Curriculum Vitae

Mohammed Benali KANOUN

Assistant Professor
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Over 880 citations in the period, 2000 – 2016,
H-number = 18

ACADEMIC PROFILE

From 2013 Qualification for the rank of full professor of Physics, CNU (university national council), ministry of higher education and scientific research, France
Section 28: condensed matter and materials

2000 – 2004 **Doctor of Philosophy**, University of Tlemcen – University of Grenoble 1.
Degree in **Materials Science**, PhD Thesis titled, *First principles study of structural, elastic and electronic properties of AlN and GaN semiconductors under pressure and magnetism in AlN:Mn and GaN:Mn systems.*

HONORS AND AWARDS

2009: *CERUNA project Award, from* University of Namur, Belgium,

2006: Awards Fall 06, University of Poitiers, France.

2005: Awards Fall 05, Institut d'Electronique de Microélectronique et de Nanotechnologie (IEMN), University of Lille I, France.

PROFESSIONAL AND RESEARCH EXPERIENCE

2016–present Assistant Professor, College of Sciences, Alfaisal University

2014 –2015 Research Scientist, in School of Chemistry and Biochemistry - School of Physics, at the Georgia Institute of Technology
- Graphene oxide films and like graphene materials

2012 – 2014 Research fellow, in KAUST Catalysis Center, KAUST
- Quantum chemistry investigations of the chemical properties, reactivity, composition and structure of metal and bimetallic nanoparticles: for example oxygen activation on gold nanoparticles.

- Development of new theoretical tools in order to understand the mechanism of catalytic activities of sub nanometer gold nanoparticles.

2010 – 2012 Research fellow in Physical Science & Engineering division, KAUST
- Understanding physical and chemical properties of thin film, nanowires
- Metal and organic interface
- Inorganic and organic hybrid materials
- Transport properties of interface metal semiconductors

2009 – 2010 Research fellow, supported by *CERUNA project,* at University of Namur, Belgium, Theoretical chemistry laboratory
- Studying the linear and nonlinear optical properties of new molecules by *ab initio* methods: Hartree-Fock, hybrid methods, MP2, TDDFT
- Development of new programs to determine the linear and nonlinear responses of organic materials.
- Predicting the macroscopic properties of molecular crystals newly synthesized

2008 – 2009 Research fellow, supported by *industrial project between* University of Namur *and AGFA-Graphics-Gevaert,* Belgium
- Assisting the R&D projects of the industrial partner.
- Applying and assessing the computational chemistry methods to industrially oriented research projects, development and installation of scientific programs, and related maintenance and formation.
- Organizing work meeting and preparation of annual reports

2006 – 2007 Temporary Assistant Professor at University of Poitiers, France.
- Experimental and theoretical prediction of new ceramic phases.

2005 – 2006 Temporary Assistant Professor at University of Lille I, France.
(Research collaboration between Institut d'Electronique de Microélectronique et de Nanotechnologie (IEMN) and THALES-France (TIGER Industrial Project)
- Investigation of InAlN, AlGaN and GaN/AlGaN alloys by ab initio and Monte Carlo methods.
- Study the effect of boron impurity in AlN and GaN semiconductors and its interest in optoelectronics

2000 – 2004 Doctoral research at University of Grenoble (Atomic Energy Commission, CEA, mixed team CEA/DRFMC/SP2M- CNRS) and University of Tlemcen.
- Performing experiments on epilayers (nanolayers) of wurzite (Ga,Mn)N were grown by nitrogen plasma- assisted molecular beam epitaxy (MBE), on a GaN buffer layer.
- Modeling and simulation of physical properties of (Ga,Mn)N.

TEACHING EXPERIENCE

- Teaching of physics and materials science courses (lecture and labs) for several undergraduate and graduate levels at different institutions since 2000.
- Trained and co-supervised graduate and undergraduate students.

SUPERVISED GRADUATE STUDENTS

Julien Guenole, M.Sc, at University of Poitiers, 2007.
Nicolas Nivault, M.Sc. at University of Poitiers, 2007.

Teaching courses

- Course and tutorials : force, energy and optics
- Course and tutorials : electrostatic, electromagnetic, and oscillations
- Course and tutorials : fundamental properties of semiconductors
- Course : Thermal transfer and solar energy for Master students
- Course : fundamentals of materials
- Course and tutorials : electro-kinetics
- Tutorials theory of signal and treatment of signal using MATLAB
- Tutorials wave functions
- Course : introduction to solid state physics
- Course and tutorials : forces and Newton's law of motion, conservation of energy.
- Course and tutorials : electrostatic, electromagnetic and electricity
- Course : physical and chemical properties of materials
- Tutorial : quantum mechanical, molecular dynamics and tight binding methods
- Tutorial "Computational physics and programming: FORTRAN
- General Chemistry II Lab CHM102

RESEARCH INTERESTS

- Reaction mechanisms, catalytic activities, physical organic and coordination chemistry of metal nanoparticles
- Investigating new materials related to photo-catalysis, photovoltaic and solar cell conversion
- Energy Storage and Conversion
- Catalysis for sustainable energy technologies
- Photovoltaic heterojunctions of hybrid organic/inorganic materials
- Nano-structured materials as well as thin film, nanowires and metal nanoparticles.
- Graphene and like graphene
- Spintronics materials

SYNERGISTIC ACTIVITIES

Conference Organization

- 2013 International Scientific Committee of Symposium, E-MRS spring meeting protective coatings and thin films, Strasbourg, France.
- 2001 Organization Committee of Euro-Mediterranean conference of the Condensed Matter, Algeria

Reviewer

2011: Evaluate the project proposal for Croatian Science Foundation.
2004 – Present: Journal Referee for J. Applied Physics, Solid State Communications, Computational Materials Science, Journal of Physics and Chemistry of Solids, Diamond and related materials, Journal of the American Ceramic Society.

PUBLICATIONS

Refereed Journals

60/ N. Shahzad, A. Hussain, N. Mustafa, N. Ali, **M. B. Kanoun**, S. Goumri-Said, First principles study of the adsorption and dissociation of H_2S on TiO_2 anatase (001) surfaces. *RSC* Advances, **6**, 7941-7949 (2016).

59/ S. Goumri-Said, Rashid Ahmed and **M. B. Kanoun**, Density-functional theory study of high hydrogen content complex hydrides $Mg(BH_4)_2$ at low temperature. Renewable Energy, 90 114–119 (2016)

58/ B. U. Haq, R. Ahmed, G. Abdellatif, A. Shaari, F. K. Butt, **M. B. Kanoun**, S Goumri-Said, Dominant ferromagnetic coupling over antiferromagnetic in Ni doped ZnO: First-principles calculations. Front. Phys. 11(3), 117101 (2016)

57/ N. H. Hong, N T. Huong, T-Y. Kim, S. Goumri-Said and **M. B. Kanoun**. *Tuning Magnetic Properties of $BiFeO_3$ Thin Films by Controlling Rare-Earth Doping: Experimental and First-Principles Studies.* The Journal of Physical Chemistry C, 119, 14351−14357 (2015)

56/ M. Bououdina, A. A. Dakhel, M. El-Hilo, D. H. Anjum, **M. B. Kanoun** and S. Goumri-Said, Revealing a room temperature ferromagnetism in cadmium oxide nanoparticles: an experimental and first-principles study. *RSC* Advances, 5, 33233–33238 (2015).

55/ L. Li, L. Zhou, S. Ould-Chikh, D.H. Anjum, **M. B. Kanoun,** J. Scaranto, M.N., S. Khalid, P.V. Laveille, L. D'Souza, A. Clo, J-M. Basset, *Controlled Surface Segregation Leads to Efficient Coke-Resistant Nickel/Platinum Bimetallic Catalysts for the Dry Reforming of Methane*. ChemCatChem (Catalysis) 7, 819-829 (2015).

54/ **M. B. Kanoun** and L. Cavallo, *Quantifying the Impact of Relativity and of Dispersion Interactions on the Activation of Molecular Oxygen Promoted by Noble Metal Nanoparticles*. The Journal of Physical Chemistry C, 118, 13707−13714 (2014)

53/ G. Abadias, **M. B. Kanoun**, S. Goumri-Said, L. Koutsokeras, S.N. Dub, Ph. Djemia, *Electronic structure and mechanical properties of ternary ZrTaN alloys studied by ab initio calculations and thin film growth experiments*. Physical Review B 90, 144107 (1-18) (2014).

52/ **M. B. Kanoun**, S. Goumri-Said, and U. Schwingenschlogl, *Ferromagnetism in Cr-doped passivated AlN nanowires*. Journal of Materials Chemistry A 2, 9287–9290 (2014)

51/ B. U. Haq, **M. B. Kanoun**, R. Ahmed, M. Bououdina, S. Goumri-Said, *Hybrid functional calculations of potential hydrogen storage material: Complex dimagnesium iron hydride*. International Journal of Hydrogen Energy 39, 9709-9717 (2014)

50/ B. U. Haq, R Ahmed, A. Shaari, F. El Haj Hassan, **M. B. Kanoun**, and S. Goumri-Said. *Analysis of wurtzite and zincblende GaN/InN based solar cells alloys: first-principles investigation within the improved modified Becke–Johnson potential*. Solar Energy, 107, 543–552 (2014)

49/ **M. B. Kanoun**, and S. Goumri-Said, *Effect of alloying on elastic properties of ZrN based transition metal nitride alloys*. Surface & Coatings Technology, 255, 140-145 (2014)

48/ N. H. Hon, **M. B. Kanoun**, S. Goumri-Said, J-H. Song, E. Chikoidze, Y. Dumont, A. Ruyter, and M. Kurisu, *The origin of magnetism in transition-metal-doped ZrO_2 thin films: experiment and theory*, Journal of Physics: Condensed Matter, 25, 436003 (2013).

47/ M. Zarshenas, R Ahmed, **M. B. Kanoun**, B. ul. Haq, A. R. M. Isa and S. Goumri-Said, *First principle investigations of the physical properties of hydrogen-rich MgH_2*, Physica Scripta, 88, 065704-8 (2013).

46/ S. Goumri-Said, H. Ozisik, E. Deligoz and **M. B. Kanoun**, *Ab initio investigations of the strontium gallium nitride ternaries Sr_3GaN_3 and Sr_6GaN_5: promising materials for optoelectronic*, Semiconductor Science and Technology, 28, 085005 (2013).

45/ S. Goumri-Said, **M. B. Kanoun**, A. Manchon and U. Schwingenschlogl, *Spin-polarization reversal at the interface between benzene and Fe(100)*, Journal Applied Physics, 113, 013905 (2013).

44/ S. Goumri-Said and **M. B. Kanoun**, *DFT+U study of the oxide-ion conductor pentalanthanum hexamolybdenum henicosaoxide*, Journal of Solid State Chemistry 197, 304–311 (2013).

43/ **M. B. Kanoun**, S. Goumri-Said, A. Manchon and U. Schwingenschlogl, *Ferromagnetism carried by highly delocalized hybrid states in Sc-doped ZnO thin films*, Applied Physics Letters, 100, 222406 (2012).

42/ **M. B. Kanoun**, P. Hermet, and S. Goumri-Said, *Structure, Elastic Stiffness and Hardness of $Os_{1-x}Ru_xB_2$ Solid Solution Transition Metal Diborides*, The Journal of Physical Chemistry C, 116 (21), 11746-11751 (2012).

41/ **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, 96-99 (2012).

40/ **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: An ab initio study*. Journal of Magnetism and Magnetic Materials 324, 1397–1405 (2012).

39/ S. Goumri-Said, N. Kanoun-Bouayed, A. H. Reshak and **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).

38/ A. Ségerie, F. Castet, **M. B. Kanoun**, A. Plaquet, V. Liégeois, and B. Champagne, *NLO switching behavior in the solid state : A theoretical investigation on anils*. Chemistry of Materials, 23, 3993–4001 (2011).

37/ I. Bantounas, S. Goumri-Said, **M. B. Kanoun**, A. Manchon, I. Roqan and U. Schwingenschlögl, *Ab initio investigation on the magnetic ordering in Gd doped ZnO*. Journal Applied Physics, **109**, 083929-083935 (2011).

36/ **M. B. Kanoun**, and B. Champagne, *Calculating the second-order nonlinear optical susceptibilities of 3-methyl-4-nitropyridine N-oxide, 2-carboxylic acid-4-nitropyridine-1-oxide, 2-methyl-4-nitroaniline, and m-nitroaniline crystals.* International Journal of Quantum Chemistry, 111, 880-890 (2011)

35/ S. N. Labidi, **M. B. Kanoun**, M. de Wergifosse, and B. Champagne, *Theoretical assessment of new molecules for second order nonlinear optics.* International Journal of Quantum Chemistry 111, 1583–1595 (2011).

34/ **M. B. Kanoun**, E Botek, and B. Champagne, *Electrostatic modeling of the linear optical susceptibilities of 2-methyl-4-nitroaniline, m-nitroaniline, 3-methyl-4-nitropyridine N-oxide and 2-carboxylic acid-4-nitropyridine-1-oxide crystals.* Chemical Physics letters 487, 256–262 (2010).

33/ S. Goumri-Said and **M. B. Kanoun,** *Ab-initio investigations of the electronic properties of bulk wurtzite Beryllia and its derived nanofilms*. Physics Letters A 374, 3977-3981 (2010).

32/ N. Kanoun-Bouayed, **M. B. Kanoun**, and S. 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 (2010).

31/ **M. B. Kanoun**, I. R. Shein and S. Goumri-Said, *Origin of incompressibility and hardness from electronic and mechanical properties of hard material ruthenium diboride*. Solid State communication 150, 1095-1098 (2010).

30/ **M. B. Kanoun**, S. Goumri-Said, A. H. Reshak and A.E. Merad, *Electro-structural correlations, elastic and optical properties among the nanolaminated ternary carbides Zr_2AC*, Solid State Science, 12, 887-898 (2010).

29/ **M. B. Kanoun**, S. Goumri-Said and 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, 491-500 (2009).

28/ P. Hermet, S. Goumri-Said, **M. B. Kanoun**, and L. Henrard, *First-principles investigations of physical properties of the magnesium nitridoboride.* The Journal of Physical Chemistry C, *113*, 4997–5003 (2009).

27/ **M. B. Kanoun**, S. Goumri-Said, and M. Jaouen, *Steric effect on the M site of nanolaminate compounds M_2SnC (M = Ti, Zr, Hf and Nb).* Journal of Physics: Condensed Matter 21, 045404 (2009).

26/ S. Goumri-Said, **M. B. Kanoun**, and F. Calvyrac, *$PtMn_3N_{0.25}$: a potential candidate for spintronic applications by ab-initio calculations.* Journal of Magnetism and Magnetic Materials 321, 1012-1014 (2009).

25/ N. Kanoun-Bouayed, S. Goumri-Said, A. E. Merad, and **M. B. Kanoun**, *Ab initio calculation of electronic structure and magnetic properties of rare earth nitride using LDA+U approach: EuN and GaEuN*. Materials Science Forum 609, 167-172 (2009).

24/ A. E. Merad, and **M. B. Kanoun**, *Effect of chromium and vanadium on nanolayered ternary carbides: Ab-initio study*. Materials Science Forum 609, 239-242 (2009).

23/ **M. B. Kanoun**, and S. Goumri-Said, *Theoretical study of structural parameters and energy gap composition dependence of $B_xGa_{1-x}N$ alloys*. Semiconductor Science and Technology 23, 125036 (2008).

22/ **M. B. Kanoun** and M. Jaouen, *Structure of the ternary carbide Ti_3SnC_2 from ab initio calculations.* Journal of Physics: Condensed Matter 20, 085211 (2008).

21/ **M. B. Kanoun** and S. Goumri-Said, *Analysis of Mn K edge x-ray absorption spectrum in $Al_{1-x}Mn_xN$ by full potential calculations.* Physica B: Condensed Matter, 403, 2847 (2008).

20/ S. Goumri-Said and **M. B. Kanoun,** *Electronic structure and magnetism of Eu-doped GaN: first-principles study based on LDA+U*. Journal of Physics D: Applied Physics, **41,** 035004 (2008).

19/ S. Goumri-Said and **M. B. Kanoun**, *Theoretical investigations of structural, elastic, electronic and thermal properties of Damiaoite $PtIn_2$.* Computational Materials Science, 43, 243-250 (2008).

18/ **M. B. Kanoun,** S. Goumri-Said, and M. Jaouen, *Structure and mechanical stability of molybdenum nitrides: A first principles study*. Physical Review B 76, 134109 (2007).

17/ **M. B. Kanoun** and S. Goumri-Said. *Investigation of structural stability and electronic properties of CuN, AgN and AuN by first principles calculations*. Physics Letters A 362, 73-83 (2007).

16/ A. E. Merad, **M. B. Kanoun**, 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).

15/ **M. B. Kanoun**, S. Goumri-Said, A. E. Merad and H Mariette, *Ab initio study of structural parameters and gap bowing in zincblende $Al_xGa_{1-x}N$ and $Al_xIn_{1-x}N$ alloys.* Journal Applied Physics, 98, 063710 (2005).

14/ **M. B. Kanoun** and S. Goumri-Said, *Electronic properties of the binary noble metal nitride PtN : First-principles calculation.* Physical Review B 72, 113103 (2005).

13/ A. Titov, X. Biquard, D. Halley, S Kuroda, E. Bellet-Amalric, H Mariette, J Cibert, A.E. Merad, **M.B. Kanoun**, E. Kulatov, Y. A. Uspenski, *X-ray Absorption near structure and valence state of Mn in (Ga,Mn)N*. Physical Review B 72, 115209 (2005).

12/ **M. B. Kanoun**, S. Goumri-Said, A. E. Merad and J. Cibert, *First-principles investigation of electronic structure and magnetic properties in ferromagnetic $Ga_xMn_{1-x}N$ and $Al_xMn_{1-x}N$.* Journal of Physics D: Applied Physics, 38, 1853-1859 (2005).

11/ A. E. Merad, **M. B. Kanoun**, G. Merad, J. Cibert and H. Aourag, *Full potential investigation of the electronic and optical properties of stressed CdTe and ZnTe.* Materials Chemistry and Physics. 92, 333-339 (2005).

10/ **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 piezoelectric properties.* Semiconductor Science and Technology 19, 1220-1231 (2004).

9/ **M. B. Kanoun**, A. E. Merad, G. Merad, J. Cibert and H. Aourag, *Prediction study of pressure effect on elastic properties for zincblende BN, AlN, GaN and InN.* Solid-State Electronics 48, 1601-1606 (2004).

8/ **M. B. Kanoun**, A. E. Merad, J. Cibert, H. Aourag, and G. Merad. *Strained* properties *of zinc-blende cubic GaN : First principles study.* Journal of Alloys and Compounds 366, 96-93 (2004).

7/ S. Goumri-Said, **M. B. Kanoun**, A. E. Merad, G. Merad and H. Aourag, *Empirical Molecular dynamics simulation of structural and thermodynamic properties of zinc-blende SiGe.* Materials Science & Engineering B 111, 207-213 (2004).

6/ 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 –141 (2004).

5/ A. E. Merad, **M. B. Kanoun**, H. Aourag, J. Cibert and G. Merad. *Ab initio study of electronic properties of zincblende AlN and deformation potentials under hydrostatic stress*. Materials Chemistry and Physics 82, 471-477 (2003).

4/ **M. B. Kanoun**, A. E. Merad, H. Aourag, J. Cibert and G. Merad. *Molecular-dynamics simulations of structural and thermodynamic properties of ZnTe using a three body potential.* Solid State Sciences 5, 1211-1216 (2003).

3/ A. E. Merad, **M. B. Kanoun**, J. Cibert, H. Aourag, and G. Merad. *Stress-dependence tight binding study of Tellurium-based II-VI semiconductors*. Physics Letters A 315, 143-149 (2003).

2/ A. E. Merad, **M. B. Kanoun**, H. Aourag, J. Cibert and G. Merad. *Electronic and optical properties of CdTe under hydrostatic pressure effect.* Superlattices and Microstructures 32, 25-34 (2002).

1/ **M. B. Kanoun**, W. Sekkal, H. Aourag and G. Merad. *Molecular-dynamics study of the structural, elastic and thermodynamic properties of Cadmium* Telluride. Physics Letters A 272, 113-118 (2000).

Conference proceedings

A. E. Merad, **M. B. Kanoun**, G. Merad and J. Cibert, Hydrostatic pressure dependence of the direct gap, transverse effective charge and refractive index of CdTe system.
Journal of Electron Devices 2, 31-33 (2003).

A. E. Merad, **M. B. Kanoun**, G. Merad and J. Cibert, Theoretical analysis of the bowing factors in electronic and optical properties in $Cd_{1-x}Zn_xTe$ alloys.
Revue des Energies Renouvelables, ICPWE, 107-111 (2003).

CONTRIBUTION IN INTERNATIONAL BOOKS

- **M. B. Kanoun** and S. Goumri-Said, Theoretical Assessment of the Mechanical, Electronic, and Vibrational Properties of the Paramagnetic Insulating Cerium Dioxide and Investigation of Intrinsic Defects.
  Book titled, Handbook of Research on Nanoscience, Nanotechnology, and Advanced Materials. Edited by Engineering science reference, IGI Global.

- **M. B. Kanoun** and S. Goumri-Said, *Theoretical study of physical properties and oxygen incorporation effect in nanolaminated ternary carbides 211MAX phases*.
  Book titled, Advances in Science & Technology of $M_{n+1}AX_n$ Phases, Edited by Woodhead Publishing Ltd, 2012.

- M. B. Kanoun**,** Theoretical investigation of electronic structure and magnetic properties of ferromagnetic $Al_{1-x}Cr_xN$ alloys.
  Book entitled: Theoretical and Experimental Studies of Magnetic Materials Including Rare-Earth Nitrides, Semimagnetic Semiconductors, Perovskites Manganites and Metallic Multilayers and Films, Edited by Transworld Research Network, 2008

- M. B. Kanoun and S. Goumri-Said, Theoretical calculations of III-V-nitrides properties and their alloys.
  Book entitled: "Investigation of Electronic, Magnetic and Elastic Properties Using First Principles Calculations and New Empirical Approach: Application to III-V, II-VI Semiconductors and Perovskite-like Fluorides Materials, Edited by Transworld Research Network,2006.

TALK AND POSTER PRESENTATIONS MEETING

1/ **M.B. Kanoun** « Trends in the elastic response of ZrN based transition metal alloys » E-MRS spring meeting: protective coatings and thin films, May 27 – 31, 2013, Strasbourg, France. (Oral presentation).

2/ S. Goumri-said and **M.B. Kanoun** « Buckling and ripples effects on the electronic structure of graphene» E-MRS spring meeting: The route to post-Si CMOS devices: from high mobility channels to graphene-like 2D nanosheets, May 27 – 31, 2013, Strasbourg, France. (Poster presentation).

3/ **M.B. Kanoun**, *et al*, « *The origin of the ferromagnetism of Sc-doped ZnO thin-films* » The 19th International Conference on Magnetism (ICM12), July 8 – 13, 2012, BEXCO, Busan, Korea (Poster presentation).

4/ **M.B. Kanoun**, *et al*, *« The origin of the ferromagnetic ordering of zinc vacancies in Sc-doped ZnO: bulk versus thin-films* » 56th Annual Conference on Magnetism and Magnetic Materials MMM, October 30 – November 3, 2011 Scottsdale, Arizona (USA) (Poster presentation).

5/ **M.B. Kanoun**, *et al, Theoretical investigation of ferromagnetic organic-inorganic hybrid material*, Functional Metalorganics - *Magnetism, structure, transport,* May 30 – June 1, 2011, Uppsala, Sweden, (Poster presentation).

6/ M.B. Kanoun, *et al*, *Electrostatic interaction schemes to evaluate the linear and nonlinear optical susceptibilities of 3-methyl-4-nitropyridine N-oxide (POM) and 2-methyl-4-nitroaniline (MNA) crystals*, *Scientific Meeting on Chemistry related to Physics & Material Sciences*, 15 and 16 February 2010, Veldoven, Netherlands. (oral presentation)

7/ **M.B. Kanoun**, and B. Champagne, *Calculation of macroscopic linear and nonlinear optical properties for some molecular crystals*, *Journée MÉTAMORPHOSE 'Les matériaux'*, January 29, 2010, Brussels, Belgium (Poster presentation)

8/ **M.B. Kanoun**, *et al*, *Investigation of the linear optical susceptibilities of meta-nitroaniline and 2-methyl-4-nitroaniline crystals*, *Journée Scientifique Annuelle de la société royale de chimie : 'Les matériaux du futur'*, october 08, 2009, Liège, Belgium. (Poster presentation)

9/ **M.B. Kanoun**, *Electronic structure prediction of new nitrides compounds*, Journées de Simulations Numériques *: June 1 and 2 2006, Jussieu, Paris (France).* (Poster presentation)

10/ **M. B. Kanoun,** S. Goumri-Said, *Electronic structure and magnetism of Eu-doped GaN: A first-principles study, First-principles approaches to optical and photoelectron spectra*, Workshop, 9-12 Mars 2006, LMU Munich. Germany (Poster presentation).

11/ **M. B. Kanoun,** *Electronic and magnetic properties of dilute magnetic semiconductor* $Ga_{1-x}Cr_xN$. Journées de Simulations Numériques, 2 and 3 June 2005 Jussieu, Paris, France (Poster presentation).

12/ **M. B. Kanoun,** *et al, Electronic structure and spin polarization of Mn-doped diluted magnetic III-nitride semiconductors*. (Organized by ELSEVIER). Fourth International Congress on Inorganic Materials, 19-21 September *2004,* Antwerp, Belgium (Poster presentation).

13/ **M. B. Kanoun,** *et al, Pressure dependence of energy band gaps for zincblende AlN and GaN*". International Congress on Photovoltaic and Wind Energies, ICPEW'03, *20-22 December 2003, Tlemcen,* Algeria (oral presentation)

14/ **M. B. Kanoun,** *et al, Equilibrium and thermodynamic properties of GaN using a three body potential* » Second International Congress on Materials Sciences and Engineering (CISGM'2) 13 &14 November 2001, Annaba, Algeria (oral presentation).

15/ **M. B. Kanoun,** *et al, Atomistic study of zinc-blende silicon carbide from molecular-dynamics*» Congrès Euro Méditerranéen de la Matière Condensée (CEMMC) 04, 05, & 06 June 2001, Tlemcen, Algeria (oral presentation)

16/ **M. B. Kanoun,** *et al, Theoretical calculation of the optical absorption in* $Hg_{1-x}Cd_xTe$ » 5ème Séminaire International sur la Physique Energétique (SIPE'5) *07, 08 and 09 November 2000,* Béchar, Algeria (Poster presentation).

17/ **M. B. Kanoun,** *et al, Molecular-dynamics simulation of thermomechanical properties of ZnSe and CdSe*» Sixth International Meeting on Materials Science, IMMS'6, 3, 4 & 5 April 2000, M'sila, Algeria (Poster presentation).

18/ **M. B. Kanoun,** *et al, Atomistic simulation of the structural, elastic and thermodynamic properties of CdTe and ZnTe* » First Arab Congress on Materials Science, ACMS – 1, 25, 26 & 27 October 1999 Sidi Bel-Abbès, Algeria (Poster presentation).

Workshops Attended

INSA-13, satellite meeting Dicadicals and Multiradicals: Theory and Experiment, July 27 and 28 2009, Namur, Belgium.

Symposium Molecular and Nanoscale Materials for Electronic, Optics and medicine**,** May 18 and 19 2009, Brussels, Belgium

Summer School '2001 on Multiscale Materials Modelling, University of Sidi Bel-Abbès. 25-31 August, 2000.

Summer School on Applied DFT and Simulation Methods, University of Sidi Bel-Abbès. 26 august – 1 September 2000.

TECHNICAL EXPERTISE

Quantum mechanical and electronic structure packages

VASP is a complex package for performing electronic structure calculations and quantum-mechanical molecular dynamics simulations using pseudopotentials or the projector-augmented wave method and a plane wave basis set.

GAUSSIAN 03 and 09: Quantum chemistry package capable of predicting many properties of atoms, molecules, reactive systems, e.g.; molecular energies, structures, vibrational frequencies, electron densities utilizing ab initio, density functional theory, semi-empirical, molecular mechanics, and various hybrid methods.

DMol^3: is a modeling program that uses density functional theory to simulate chemical processes and predict properties of materials both rapidly and accurately. It can predict processes in gas phase, solution, and solid environments.

ADF programs are powerful computational chemistry tools based on density functional density, with an emphasis on accuracy for heavy elements and spectroscopic properties.

CASTEP package is used the density functional theory with a plane wave basis set to calculate the electronic properties of crystalline solids, surfaces, molecules, liquids and amorphous materials from first principles.

Wien2k package allows performing electronic structure calculations of solids using density functional theory (DFT). It is based on the all-electron scheme with relativistic effects full-potential (linearized) augmented plane-wave ((L)APW)+local orbitals (lo) method.

SIESTA allows computing electronic structure calculations and ab initio molecular dynamics simulations of molecules and solids. It is based on density functional method using norm-conserving pseudopotentials and numerical linear combination of atomic orbitals basis set.

Homemade code:
(1) Calculating of the linear and nonlinear optical susceptibilities of molecular crystals using electrostatic approach.

(2) Computing of structural and thermodynamic properties of materials solids by using molecular dynamic simulation with the empirical potential as Tersoff, and Leonard-Jones.

Operating systems: Windows, different versions of Linux

Programming languages: Fortran, C++, Matlab

Document preparation: Microsoft word, powerpoint, Latex, Acrobat professional.

Graphing and data analysis software: Origin, Gnuplot, Mercury, Xcrysdens, Material Studio.

MEMBERSHIPS

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