Research and Training Network (contract HPRN-CT-2002-00317) award on "elementary excitations on nano-particles and metallic nanoclusters", from Kaiserslautern University (Germany) (2005-2006).

4. Physics department of Bourgogne University (Dijon, France) Researcher- Assistant Professor, Academic Support Program Fall-2002

5.Physics department of Val de Marne University (Paris, France) Researcher- Assistant Professor, Academic Support Program Fall-2004

Academic & research Experience

Université de Bourgogne, Dijon (France), Nano-optical Near field group, Physics Department

Researcher-Assistant Professor, Academic year 2001-2002, Academic Support Program, Group : Nano-optical Near field. **Courses** : solid state physics, Analytical mechanics, optic and electromagnetism, for Undergraduate students.

Research Assistant, Spring 2002–Spring 2003 **Title** : Modeling Near-field measurements on nano-structures.

Research- Assistant Professor, Academic Support Program, Academic year 2003-2004. **Courses** : solid state physics, Analytical mechanics for Undergraduate students.

Université Val de Marne, Paris 12 (France), Condensed matter group, Department of Physics

Researcher-Assistant Professor, **Project :** Cuprates and magnetic oxides : Experience and theory Academic year 2004-2005. **Courses** : Quantum mechanics, Thermodynamics, Matlab, solid state physics for Undergraduate and Master students

Technische Universität Kaiserslautern (Germany), Condensed Matter Theory Group, Department of Physics

Postdoctoral position, Academic year 2005-2006. **Project :** Magnetic nano-clusters and femoto-seconds from ab-initio methods.

Lecturer in physics, Fall-Spring 2005. **Courses** : Quantum mechanics, solid state physics for Undergraduate students

Université du Maine, Le Mans (France), Department of Physics

Postdoctoral position, Academic year 2006-2007. **Project :** Design route for the synthesis of super transition metal nitride alloys.

Researcher- Assistant Professor, Fall 2007-Winter 2008. **Courses** : Quantum mechanics, Thermodynamics, Optic, mechanics, Matlab and Fortran languages, solid state physics for Undergraduate and Master students

University of Namur (Belgium), Department of Physics

Postdoctoral position (CERUNA Project), Spring 2008- Winter 2009. **Project:** Electromagnetic response of metallic nano-particles and plasmom excitations

Research Assistant and co-manager of Mirage project : collaboration between Arcelor Mittal-FUNDP (NAMUR) Spring 2009-Summer 2010. **Project:** Thermochromic and electrochromic properties of nano-layered tungsten oxide (WO_3) and vanadium oxide (VO_2) : from experience and theory

King Abdullah University of Science and Technology (KAUST)

Research fellow, Summer 2010- Summer 2012. **Project :** spintronic and magnetic transport in nanofilms : understanding the spin injection in organic molecular semiconductors systems.

Summer 2012- Summer 2013. **Project :** Theoretical and experimental measurement of silicon nanoparticles optical properties.

Thesis and projects supervision

1. Co-supervisor of Master, Student : Ahmed-Ali Kanoun, from "Physics departement, Faculté des Sciences Mostaganem University (Algeria), 2011–2012. Title : "Modelling and simulation of organic LED".

2. Co-supervisor of PhD thesis, Student : N. Kanoun-Bouayed from Solid state physics group, "Département de Physique, Faculté des Sciences Tlemcen University (Algeria), 2007–2011. Title : "Density functional theory study of physical properties of nitrides, rare-earth dioxides and silicon-germanium oxynitrides".

3. Co-supervisor of Master project, Student : Lagarde Foka, University of Paris 12, mention: Physics (2004-2005). Title " Theoretical study of physical properties for GaAs using the density functional theory ".

4. Co-supervisor of Master of science project, Student : Danilo Bianchi Granato, King Abdullah University of Science and Technology (KAUST), mention: Physical Sciences (2011-2012). Title : A Density Functional Theory Study of the Electronic Structure of Doped Tin Monoxide.

Research

Experimental work

1. Control of Scanning Tunnelling Microscopy (STM), Atomic Force Microscopy (AFM) or an optical near field (PSTM).

2. Ellipsometric spectra measurement.

Physical codes, packages and scientific softwares

1. Wien2K. A program package WIEN2k allows to perform electronic structure calculations of solids using density functional theory (DFT).(from 2002).

2. ABINIT. A package whose main program allows one to find the total energy, charge density and electronic structure of systems made of electrons and nuclei (molecules and periodic solids) within Density Functional Theory (DFT), using pseudopotentials and a planewave basis.(from 2006).

3. Elk FP-LAPW Code . An all-electron full-potential linearised augmented-plane wave (FP-LAPW) code with many advanced features).(from 2006).

4. Gaussian09. It provides state-of-the-art capabilities for electronic structure modeling. Gaussian 09 is licensed for a wide variety of computer systems.(from 2006).

5. VASP. Performs ab-initio quantum-mechanical molecular dynamics (MD) using pseudopotentials and a plane wave basis set.(from 2007).

6. CASTEP. Software package which uses density functional theory to provide a good atomic-level description of all manner of materials and molecules. CASTEP can give information about total energies, forces and stresses on an atomic system, as well as calculating optimum geometries, band structures, optical spectra, phonon spectra and much more. It can also perform molecular dynamics simulations.(from 2006).

7. DMol3. It allows to model the electronic structure and energetics of molecules, solids, and surfaces using density functional theory (DFT). We can study a broad range of systems using DMol3, including organic and inorganic molecules, molecular crystals, covalent solids, metallic solids, and infinite surfaces of a material. With DMol3.(from 2006).

8. GULP, is a program for performing a variety of types of simulation on materials using boundary conditions of 0-D (molecules and clusters), 1-D (polymers), 2-D (surfaces, slabs and grain boundaries), or 3-D (periodic solids). The focus of the code is on analytical solutions, through the use of lattice dynamics, where possible, rather than on molecular dynamics).(from 2007).

9. ASW program package, The Augmented Spherical Wave method based on the Born-Oppenheimer approximation and Density Functional Theory (DFT)).(from 2009).

10. XCrysden, a crystalline and molecular structure visualization program which aims to display isosurfaces and contours.(from 2001).

11. Smeagol, DFT code, designed to calculate transport properties of atomic scale devices.(from 2011).

12. SIESTA is both a method and its computer program implementation, to perform efficient electronic structure calculations and ab initio molecular dynamics simulations of molecules and solids. SIESTA's efficiency stems from the use of strictly localized basis sets and from the implementation of linear-scaling algorithms which can be applied to suitable systems. A very important feature of the code is that its accuracy and cost can be tuned in a wide range, from quick exploratory calculations to highly accurate simulations matching the quality of other approaches, such as plane-wave and all-electron methods.

13. Quantum Espresso is an integrated suite of Open-Source computer codes for electronic-structure calculations and materials modeling at the nanoscale. It is based on density-functional theory, plane waves, and pseudopotentials.(from 2008).

International Recognition

1. SciVerse ScienceDirect TOP25 Hottest Articles : http://top25.sciencedirect.com/subject/materials-science/15/journal/computational-materials-science/09270256/archive/19 Theoretical investigations of structural, elastic, electronic and thermal properties of Damiaoite PtIn"2 Computational Materials Science, Volume 43, Issue 2, August 2008, Pages 243-250 Goumri-Said, S.; Kanoun, M.B.

Conference Presentations & Workshop

1. E-MRS 2013 Spring Meeting, "Buckling and ripples effects on the electronic structure of graphene" Strasbourg (France) 27 to 31 May 2013. Poster presentation.

2. E-MRS 2013 Spring Meeting, "Exploring the physical properties of the microporous zirconogermanate" Strasbourg (France) 27 to 31 May 2013. Poster presentation.

3. GDR-CoDFT 2013, Lorient (France) 21 to 24 May 2013. Poster presentation.

2. The 19th International Conference on Magnetism with Strongly Correlated Electron Systems 2012 (ICM2012) Busan, Korea From July 8th to 13th, 2012. Poster presentation

2. 56th Annual Conference on Magnetism and Magnetic Materials,Scottsdale, Arizona (USA). Poster presentation : "The origin of the ferromagnetic ordering of zinc vacancies in Sc-doped ZnO: bulk versus thin-films". From October 30 to November 3, 2011.

3. 56th Annual Conference on Magnetism and Magnetic Materials,Scottsdale, Arizona (USA). Poster presentation : "Ab-initio understanding of the spin injection in organic molecular semiconductors systems". From October 30 to November 3, 2011.

4. Functional Metalorganics Magnetism, structure, transport, May 30 to June 1, 2011, Uppsala (Sweden). Poster presentation : "Ab-initio study of organic molecules for spintronic applications".

5. ECNF - European Conference on Nano Films, March 22 - 25, 2010 Liège, (Belgium). Oral Presentation : "Optical Modeling of Electrochromic and thermochromic thin films".

6. EDGE 2009 International EELS Workshop Banff, Alberta, (Canada), May 17 to 22, 2009. Poster presentation : "Low-loss simulation with a discrete dipole approximation".

7. "Journées de la Matière Condensée" (JMC11) - Strasbourg, August 25 to 29 2008. Tow posters: (1) "EELS characterisation of subwavelength excitation in metallic nanoparticles : a DDA study". (2)"First-principles calculation of molybdenum nitrides : Structure and mechanical properties"

8. Workshop: "Ion dynamics and relaxation in ion conducting disordered solids" March 26 to 29, 2007. Université du Maine - Le Mans, (France). Oral Presentation: " First principles investigation of LAMOX derived from La2Mo2O9 .

9. JSNUM2006, June 01 to 02, 2006. Paris (France). Oral presentation : "Electronic structure and magnetism of small TM and RE clusters by first principles calculations".

10. Exciting Workshop : First-principles approaches to optical and photoelectron spectra, ", March 9 to 12, 2006, LMU Munich. (Germany). Poster presentation : "First principles calculations of electronic and magnetic properties of Co_5 cluster" .

11. Exciting Workshop : Symposium on Excited State Properties of Solids, May 16 to 19, 2005, Mannheim, (Germany). Poster presentation, title : "Theoretical study of electronic and magnetic properties of Diluted magnetic semiconductor zincblende $Al_{1-x}Cr_xN$ ". Organization and participation.

12. Fourth International Congress on Inorganic Materials, University of Antwerp, (Belgium) 19 to 21, 2004. Poster presentation: "Electronic structure and spin polarization of Mn-doped diluted magnetic III-nitride semiconductors. (organized by ELSEVIER). Participation".

13. GDR " Ondes Groupe Thématique " 5th edition, Dijon (France), December, 15 and 16 (2004). Oral communication, title : "Two-dimensional Simulations of Photon Scanning Tunneling Microscopy: the role of the probe tip characteristics in image formation".

14. 1st International conference on electromagnetic Near-Field Characterisation, June 18 to 20 (2003), Rouen (France). Oral presentation, title :" Two-dimensional model for Photon Scanning Tunneling Microscopy (PSTM): differential method".

15. Congress: "Journées européennes sur les méthodes numériques en électromagnétisme", March 6 to 8(2002), Toulouse (France). Oral presentation, title :"Numerical Study of Photolithography System: Electromagnetic Differential Method".

16. Congress: Congrès Euro-Méditerranéen de la Matière Condensée, CEMMC, Université de Tlemcen, June 04 and 05 (2001), Tlemcen, (Algeria). Poster presentation, title : "Numerical Study of Photolithography Systems based on electromagnetic Modal Method".

17. Spring College on Numerical Methods in Electronic Structure Theory, the Abdus Salam International Centre for Theoretical Physics, Trieste (Italy), May 7 to 25 (2001). Oral presentation : "Numerical study of the one-dimensional Hubbard model in determination of trans-polyacetylene properties".

18. Winter College on INTERFEROMETRY and APPLICATIONS IN MODERN PHYSICS , February, 2-13 (2004). ICTP center, Trieste (Italy). Poster communication, title : "Numerical Study of PSTM device based on Modal Method".

19. Summer School'2001 on Multiscale Materials Modelling, organized by Prof. Hafid Aourag from "Computational Materials Science Laboratory", Physics Department of University of Sidi Bel-Abbès (Algeria). August 25th - 31th, (2001). Organizations and tutorials about Monte carlo method applied to Hubbard model and quantum systems.

20. Algerian Summer School on Applied DFT and Simulation Methods, organized by Prof. Hafid Aourag from "Computational Materials Science Laboratory", Physics Department of University of Sidi Bel-Abbès (Algeria). August 26th - September 1st, (2000). Organization and tutorials.

Professional Activities

1. Technical Committee of the "2013 International Conference on Advances in Industrial Control, Electronics and Computer Engineering (AICECE'13)" . http://www.aicece.net/committee.htm

Member of Société Française de Physique , 2008–Present.

Member of American Physical Society , 2010–Present.

I. **Referee** for:

1. Journal of Applied Physics. (AIP, American Institute of Physics).

2. Polymer (Elsevier).

3. Material chemistry and physics (Elsevier).

4. Physica B (Elsevier).

5. physica status solidi (Wiley-VCH Verlag GmbH and Co. KGaA).

6.Philosophical Magazine and Philosophical Magazine Letters (Taylors and Francis Group).

7.Journal of Magnetism and Magnetic Materials (Elsevier).

8. Journal of Physics and Chemistry of Solids (Elsevier).

II. **Associate Editor (AE)** for : Central European Journal of Physics
`http://www.versita.com/science/physics/cejp/`

Miscellaneous

Computer Skills: C, C++, Fortran, LaTeX, Linux, Mathematica, Matlab, OpenMP.

Languages: French, English and Arabic.

Last updated: May 4, 2013
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Published Papers

1. R. Moussa, **S. Goumri-Said,** and H. Aourag, "Unperturbed and perturbed non-linear Schrödinger system for optical fibers Solitons". Phys. Lett. A 266 173 (2000).

2. **S. Goumri-Said**, R. Moussa, J.-P. Dufour, L. Salomon, and H. Aourag, "Numerical Study of the one-dimensional Hubbard model in determination of Trans-polyacetylene properties". Physica B 296 377 (2001).

3. **S. Goumri-Said**, F. de Fornel,. L. Salomon and H. Aourag; "Quantum Monte Carlo study of the alternating Extended Peierls-applied to the trans-polyacetylene properties". Physica B 301 299 (2001).

4. **S. Goumri-Said**, H. Aourag, L. Salomon and J. -P. Dufour "The behavior of correlation functions in trans-polyacetylene: quantum Monte Carlo study", Solid State Sciences, 4 757. (2002).

5. **S. Goumri-Said**, H. Aourag, L. Salomon and J. -P. Dufour "Electronic momentum distribution in the one-dimensional extended Hubbard model: determinantal Monte Carlo study", Polymer, 43 6323(2002).

6. **S. Goumri-Said** and H. Aourag. "Quantum Monte Carlo study of insulating state in NaV2O5", Journal of Alloys and Compounds, Volume 354, 24 (2003).

7. **S. Goumri-Said**, H. Aourag, L. Salomon and J. -P. Dufour, "Quantum Monte-Carlo calculation of correlation functions of undistorted, cis-distorted and trans-distorted polyacene", Polymer 44, 1765 (2003).

8. **S. Goumri-Said**, H. Aourag, "New Quantum Monte Carlo formulation for modeling trans-polyacetylene properties: specific heat calculation", Polymer 45 2443 (2004).

9. **S. Goumri-Said**, M. B. Kanoun, A.E. Merad, G. Merad and H. Aourag, "Prediction of structural and thermodynamic properties of zinc-blende AlN:molecular dynamics simulation", Chemical Physics 302 135 (2004).

10. **S. Goumri-Said**, M. B. Kanoun, A.E. Merad, G. Merad and H. Aourag, "Empirical molecular dynamics study of structural, elastic and thermodynamic properties of zinc-blende-like SiGe compound', Materials Science and Engineering B, 111, 207 (2004).

11. M. B. Kanoun, **S. Goumri-Said**, A.E. Merad, G. Merad, J. Cibert and H. Aourag, "Zinc-blende AlN and GaN under pressure : " structural, electronic, elastic and piezelectric properties" , Semicond. Sci. Technol. 19, 1220 (2004).

12. **S. Goumri-Said**, R.Moussa, B. Belgoumène and H. Aourag, "Analytical investigation of solitary waves in nonlinear Kerr medium', Optical Materials 27, 203 (2004).

13. **S. Goumri-Said**, L. Salomon, J. -P. Dufour, H. Aourag, "Numerical Study of photolithography system: Electromagnetic Differential Method", Journal of Materials Processing Technology 148, 50 (2004).

14. **S. Goumri-Said**, L. Salomon, J. -P. Dufour and F. Defornel "Two-Dimensional Numerical Simulations of Photon Scanning Tunneling Microscopy: Fourier Modal Method and R-Matrix Algorithm", Optical and Quantum Electronics 36, 787 (2004).

15. A. Dazzi, **S. Goumri-Said** and L. Salomon, "Theoretical study for an absorbing sample in Infrared Near Field Spectromicroscopy", Optics Communications 235, 351 (2004).

16. **S. Goumri-Said**, L. Salomon, J. -P. Dufour, F. Defornel and A. Zayats, ”Numerical Simulations of Photon Scanning Tunneling Microscopy: role of a probe tip geometry in image formation” , Optics Communications 244 245 (2005).

17. M. B. Kanoun, **S. Goumri-Said,** A. E. Merad and J. Cibert " First-principles investigation electronic structure and magnetic properties in ferromagnetic Gax Mn1-xN and AlxMn1-xN ". J. Phys. D: Appl. Phys. 38 1 (2005).

18. M. B. Kanoun, **S. Goumri-Said**, A. E. Merad and H. Mariette " Ab initio study of structural parameters and gap bowing in Zincblende AlxGa1-xN and AlxIn1-xN alloys". J. Appl. Phys. 98, 063710 (2005).

19. M. B. Kanoun and **S. Goumri-Said** " Electronic properties of binary noble metal nitride PtN: First principles calculations". Phys. Phys. Rev. B. 72 113103 (2005) .

20. A. E. Merad, M. B. Kanoun, and **S. Goumri-Said**, " Ab Initio Study of Electronic Structures and Magnetism in ZnMnTe and CdMnTe Diluted Magnetic Semiconductors ". Journal of Magnetism and Magnetic Materials, 302 536 (2006).

21. M. B. Kanoun, **S. Goumri-Said**, "Investigation of structural stability and electronic properties of CuN, AgN and AuN by first principles calculations". Physics Letters A, Volume 362, 73 (2007).

22. M. B. Kanoun, **S. Goumri-Said**, and M. Jaouen, " Structure and mechanical stability of molybdenum nitrides: a first principles study, Phys. Rev. B 76, 134109 (2007).

23. M. B. Kanoun and **S. Goumri-Said**, "Analysis of Mn K-edge x-ray absorption spectrum in Al1-xMnxN by full potential calculations". Physica B: Condensed Matter, 403, 2847 (2008).

24. **S. Goumri-Said**, M. B. Kanoun, "Electronic structure and magnetism of Eu-doped GaN: first-principles study based on LDA+U ". J. Phys. D: Appl. Phys. 41 035004 (2008).

25. **S. Goumri-Said**, M. B. Kanoun, "Theoretical investigations of structural, elastic, electronic and thermal properties of Damiaoite PtIn2", Computational Materials Science, 43, 243 (2008).

26. **S. Goumri-Said**, M. B. Kanoun and F. Calvayrac, "PtMn3No.25: A potential candidate for spintronic applications by ab initio calculations", Journal of Magnetism and Magnetic Materials, 321, 1012 (2009).

27. M. B. Kanoun and **S. Goumri-Said**, "Theoretical study of structural parameters and energy gap composition dependence of $Ga_{1-x}B_xN$ alloys" Semicond. Sci. Technol. 23, 125036 (2008)

28. M. B. Kanoun, **S. Goumri-Said** and M. Jaouen, "Steric effect on the M site of nanolaminate compounds M2SnC (M = Ti, Zr, Hf and Nb)" J. Phys.: Condens. Matter 21, 045404 (2009) .

29. P. Hermet, **S. Goumri-Said**, M. B. Kanoun, and L. Henrard, "First-principles investigations of physical properties of the magnesium nitridoboride" J. Phys. Chem. C,113, 4997 (2009).

30. M.B. Kanoun, **S. Goumri-Said**, A. H. Reshak, "Theoretical study of mechanical, electronic, chemical bonding and optical properties of Ti_2SnC, Zr_2SnC, Hf_2SnC and Nb_2SnC", Computational Materials Science 47, 491 (2009).

31. N. Kanoun-Bouayed, S. Goumri-Said, A. E. Merad, and M. B. Kanoun, "Ab initio calculation of electronic structure and magneties properties of rare earth nitride using LDA plus U approach: EuN and GaEuN". THIN FILMS AND POROUS MATERIALS, MATERIALS SCIENCE FORUM 609, 167-172 (2009).

32. M.B. Kanoun, **S. Goumri-Said**, A. H. Reshak, A. E. Merad, "Electro-structural correlations, elastic and optical properties among the nanolaminated ternary carbides Zr_2AC Solid Solid State Sciences, Volume 12, Issue 5, May 2010, Pages 887-898

33. **S. Goumri-Said**, M. B. Kanoun, "Ab-initio investigations of the electronic properties of bulk wurtzite Beryllia and its derived nanofilms", Physics Letters A, Volume 374, Issue 38, 23 August 2010, Pages 3977-3981.

34. M. B. Kanoun, I. R. Shein, S. Goumri-Said, "Origin of incompressibility and hardness from electronic and mechanical properties of hard material ruthenium diboride", Solid State Communications, Volume 150, Issues 23-24, June 2010, Pages 1095-1098.

35. N. Kanoun-Bouayed, M. B. Kanoun, **Souraya Goumri-Said**, "Structural stability, elastic constants, bonding characteristics and thermal properties of zincblende, rocksalt and fluorite phases in copper nitrides: plane-wave pseudo-potential ab initio calculations", CENTRAL EUROPEAN JOURNAL OF PHYSICS, 9 205-212 (2011).

36. B. Amin, Iftikhar Ahmad, M. Maqbool, **S. Goumri-Said**, and R. Ahmad, "Ab initio study of the bandgap engineering of Al1-xGaxN for optoelectronic applications". Journal of Applied Physics 109, 023109 (2011).

37. B. Amin, S. Arif, Iftikhar Ahmad, M. Maqbool, R. Ahmad, **S. Goumri- Said**, K. Pribrey, "Cr doped III-V (nitrides) dilute magnetic alloys: potential candidates for spintronics". Journal of ELECTRONIC MATERIALS, Vol. 40, No. 6, (2011).

48. A. Lafort, H. Kebaili, **S. Goumri-Said**, O. Deparis, R. Cloots, J. De Coninck, M. Voué, F. Mirabella, F. Maseri, S. Lucas, "Optical properties of thermochromic VO2 thin films on stainless steel: experimental and theoretical studies", Thin Solid Films, Volume 519, Issue 10, 1 March 2011, Pages 3283-3287.

39. Abdullah Al-Sunaidi, **Souraya Goumri-Said**, "Investigating the adsorption of H2O on ZnO nanoclusters by first principle calculations". Chemical Physics Letters, Volume 507, 111 (2011).

40. I. Bantounas, **S. Goumri-Said**, M. B. Kanoun, A. Manchon, I. Roqan and U. Schwingenschlogl, "Ab initio investigation on the magnetic ordering in Gd doped ZnO" . J. Appl. Phys. 109, 083929 (2011).

41. **S. Goumri-Said**, N. Kanoun-Bouayed, A. H. Reshak, M. B. Kanoun, "On the electronic nature of silicon and germanium based oxynitrides and their related mechanical, optical and vibrational properties as obtained from DFT and DFPT" Computational Materials Science 53, 158-168 (2012).

42. M. B. Kanoun, A. H. Reshak, N. Kanoun-Bouayed, and **S. Goumri-Said**, "Evidence of Coulomb correction and spin-orbit coupling in rare-earth dioxides : CeO_2, PrO_2 and TbO_2", Journal of Magnetism and Magnetic Materials 324, 1397-1405 (2012).

43. M. B. Kanoun,**S. Goumri-Said**, U. Schwingenschlogl, and A. Manchon, "Magnetism in Sc-doped ZnO with zinc vacancies: A hybrid density functional and GGA+U approaches", CHEMICAL PHYSICS LETTERS 532, 96 (2012)

44. M. B. Kanoun, P. Hermet, and **S. Goumri-Said** "Structure, elastic stiffness and hardness of $Os_{1-x}RuxB_2$ solid solution transition metal diborides", JOURNAL OF PHYSICAL CHEMISTRY C, 116, 11746 (2012).

45. M. B.Kanoun, **S. Goumri-Said**, A. Manchon, and U. Schwingenschlogl, "Ferromagnetism carried by highly delocalized hybrid states in Sc-doped ZnO thin films", Appl. Phys. Lett. 100, 222406 (2012).

46. **S. Goumri-Said** and M. B. Kanoun, "DFT+U study of the oxide-ion conductor pentalanthanum hexamolybdenum henicosaoxide " Journal of Solid State Chemistry 197, 304(2013).

47. Bakhtiar Ul Haq, R. Ahmed, **S.Goumri-Said**, A. Shaari and A. Afaq. "Electronic structure engineering of ZnO with the modified BeckeŰJohnson exchange versus the classical correlation potential approaches Electronic structure engineering of ZnO with the modified Becke-Johnson exchange versus the classical correlation potential approaches", Phase Transitions (2013).

48. **S. Goumri-Said** and M. B. Kanoun, Aurelien Manchon and Udo Schwingenschlögl ,"Spin-polarization reversal at the interface between benzene and Fe(100)" Journal of Applied Physics 113, 013905 (2013)

49. **S. Goumri-Said** H. Ozisik, E. Deligoz and M. B. Kanoun, "Ab-initio investigations of the Strontium Gallium Nitrides ternaries Sr3GaN3 and Sr6GaN5: promising materials for optoelectronic" Semiconductor science and technology (IOP, accepted for publication).

50. **S. Goumri-Said** R. Ahmed and M. B. Kanoun, "Density-functional study of High hydrogen content complex hydrides Mg(BH4)2 : a promising conducting hydride" Materials Chemistry and Physics (Under review).

Published Books and chapters in books

1. **Chapter title** : "DFT fundamental understanding of the structure-physical properties relationships for borides: ZrB_2 and ZrB_{12}". By S. Goumri-Said and M. B. Kanoun . **Book title** "MAX Phases and Ultra-High Temperature Ceramics for Extreme Environments", edited by Woodhead Publishing Ltd. Book Editors : Prof. Jim Low (Department of Applied Physics Curtin University, Perth, Australia), Yoshio Sakka (NIMS, Tsukuba, Japan) and Prof. Chunfeng Hu of the Chinese Academy of Science. (date of edition : May 2013).

2. **Chapter title** : "Theoretical study of physical properties and oxygen incorporation effect in nanolaminated ternary carbides 211MAX phases". By M. B. Kanoun and S. Goumri-Said. **Book title** "Advances in Science & Technology of Mn+1AXn Phases", edited by Woodhead Publishing Ltd. Book Editor : Prof. Jim Low (Department of Applied Physics Curtin University, Perth, Australia). (date of edition : September 2011).

3. **Book edition** : Applied Physics series: "Investigation of Electronic, Magnetic and Elastic Properties Using First Principles Calculations and New Empirical Approach: Application of III-V, II-VI Semiconductors and Perovskite-Like Fluorides Materials ", by Dr. S.G. Pandalai, Managing Editor. Research Signpost. 37/661 (2), Fort P.O. Trivandrum-695 023, Kerala (India). (Year of edition 2006). Book Editor : Souraya Goumri-Said

4. **Participation by two chapters** in physical book entitled "Theoretical and Experimental Studies of Magnetic Materials Including Rare-Earth Nitrides, Semimagnetic Semiconductors, Perovskites Manganites and Metallic Multilayers and Films, 2008: ISBN: 978-81-7895-365-6 Editor: Abdelkrim El-Hasnaïne Merad. Titles of Chapters are (1) Electronic and magnetic structure of rare-earth nitrides using the LDA+U approach: EuN and GaEuN. (2) PtMn3No.25: Looking for a new candidate for spintronic applications.