

# CURRECULUM VITAE



## 1- PERSONAL DATA

**Name:** KHENATA RABAH

**Designation:** Full Professor.

**Date and Place of Birth:** 27 January 1967 - El Hachem- Algeria

**Nationality:** Algerian

**Qualification:** Computational Physics, Materials Physics, PhD.

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University of Mascara, P. B. 763-29000 Mascara, Algeria.

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## 2- EDUCATION

July 1987 Baccalaureate (Mathematic), - (Mascara-Algeria)

July 1992 "Engineer in electronics", University of Sidi Bel Abbès- Algeria

July 1995 Magister in Physics, University of Sidi-Bel Abbès- Algeria

June 2005 Ph.D (Doctorat), University of Sidi-Bel Abbès- Algeria

## 3- EMPLOYMENT HISTORY

1992-1993 Assistant Professor, Institute of Science- Sidi Bel Abbès University.

1995-2004 Assistant Professor of Physics, Institute of Biology- Mascara University.

2005-2009, Associate Professor of Physics, Faculty of Sciences and Technology at Mascara University.

2010-2017, Professor of Physics, Faculty of Sciences and Technology at Mascara University.

## 4- RESEARCH ACTIVITIES

In our research, we use the program package WIEN2k, which allows to performing electronic structure calculations of solids using density functional theory (DFT). It is based on the full-potential (linearized) augmented plane-wave ((L)APW) + local orbitals (lo) method, one among the most accurate schemes for band structure calculations. In DFT the local (spin) density approximation (LDA) or the improved version of the generalized gradient approximation (GGA) can be used. WIEN2k is an all-electron scheme including relativistic effects and has many features. Using this program we can studied: the structural (Structural stability, transition pressures), the mechanical (elastic properties), electronic (Band structure,

energy gaps, density of states, bonding properties) and optical properties; including the different optical transitions, refractive index, reflectivity, loss function, of solids. The effect of pressure and temperature on different physical properties can also study. The Plane Wave Pseudo potential PWP as well as FPLMTO methods are also used to calculate the above properties.

## **5-SCIENTIFIC PRODUCTIONS:**

### **5-1. PUBLICATIONS in (ISI)**

[https://www.researchgate.net/profile/Rabah\\_Khenata](https://www.researchgate.net/profile/Rabah_Khenata)

<https://scholar.google.com/citations?user=4FYHetYAAAAJ&hl=fr>

**With h-index: 35 in Google scholar with More than 5000 Citations**

1. D.P. Rai, Sanddeep, A. Shankar, Anup Pradhan Sakhya, T.P. Sinha, P. Grima-Gallardo, H. Cabrera, R. Khenata, M.P. Ghimire, R.K. Thapa: ***Electronic, optical and thermoelectric properties of bulk and surface (001) CuInTe2: A first principles study.*** Journal of Alloys and Compounds 01/2017;, DOI:10.1016/j.jallcom.2016.12.443
2. Sandeep; Rai, D. P.; Shankar, A.; et al.; **Investigation of the structural, electronic and optical properties of the cubic RbMF<sub>3</sub> perovskites (M = Be, Mg, Ca, Sr and Ba) using modified Becke-Johnson exchange potential**; MATERIALS CHEMISTRY AND PHYSICS Volume: 192 Pages: 282-290 Published: MAY 1 2017
3. Ammour, B.; Slimani, M.; Sifi, C.; et al. ;**Computational investigations of the band structure and thermodynamic properties of calcium-doped BaS using the FP-LAPW approach**; CHINESE JOURNAL OF PHYSICS Volume: 55 Issue: 2 Pages: 367-377 Published: APR 2017
4. Zenasni, M.; Monir, Mohammed El Amine; Baltach, H.; et al.; **First-principles investigation on the mechanical and electronic properties of novel Pb<sub>1-x</sub>Ce<sub>x</sub>Y alloys (Y = S, Se, and Te): an ab initio study**; MATERIALS RESEARCH EXPRESS Volume: 4 Issue: 9 Article Number: 095903 Published: SEP 2017
5. Drablia, S.; Boukhris, N.; Boulechfar, R.; et al. ; **Ab initio calculations of the structural, electronic, thermodynamic and thermal properties of**

6. D. P. Rai, Sandeep, A. Shankar, R. Khenata, A. H. Reshak, C. E. Ekuma, R. K. Thapa, San-Huang Ke: **Electronic, optical, and thermoelectric properties of Fe 2+ x V 1- x Al.** AIP Advances 04/2017; 7(4):045118., DOI:10.1063/1.4982671
7. Monir, Mohammed El Amine; Ullah, Hayat; Baltach, Hadj; et al.; **Mechanical and magneto-electronic properties of half-metallic ferromagnetism in Ti-doped ZnSe and CdSe alloys: Ab initio study;** JOURNAL OF MAGNETISM AND MAGNETIC MATERIALS Volume: 442 Pages: 107-117 Published: NOV 15 2017
8. K. Boudiaf, A. Bouhemadou, O. Boudrifa, K. Haddadi, F. Saad Saoud, R. Khenata, Y. Al-Douri, S. Bin-Omran, M. A. Ghebouli: **Structural, Elastic, Electronic and Optical Properties of LaOAgS-Type Silver Fluoride Chalcogenides: First-Principles Study.** Journal of Electronic Materials 03/2017;, DOI:10.1007/s11664-017-5452-6
9. L. Tairi, S. Touam, A. Boumaza, M. Boukhtouta, H. Meradji, S. Ghemid, S. Bin Omran, F. El Haj Hassan, R. Khenata: **Phase stability and electronic behavior of MgS, MgSe and MgTe compounds.** Phase Transitions 03/2017;, DOI:10.1080/01411594.2017.1302085
10. Roopam Sharma, Namita Singh, Khurshid Akhtar, R. Khenata, Dinesh Varshney: **Phonon drag and carrier diffusion contribution to heat transport of superconductor MgB 2.** International Journal of Computational Materials International Journal of Computational Materials Science and Engineeringnce and Engineering 03/2017;, DOI:10.1142/S2047684117500087
11. T. Chihi, A. Bouhemadou, M. Reffas, R. Khenata, M.A. Ghebouli, B. Ghebouli, L. Louail: **Structural, elastic and thermodynamic properties of iron carbide Fe 7 C 3 phases: an ab initio study.** DOI:10.1016/j.cjph.2016.12.014
12. A. K. Kushwaha, R. Khenata, A. Bouhemadou, S. Bin-Omran, K. Haddadi: Lattice **Dynamical Properties and Elastic Constants of the Ternary Chalcopyrite Compounds CuAlS2, CuGaS2, CuInS2, and AgGaS2.** Journal of Electronic Materials 02/2017;, DOI:10.1007/s11664-017-5290-6

13. Raed Jaradat, Mohammed Abu-Jafar, Issam Abdelraziq, Rabah Khenata, Dinesh Varshney, Saad Bin Omran, Samah Al-Qaisi: ***High-pressure structural phase transition and electronic properties of the alkali hydrides compounds XH (X D Li, Na).*** Phase Transitions 02/2017;, DOI:10.1080/01411594.2017.1286488
14. N. Ali, A. Hussain, R. Ahmed, W. N. Wan Shamsuri, Naser M. Abdel Salam, R. Khenata: ***Fabrication and characterization of 150 nm tin antimony sulfide thin films, a promising window layer material for homojunction solar cells.*** Applied Physics A 02/2017; 123(4):242., DOI:10.1007/s00339-017-0879-4
15. Mohammed El Amine Monir, H. Baltach, A. Abdiche, Y. Al-Douri, R. Khenata, S. Bin Omran, X. Wang, D. P. Rai, A. Bouhemadou, W. K. Ahmed, C. H. Voon: ***Doping-Induced Half-Metallic Ferromagnetism in Vanadium and Chromium-Doped Alkali Oxides K<sub>2</sub>O and Rb<sub>2</sub>O: Ab Initio Method.*** Journal of Superconductivity and Novel Magnetism 02/2017;, DOI:10.1007/s10948-017-4021-9
16. Bedjaoui, A.; Bouhemadou, A.; Aloumi, S.; et ; ***Structural, elastic, electronic and optical properties of the novel quaternary diamond-like semiconductors Cu<sub>2</sub>MgSiS<sub>4</sub> and Cu<sub>2</sub>MgGeS<sub>4</sub> ;*** SOLID STATE SCIENCES Volume: 70 Pages: 21-35 Published: AUG 2017
17. B. Amimour, M. Slimani, C. Sifi, R. Khémissi, H. Meradji, S. Ghemid, S. Bin Omran, R. Khenata: ***Computational investigations of the band structure and thermodynamic properties of calcium-doped BaS using the FP-LAPW approach.*** DOI:10.1016/j.cjph.2017.02.002
18. Sandeep, D.P. Rai, A. Shankar, M.P. Ghimire, R. Khenata, S. Bin Omran, S.V. Syrotyuk, R.K. Thapa: ***Investigation of the structural, electronic and optical properties of the cubic RbMF<sub>3</sub> perovskites (M = Be, Mg, Ca, Sr and Ba) using modified Becke-Johnson exchange potential.*** DOI:10.1016/j.matchemphys.2017.02.005
19. Diana Dahliah, M. Abu-Jafar, R. Khenata, A. Mousa, Raed Jaradat, Samah Al-Qaisi, S. Bin Omran: ***Structural stabilities and band structure characteristics of Platinum Nitride (PtN) via first-principles calculations.*** DOI:10.1016/j.cjph.2016.12.007
20. Samah Al-Qaisi, M.S. Abu-Jafar, G.K. Gopir, R. Ahmed, S. Bin Omran, Raed Jaradat, Diana Dahliah, R. Khenata: ***Structural, Elastic, Mechanical and Thermodynamic Properties of Terbium Oxide: First-Principles***

21. Diana Dahliah, M. Abu-Jafar, R. Khenata, Ahmad Mousa, Raed Jaradat, Samah Al-Qaisi, S. Bin Omran: **Structural stabilities and band structure characteristics of platinum nitride (PtN) via first-principles calculations.** Chinese Journal of Physics- Taipei- 01/2017; 55(2):211.
22. I. Hattabi, A. Abdiche, F. Soyalp, R. Moussa, R. Riane, K. Hadji. Bin-Omran, R. Khenata: **First-principles study of the structural, electronic and optical properties of cubic InAsxNyP1-x-y triangular quaternary alloys.** Chinese Physics B 01/2017; 26(1):017303.
23. D. P. Rai, Sandeep, R. Khenata, R. K. Thapa, Anup Pradhan Sakhya, T. P. Sinha, Boualem Merabet, Shahram Solaymani, M. Musa Saad H.-E, Arash Boochani, A. Shankar: **Electronic and optical properties of cubic SrHfO<sub>3</sub> at different pressures: A first principles study.** Materials Chemistry and Physics 11/2016; 186., DOI:10.1016/j.matchemphys.2016.11.045
24. S. Amari, F. Dahmane, S. Bin Omran, B. Doumi, I. E. Yahiaoui, A. Tadjer, R. Khenata: **Theoretical Investigation of the Structural, Magnetic and Band Structure Characteristics of Co<sub>2</sub>FeGe<sub>1-x</sub>Si<sub>x</sub> (x = 0, 0.5, 1) Full-Heusler Alloys.** Journal- Korean Physical Society 11/2016; 69(9)., DOI:10.3938/jkps.69.1462
25. R.K. You, Guodong Liu, Xiaotian Wang, Habib Rozale, L.Y. Wang, Rabah Khenata, Z.M. With, X.F. Dai: **First-principles study on quaternary Heusler compounds ZrFeVZ (Z = Al, Ga, In) with large spin-flip gap.** RSC Advances 11/2016; 6(111)., DOI:10.1039/C6RA18873G
26. T. Seddik, G. Uğur, F. Soyalp, R. Khenata, Deo Prakash, I.V. Kityk, Saleem Ayez Khan, A. Bouhemadou, S. Bin-Omran, D.P. Rai, K.D. Verma: **Computational investigations on band structure and electronic features of chromium-based carbides and nitride Cr<sub>3</sub>PX (X = C and N) through the FP-APW+LO approach.** SUPERLATTICES AND MICROSTRUCTURES Volume: 109 Pages: 1-12 Published: SEP 2017
27. Souadie, Z.; Bouhemadou, A.; Khenata, R.; et al. ; **Structural, elastic and lattice dynamical properties of the alkali metal tellurides: First-principles study ;** PHYSICA B-CONDENSED MATTER Volume: 521 Pages: 204-214 Published: SEP 2017
28. K. Hadji, A. Abdiche, F. Soyalp, S.Bin Omran, R. Khenata: **Computational investigations on band structure and optical properties of the BeSexTe1-**

**xalloys through the FP-LAPW approach.** Optik - International Journal for Light and Electron Optics 11/2016; DOI:10.1016/j.ijleo.2016.11.105

29. A. Shankar, D. P. Rai, Sandeep, R. Khenata, R. K. Thapa, P. K. Mandal: **Energy Bands and Thermoelectricity of Filled Skutterudite EuRu<sub>4</sub>As<sub>12</sub>.** International Journal of Thermophysics 11/2016; 37(37)., DOI:10.1007/s10765-016-2112-7
30. T Seddik, G U̇gur, R Khenata, S, U̇gur, F Soyalp, G Murtaza, D P Rai, A Bouhemadou, S Bin Omran: **Optoelectronic and thermoelectric properties of Zintl YLi<sub>3</sub>A<sub>2</sub>(A = Sb, Bi) compounds through modified Becke-Johnson potential.** Chinese Physics B 10/2016; 25(10)., DOI:10.1088/1674-1056/25/10/107801
31. M FAIZAN, G MURTAZA, S H KHAN, A KHAN, ASIF MEHMOOD, R KHENATA, S HUSSAIN: **First-principles study of the double perovskites Sr<sub>2</sub>XOsO<sub>6</sub> (X = Li, Na, Ca) for spintronics applications.** Bulletin of Materials Science 09/2016; 39(6)., DOI:10.1007/s12034-016-1288-6
32. X.T. Wang, Zhenxiang Cheng, Rabah Khenata, Habib Rozale, J.L. Wang, L.Y. Wang, R.K. Guo, G.D. Liu: **A first-principle investigation of spin-gapless semiconductivity, half-metallicity, and fully-compensated ferrimagnetism property in Mn<sub>2</sub>ZnMg inverse Heusler compound.** Journal of Magnetism and Magnetic Materials 09/2016; 423., DOI:10.1016/j.jmmm.2016.09.043
33. Fatma Saad Saoud, Khenata Rabah, Abdelmadjid Bouhemadou, Jean Claude Plenet, Mohamed Henini, Rihibe El Houda Djabou: **Structural Stabilities and Elastic Thermodynamic Properties of SrTe Compound and SrTe<sub>1-x</sub>Ca<sub>x</sub> Alloy Under High Pressure.** Journal of Electronic Materials 09/2016;, DOI:10.1007/s11664-016-4830-9
34. G MURTAZA, MAZHAR ULLAH, NAEEM ULLAH, MALIKA RANI, M MUZAMMIL, R KHENATA, SHAHID M RAMAY, UMAIR KHAN: **Structural, elastic, electronic and optical properties of bi-alkali antimonides.** Bulletin of Materials Science 09/2016; 39(6)., DOI:10.1007/s12034-016-1300-1
35. Naeem Ullah, G. Murtaza, M. A. Iqbal, Asif Mahmood, R. Khenata: **Computational study of Cu<sub>2</sub>ZnSn(X<sub>1-x</sub>Tex)<sub>4</sub> (X = S, Se) for optoelectronic applications.** International Journal of Modern Physics B 08/2016; DOI:10.1142/S021797921650137X
36. F. Dahmane, R. Khenata, B. Doumi, S. Bin Omran, I. V. Kityk, Sandeep, A. Tadjer, S. V. Syrotyuk, D. P. Rai: **Band Structure Simulations of the Structural, Electronic, Magnetic, and Half-Metallic Features of the Ti<sub>2</sub>CoAl<sub>1-x</sub>Sn<sub>x</sub> (x = 0, 0.25, 0.50, 0.75, 1) Heusler Alloys.** Journal of

Superconductivity and Novel Magnetism 08/2016;, DOI:10.1007/s10948-016-3711-z

37. S. Reguieg, R. Baghdad, A. Abdiche, M. A. Bezzerrouk, B. Benyoucef, R. Khenata, S. Bin-Omran: ***First-Principles Study of Structural, Optical, and Thermodynamic Properties of ZnIn<sub>2</sub>X<sub>4</sub> (X = Se, Te) Compounds with DC or DF Structure.*** Journal of Electronic Materials 08/2016;, DOI:10.1007/s11664-016-4831-8
38. A. Benahmed, A. Bouhemadou, R. Khenata, S. Bin-Omran: ***Ab initio study of the electronic, optical and thermodynamic properties of the ternary phosphides LiAeP (Ae = Sr, Ba),*** Indian Journal of Physics 08/2016;, DOI:10.1007/s12648-016-0909-7
39. D. P. Rai, Sandeep, M.P. Ghimire, A. Shankar, Anup Pradhan Sakhya, T. P. Sinha, R. Khenata, R. K. Thapa: ***Electronic and magnetic properties of X<sub>2</sub>YZ and XYZ Heusler compounds: a comparative study of density functional theory with different exchange-correlation potentials.*** Materials Research Express 07/2016; 3(7).
40. Fafa Chiker, Fatiha Boukabrine, H. Khachai, R. Khenata, C. Mathieu, S. Bin Omran, S. V. Syrotyuk, W. K. Ahmed, G. Murtaza: ***Investigating the Structural, Thermal, and Electronic Properties of the Zircon-Type ZrSiO<sub>4</sub>, ZrGeO<sub>4</sub> and HfSiO<sub>4</sub> Compounds.*** Journal of Electronic Materials 07/2016; 45(11)., DOI:10.1007/s11664-016-4767-z
41. Wilayat Khan, G. Murtaza, T. Ouahrani, Asif Mahmood, R. Khenata, Mohammed El Amine Monir, H. Baltache: ***Electronic, bonding, linear and non-linear optical properties of novel Li<sub>2</sub>Ga<sub>2</sub>GeS<sub>6</sub> compound.*** Journal of Alloys and Compounds 07/2016; 674., DOI:10.1016/j.jallcom.2016.02.213
42. O. Boudrifia, A. Bouhemadou, Ş. Uğur, R. Khenata, S. Bin-Omran, Y. Al-Douri: ***Structural, electronic, optical and elastic properties of the complex K<sub>2</sub>PtCl<sub>6</sub> -structure hydrides A RuH<sub>6</sub> (A = Mg, Ca, Sr and Ba): first-principles study.*** Philosophical Magazine 06/2016; 96(22), DOI:10.1080/14786435.2016.1198874
43. Sandeep, D P Rai, A Shankar, M P Ghimire, Anup Pradhan Sakhya, T P Sinha, R Khenata, S Bin Omran, R K Thapa: ***Band-gap engineering of La<sub>1-NdAlO<sub>3</sub> ( = 0,0.25,0.50,0.75,1) perovskite using density functional theory: A modified Becke Johnson potential study.</sub>*** Chinese Physics B 06/2016; 25(6)., DOI:10.1088/1674-1056/25/6/067101
44. A. Shankar, D. P. Rai, Sandeep, R. Khenata, M. P. Ghimire, R. K. Thapa: ***FP-LAPW study of energy bands and optical properties of the filled skutterudite \$\\$\\hbox {CeRu}\_{\{4\}}\\hbox {As}\_{\{12\}}\$ CeRu<sub>4</sub>As<sub>12</sub> with***

**spin-orbit coupling.** Journal of Computational Electronics 05/2016; 15(3)., DOI:10.1007/s10825-016-0836-z

45. M. Faizan, S. H. Khan, G. Murtaza, A. Khan, R. Khenata, Asif Mahmood, S. Hussain, M. A. Ali: **Structural, elastic, electronic and magnetic properties of Ba<sub>2</sub>XOsO<sub>6</sub> (X = Li, Na, Ca) double perovskites.** Indian Journal of Physics 05/2016; 90(11)., DOI:10.1007/s12648-016-0872-3
46. A. S. Ibraheam, Y. Al-Douri, U. Hashim, M. Ameri, A. Bouhemadou, R. Khenata: **Structural, optical and electrical investigations of Cu<sub>2</sub>Zn<sub>1-x</sub>Cd<sub>x</sub>SnS<sub>4</sub>/Si quaternary alloy nanostructures synthesized by spin coating technique.** Microsystem Technologies 05/2016;, DOI:10.1007/s00542-016-2986-0
47. Samad Iqbal, G. Murtaza, R. Khenata, Asif Mahmood, Abdullah Yar, M. Muzammil, Matiullah Khan: **Electronic and Optical Properties of Ca<sub>3</sub>MN (M = Ge, Sn, Pb, P, As, Sb and Bi) Antiperovskite Compounds.** Journal of Electronic Materials 05/2016; 45(8)., DOI:10.1007/s11664-016-4563-9
48. L. Hamioud, A. Boumaza, S. Touam, H. Meradji, S. Ghemid, F. El Haj Hassan, R. Khenata, S. Bin Omran: **First-principles calculations of the structural, electronic, optical and thermal properties of the BN x As 1-x alloys.** Philosophical Magazine 05/2016; 96(16)., DOI:10.1080/14786435.2016.1177669
49. Sandeep, D.P. Rai, A. Shankar, M.P. Ghimire, R. Khenata, R.K. Thapa: **A first principles study of Nd doped cubic LaAlO<sub>3</sub> perovskite: MBJ+U study.** Journal of Magnetism and Magnetic Materials 05/2016; 417., DOI:10.1016/j.jmmm.2016.05.093
50. A. Shankar, D.P. Rai, Sandeep, R. Khenata, R.K. Thapa: **FP-LAPW calculations of the elastic, electronic and thermoelectric properties of the filled skutterudite CeRu<sub>4</sub>Sb<sub>12</sub>.** Journal of Solid State Chemistry 05/2016; 240., DOI:10.1016/j.jssc.2016.05.027
51. Dinesh Varshney, S. Jain, S. Shriya, R. Khenata: **High-pressure and temperature-induced structural, elastic, and thermodynamical properties of strontium chalcogenides.** 04/2016; 10(3)., DOI:10.1007/s40094-016-0214-z
52. Sandeep Chettri, D. P. Rai, A. Shankar, R. Khenata, M. P. Ghimire, R. K. Thapa, S. Bin Omran: **GGA + U and mBJ + U study of the optoelectronic, magnetic and thermoelectric properties of the SmAlO<sub>3</sub> compound with spin-orbit coupling.** International Journal of Modern Physics B 04/2016;, DOI:10.1142/S0217979216500788

53. K. Bencherif, A. Yakoubi, N. Della, O. Miloud Abid, H. Khachai, R. Ahmed, R. Khenata, S. Bin Omran, S. K. Gupta, G. Murtaza: ***First Principles Investigation of the Elastic, Optoelectronic and Thermal Properties of XRuSb: (X = V, Nb, Ta) Semi-Heusler Compounds Using the mBJ Exchange Potential.*** Journal of Electronic Materials 04/2016; 45(7)., DOI:10.1007/s11664-016-4488-3
54. M. CAID, H. RACHED, D. RACHED, R. KHENATA, S. BIN OMRAN, D. VASHNEY, B. ABIDRI, N. BENKHETTOU, A. CHAHED, O. BENHELLAL: ***Electronic structure and optical properties of (BeTe)n/(ZnSe)m superlattices.*** MATERIALS SCIENCE-POLAND 04/2016; 34(1)., DOI:10.1515/msp-2016-0004
55. F. Boukabrine, F. Chiker, R. Miloua, Z. Kebab, R. Khenata, Deo Prakash, S. Bin Omran, K.D. Verma: ***Combined theoretical studies of the optical characteristics of II-IV-V2 semiconductor thin films.*** Optical Materials 04/2016; 54., DOI:10.1016/j.optmat.2016.01.061
56. Samah Al-Qaisi, M. S. Abu-Jafar, G. K. Gopir, R. Khenata: ***Electronic, structural and magnetic properties of TbO under pressure: FP-LAPW study.*** Phase Transitions 03/2016; 89(12)., DOI:10.1080/01411594.2016.1156111
57. Sikander Azam, Saleem Ayaz Khan, Haleem Ud Din, Rabah Khenata, Souraya Goumri-Said: ***Exploring the thermoelectric and magnetic properties of uranium selenides: Tl<sub>2</sub>Ag<sub>2</sub>USe<sub>4</sub> and Tl<sub>3</sub>Cu<sub>4</sub>USe<sub>6</sub>.*** Journal of Magnetism and Magnetic Materials 03/2016; 413., DOI:10.1016/j.jmmm.2016.03.0733
58. DINESH VARSHNEY, SWARNA SHRIYA, SANJAY JAIN, MEENU VARSHNEY, R. KHENATA: ***Mechanically induced stiffening, thermally driven softening, and brittle nature of SiC.*** 03/2016; 5(5)., DOI:10.1007/s40145-015-0166-9
59. P. Upadhaya, Deo Prakash, E.R. Shaaban, Y. Al-Douri, R. Khenata, A.H. Reshak, Majid Darroudi, K.D. Verma: ***Realization and Computational Analysis of splitting in higher order optical vortices.*** Optik - International Journal for Light and Electron Optics 03/2016; 127(14)., DOI:10.1016/j.ijleo.2016.03.051
60. Sajjad Hussain, G. Murtaza, Shah Haider Khan, Afzal Khan, Malak Azmat Ali, M. Faizan, Asif Mahmood, R. Khenata: ***First principles study of structural, optoelectronic and thermoelectric properties of Cu<sub>2</sub>CdSnX<sub>4</sub> (X=S, Se, Te) chalcogenides.*** Materials Research Bulletin 03/2016; 79., DOI:10.1016/j.materresbull.2016.03.001
61. Mohammed El Amine Monir, H. Baltache, R. Khenata, G. Murtaza, R. Ahmed, Waleed. K. Ahmed, S. Bin Omran, A. Bouhemadou: ***Half-metalllicity and***

**optoelectronic properties of V-doped zincblende ZnS and CdS alloys.**  
International Journal of Modern Physics B 03/2016; 30(8).,  
DOI:10.1142/S021797921650034X

62. M.H. ELAHMAR, H. RACHED, D. RACHED, S.BENALIA, R. KHENATA, Z.E. BISKRI, S. BIN OMRAN: **Structural stability, electronic structure and magnetic properties of the new hypothetical half-metallic ferromagnetic full-Heusler alloy CoNiMnSi.** 03/2016; 34(1)., DOI:10.1515/msp-2016-0011
63. A. Bendjedid, H. Baltache, T. Ouahrani, R. Khenata, G. Murtaza, Y. Al-Douri, S. Bin Omran, D. Rached, S. Benalia: **Structural, Electronic, Bonding and Thermo-Elastic Properties of Orthorhombic and Cubic CeO<sub>2</sub> Compound.** Chinese Journal of Physics- Taipei- 03/2016; 54(01).,  
DOI:10.1016/j.cjph.2016.02.001
64. Abdul Basit, Saleem Ayaz Khan, G. Murtaza, Asif Mahmood, R. Khenata, S. Bin Omran, M. Yaseen: **Electronic, optical and thermoelectric properties of XNMg<sub>3</sub> (X<sup>1/4</sup>P, As, Sb, Bi) compounds.** Materials Science in Semiconductor Processing 03/2016; 43., DOI:10.1016/j.mssp.2015.12.001
65. M. Labair, H. Rached, D. Rached, S. Benalia, B. Abidri, R. Khenata, R. Ahmed, S. Bin Omran, A. Bouhemadou, S. V. Syrotyuk: **Prediction of phase transition, mechanical and electronic properties of inverse Heusler compound Y<sub>2</sub>RuPb, Via FP-LMTO method.** International Journal of Modern Physics C 02/2016;, DOI:10.1142/S0129183116501072
66. A. Shankar, D.P. Rai, Sandeep, R. Khenata, R.K. Thapa, P.K. Mandal: **Electronic structure and thermoelectricity of filled skutterudite CeRu<sub>4</sub>Sb<sub>12</sub>.** Journal of Alloys and Compounds 02/2016; 672.,  
DOI:10.1016/j.jallcom.2016.02.192
67. A. Benmakhlof, A. Bentabet, A. Bouhemadou, S. Maabed, A. Benghia, R. Khenata, S. Bin-Omran: **Structural, half-metallic magnetism and elastic properties of the KMnQ<sub>2</sub> (Q=O, S, Se, Te) chalcogenides from first-principles calculations.** Journal of Magnetism and Magnetic Materials 02/2016; 408., DOI:10.1016/j.jmmm.2016.02.058
68. Mohammed El Amine Monir, H. Baltache, R. Khenata, G. Murtaza, Asif Mahmood: **Structural, Magnetic, and Optoelectronic Properties of TbNi<sub>5</sub>, TbNi<sub>3</sub>Ti<sub>2</sub> and TbNi<sub>3</sub>V<sub>2</sub> Compounds.** Journal of Superconductivity and Novel Magnetism 01/2016;, DOI:10.1007/s10948-016-3408-3
69. Mohammed El Amine Monir, H. Baltache, R. Khenata, G. Murtaza, Asif Mahmood: **Structural, Magnetic, and Optoelectronic Properties of TbNi 5 , TbNi 3 Ti 2 and TbNi 3 V 2 Compounds.** Journal of Superconductivity and Novel Magnetism 01/2016;

70. R. Khenata A. K. Kushwaha, S. Bin Omran: ***Vibrational, mechanical and thermodynamical properties of indium thiospinels MIn<sub>2</sub>S<sub>4</sub> (M = Cd, Zn and Mg)***. International Journal of Modern Physics B 01/2016; 30(6)., DOI:10.1142/S0217979216500181
71. Imran Ullah, G. Murtaza, R. Khenata, Asif Mahmood, M. Muzzamil, N. Amin, M. Saleh: ***Structural and Optoelectronic Properties of X<sub>3</sub>ZN (X = Ca, Sr, Ba; Z = As, Sb, Bi) Anti-Perovskite Compounds***. Journal of Electronic Materials 01/2016;, DOI:10.1007/s11664-015-4330-
72. F. Dahmane, Y. Mogulkoc, B. Doumi, A. Tadjer, R. Khenata, S. Bin Omran, D.P. Rai, G. Murtaza, Dinesh Varshney: ***Structural, electronic and magnetic properties of Fe<sub>2</sub>-based full Heusler alloys: A first principle study***. Journal of Magnetism and Magnetic Materials 01/2016; 407., DOI:10.1016/j.jmmm.2016.01.074
73. Naeemullah, G. Murtaza, R. Khenata, S. Bin Omran: ***Direct band gap nature and optical response of B<sub>x</sub>Mg<sub>y</sub>Zn<sub>1-(x+y)</sub>Se***. Modern Physics Letters B 01/2016; 30(3)., DOI:10.1142/S021798491650007X
74. O.Miloud Abid, S. Menouer, A. Yakoubi, H. Khachai, S. Bin Omran, G. Murtaza, Deo Prakash, R. Khenata, K.D. Verma: ***Structural, Electronic, Elastic, Thermoelectric and Thermodynamic properties of the NbMSb half heusler (M=Fe, Ru, Os) compounds with first principle calculations***. Superlattices and Microstructures 01/2016; 93., DOI:10.1016/j.spmi.2016.01.001
75. I. Hattabi, A. Abdiche, R. Moussa, R. Riane, K. Hadji, F. Soyalp, Dinesh Varshney, S.V. Syrotyuk, R. Khenata: ***First-Principle Study of the Structural, Electronic, and Optical Properties of Cubic InNxP1-x Ternary Alloys under Hydrostatic Pressure***. Zeitschrift fur Naturforschung a 01/2016; 71(9)., DOI:10.1515/zna-2016-01005
76. F. Dahmane, D. Mesri, A. Tadjer, R. Khenata, S. Benalia, L. Djoudi, B. Doumi, L. Boumia, H. Aourag: ***Electronic structure; magnetism and stability of Co<sub>2</sub>CrX (X=Al, Ga, In) ab initio study***. Modern Physics Letters B 01/2016; 30(1)., DOI:10.1142/S0217984915502656
77. F. Dahmane, B. Doumi, Y. Mogulkoc, A. Tadjer, Deo Prakash, K. D. Verma, Dinesh Varshney, M. A. Ghebouli, S. Bin Omran, R. Khenata: ***Investigations of the Structural, Electronic, Magnetic, and Half-Metallic Behavior of Co<sub>2</sub>MnZ (Z = Al, Ge, Si, Ga) Full-Heusler Compounds***. Journal of Superconductivity and Novel Magnetism 01/2016; 29(3)., DOI:10.1007/s10948-015-3357-2
78. D.P. Rai, A. Shankar, Sandeep, M.P. Ghimire, R. Khenata, R.K. Thapa: ***Erratum: Study of the enhanced electronic and thermoelectric (TE)***

***properties of ZrxHf1-x-yTayNiSn: A first principles study*** (RSC Advances (2015) 5 (95353-95359)). DOI:10.1039/c6ra90008a

79. K. C. Bhamu, R. Khenata, Saleem Ayaz Khan, Mangej Singh, K. R. Priolkar: ***Electronic, Optical and Thermoelectric Properties of 2H-CuAlO<sub>2</sub>: A First Principles Study.*** Journal of Electronic Materials 11/2015; 45(1)., DOI:10.1007/s11664-015-4160-3
80. D. P. Rai, Sandeep, A. Shankar, M. P. Ghimire, R. Khenata, R. K. Thapa: ***Ferromagnetism in d<sup>0</sup> Binary Compounds MC (M = Be, Mg, Ca, Sr, Ba and Ra): A Modified Becke Johnson Potential Study.*** 01/2016; 5., DOI:10.1166/jap.2016.1280
81. M. Arif, G. Murtaza, R. Ali, R. Khenata, Y. Takagiwa, M. Muzammil, S. Bin Omran: ***Elastic and electro-optical properties of XYZ (X = Li, Na and K; Y = Mg; Z = N, P, As, Sb and Bi) compounds.*** Indian Journal of Physics 12/2015; 90(6)., DOI:10.1007/s12648-015-0791-8
82. G. Murtaza, A. Sajid, M. Rizwan, Y. Takagiwa, H. Khachai, M. Jibran, R. Khenata, S. Bin Omran: ***First principles study of Mg<sub>2</sub>X (X=Si, Ge, Sn, Pb): Elastic, optoelectronic and thermoelectric properties.*** Materials Science in Semiconductor Processing 12/2015; 40., DOI:10.1016/j.mssp.2015.06.075
83. Abdelmadjid Bouhemadou, K. Haddadi, S. Bin-Omran, R. Khenata, Y. Al-Douri, S. Maabed: ***Structural, elastic, electronic and optical properties of the quaternary nitridogallate LiCaGaN<sub>2</sub>: First-principles study.*** Materials Science in Semiconductor Processing 12/2015; 40., DOI:10.1016/j.mssp.2015.06.021
84. Y. Al-Douri, H. Khachai, R. Khenata: ***Chalcogenides-based quantum dots: Optical investigation using first-principles calculations.*** Materials Science in Semiconductor Processing 11/2015; 39., DOI:10.1016/j.mssp.2015.05.016
85. M Khalfa, H Khachai, F Chiker, N Baki, K Bougerara, A Yakoubi, G Murtaza, M Harmel, M S Abu-Jafar, S Bin, R Khenata: ***Mechanical, electronic and thermodynamic properties of full Heusler compounds Fe<sub>2</sub>VX(X = Al, Ga).*** International Journal of Modern Physics B 11/2015; 29(31)., DOI:10.1142/S021797921550229X
86. B. Ghebouli, M.A. Ghebouli, H. Choutri, M. Fatmi, T. Chihi, L. Louail, A. Bouhemadou, S. Bin-Omran, R. Khenata, H. Khachai: ***An ab initio study of the structural, elastic, electronic, optical properties and phonons of the double perovskite oxides Sr<sub>2</sub>AlXO<sub>6</sub> (X=Ta, Nb, V).*** Materials Science in Semiconductor Processing 11/2015; 42., DOI:10.1016/j.mssp.2015.09.026
87. Deo Prakash, Chernet Amente, Keya Dharamvir, Bedvir Singh, Rishipal Singh, E.R. Shaaban, Y. Al-Douri, R. Khenata, Majid Darroudi, K.D. Verma:

**Synthesis, Purification and Microstructural Characterization of Nickel Doped Carbon Nanotubes for spintronic applications.** Ceramics International 11/2015; 42(5)., DOI:10.1016/j.ceramint.2015.11.074

88. M.H. Elahmar, H. Rached, D. Rached, R. Khenata, G. Murtaza, S. Bin Omran, W.K. Ahmed: **Structural, mechanical, electronic and magnetic properties of a new series of quaternary Heusler Alloys CoFeMnZ (Z =Si, As, Sb): a first-principle study.** Journal of Magnetism and Magnetic Materials 05/2015; 393., DOI:10.1016/j.jmmm.2015.05.019.
89. H Ullah, G. Murtaza, R. Khenata, S. Mohammad, A. Manzar, S. Bin Omran, Aman Ullah, M. Muzammil: **Mechanical, electronic and magnetic properties of Sm-based perovskite-type oxides SmMO<sub>3</sub> (M = V, Fe and Co): an ab initio study.** Indian Journal of Physics 11/2015; 89(11)., DOI:10.1007/s12648-015-0690-z
90. A. Bouhemadou, D. Allali, S. Bin-Omran, E. Muhammad Abud Al Safi, R. Khenata, Y. Al-Douri: **Elastic and thermodynamic properties of the SiB<sub>2</sub>O<sub>4</sub> (B=Mg, Zn and Cd) cubic spinels: An ab initio FP-LAPW study.** Materials Science in Semiconductor Processing 10/2015; 38., DOI:10.1016/j.mssp.2015.04.021
91. H. Louhab, A. Yakoubi, H. Khachai, O. Miloud Abid, R. Khenata, R. Ahmed, G. Murtaza, S. Bin Omran: **First-principles study of structural, electronic, elastic and thermal properties of intermetallic ternary compounds (RMn<sub>2</sub>Si<sub>2</sub>: R=Ce and Nd).** Materials Science in Semiconductor Processing 10/2015; 38., DOI:10.1016/j.mssp.2015.04.004
92. R. Graine, R. Chemam, F. Z. Gasmi, R. Nouri, H. Meradji, R. Khenata: **First principles calculations of structural, electronic and optical properties of InN compound.** International Journal of Modern Physics B 10/2015; 29(5)., DOI:10.1142/S02179792155002897
93. D. P. Rai, A. Shankar, Sandeep, M. P. Ghimire, R. Khenata, R. K. Thapa: **Study of electronic and an enhanced thermoelectric properties of Zr x Hf 1-x-y Ta y NiSn: A first principles study..** RSC Advances 10/2015;, DOI:10.1039/C5RA12897H
94. M. Benkabou, H. Rached, A. Abdellaoui, D. Rached, R. Khenata, M.H. Elahmar, B. Abidri, N. Benkhettou, S. Bin-Omran: **Electronic structure and magnetic properties of quaternary Heusler alloys CoRhMnZ (Z = Al, Ga, Ge and Si) via first-principle.** Journal of Alloys and Compounds 10/2015; 647., DOI:10.1016/j.jallcom.2015.05.273
95. R Moussa, A Abdiche, R Khenata, D P Rai, W K Ahmed, S Bin Omran, G Murtaza, F Soyalp: **Studying structural, electronic and optical properties of zinc-blende Ga 1 - x Al x P at normal and under pressure by means of**

96. Arshad Hussain, R. Ahmed, N. Ali, Faheem K. Butt, A Shaari, Wan W N Shamsuri, R. Khenata, Deo Prakash, K.D.Verma: ***Post annealing effects on structural, optical and electrical properties of CuSbS<sub>2</sub> thin films fabricated by combinatorial thermal evaporation technique.*** Superlattices and Microstructures 10/2015;, DOI:10.1016/j.spmi.2015.10.024
97. N.Baki, R.D.Eithiraj, H.Khachai, R.Khenata, G.Murtaza, A.Bouhemadou, T.Seddik, S.Bin-Omran: ***Elastic, Electronic, Optical and Thermal Properties of Na<sub>2</sub>Po: An Ab Initio Study.*** Journal of Electronic Materials 10/2015;, DOI:10.1007/s11664-015-4119-4
98. Shah Fahad, G. Murtaza, T. Ouahrani, R. Khenata, Masood Yousaf, S.Bin Omran, Saleh Mohammad: ***ChemInform Abstract: Structural, Elastic, Electronic, Bonding, and Optical Properties of BeAZ 2 (A: Si, Ge, Sn; Z: P, As) Chalcopyrites.*** ChemInform 10/2015; 46(41)., DOI:10.1002/chin.201541001
99. A. Benmakhlof, A. Bentabet, A. Bouhemadou, S. Maabed, R. Khenata, S. Bin-Omran: ***Structural, elastic, electronic and optical properties of KAlQ<sub>2</sub> (Q = Se, Te): A DFT study.*** Solid State Sciences 01/2015; 48.
100. Sikander Azam, Saleem Ayaz Khan, Wilayat Khan, Saleh Muhammad, Haleem Udin, G. Murtaza, R. Khenata, Fahad Ali Shah, Jan Minar, W.K. Ahmed: ***Detailed DFT studies of the electronic structure and optical properties of KBaMSe<sub>3</sub> (M = As, Sb).*** Journal of Alloys and Compounds 09/2015; 644., DOI:10.1016/j.jallcom.2015.04.181
101. R. Moussa, A. Abdiche, B. Abbar, M. Guemou, R. Riane, G. Murtaza, SAAD Bin Omran, R. Khenata, F. Soyalp: ***Ab Initio Investigation of the Structural, Electronic and Optical Properties of Cubic GaAs<sub>1-x</sub> P<sub>x</sub> Ternary Alloys Under Hydrostatic Pressure.*** Journal of Electronic Materials 09/2015; 44(12)., DOI:10.1007/s11664-015-4048-2
102. R. Zine El-Kelma, L. Beldi, F. El Haj Hassan, G. Murtaza, R. Khenata, M. S. Abu-Jafar, S. Bin Omran, B. Bouhafs: ***Magnetic ordering and electronic structure of the ternary iron arsenide BaFe<sub>2</sub>As<sub>2</sub>.*** International Journal of Modern Physics B 09/2015; 29(23)., DOI:10.1142/S0217979215501829
103. NAEEM ULLAH, H. ULLAH, G. MURTAZA, R. KHENATA, S. ALI: ***Structural phase transition and optoelectronic properties of ZnS under pressure.*** Journal of Optoelectronics and Advanced Materials 09/2015; 17(9-10).
104. Dinesh Varshney, S. Shriya, M. Varshney, N. Singh, R. Khenata: ***Elastic and thermodynamical properties of cubic (3C) silicon carbide under high***

**pressure and high temperature.** 09/2015; 9(3)., DOI:10.1007/s40094-015-0183-7

105. A. Bendjedid, T. Seddik, R. Khenata, H. Baltache, G. Murtaza, A. Bouhemadou, S. Bin Omran, Sikander Azam, Saleem Ayaz Khan: **GGA+U study on phase transition, optoelectronic and magnetic properties of AmO<sub>2</sub> with spin-orbit coupling.** Journal of Magnetism and Magnetic Materials 08/2015; 396., DOI:10.1016/j.jmmm.2015.08.020
106. M. El Amine Monir, R. Khenata, H. Baltache, G. Murtaza, M.S. Abu-Jafar, A. Bouhemadou, S. Bin Omran, D. Rached: **Study of structural, electronic and magnetic properties of CoFeIn and Co<sub>2</sub>FeIn Heusler alloys.** Journal of Magnetism and Magnetic Materials 07/2015; 394., DOI:10.1016/j.jmmm.2015.06.077
107. A. Haddou, G. Murtaza, H. Khachai, R. Khenata, S. Bin Omran, Naeem Ullah, Dinesh Varshney, A. Bouhemadou: **Structural, Elastic, Electronic Optical and Thermodynamic Properties of ZnAl<sub>2</sub>S<sub>4</sub>.** International Journal of Thermophysics 08/2015; 2015;, DOI:10.1007/s10765-015-1941-0
108. Y. Al-Douri, H. Khachai, R. Khenata, A. Bouhemadou: **First-principles calculations for optical investigations of PbX (X=S,Te) compounds under quantum dots diameter effect.** Canadian Journal of Physics 07/2015; 93(12)., DOI:10.1139/cjp-2015-0145
109. A. Shankar, D.P. Rai, Sandeep, R. Khenata, R.K. Thapa: **An ab initio study of filled skutterudites RO<sub>0.4</sub>Pt<sub>12</sub> (R = Sm, Eu and Gd).** Phase Transitions 07/2015; [http://dx.doi.org/10.1080/01411594.2015.1031133\(11\).,](http://dx.doi.org/10.1080/01411594.2015.1031133) DOI:10.1080/01411594.2015.1031133
110. M.Harmel, H.khachai, A.Haddou, R.Khenata, G.murtaza: **Ab Initio Study of the Mechanical, Thermal and Optoelectronic Properties of the Cubic CsBaF<sub>3</sub>.** Acta Physica Polonica Series a 07/2015;, DOI:10.12693/APhysPolA.128.34
111. I. Benkaddour, H. Khachai, F. Chiker, N. Benosman, Y. Benkaddour, G. Murtaza, S. Bin Omran, R. Khenata: **Ab Initio Study of the Structural, Electronic, and Thermal Properties of BaS<sub>1-x</sub>Te<sub>x</sub> Alloy.** International Journal of Thermophysics 07/2015; 36(7)., DOI:10.1007/s10765-015-1908-1
112. F. Dahmane, S. Benalia, L. Djoudi, A. Tadjer, R. Khenata, B. Doumi, H. Aourag: **First-Principles Study of Structural, Electronic, Magnetic and Half-Metallic Properties of the Heusler Alloys Ti<sub>2</sub>ZAl (Z = Co, Fe, Mn).** Journal of Superconductivity and Novel Magnetism 06/2015; 28(10)., DOI:10.1007/s10948-015-3109-3

113. Y. Al-Douri, M. Ameri, A. Bouhemadou, R. Khenata: **Annealing temperature effect on structural, optical, morphological and electrical properties of CdS/Si(100) nanostructures.** Microsystem Technologies 06/2015;, DOI:10.1007/s00542-015-2584-6
114. Shah Fahad , G. Murtaza , T. Ouahrani , R. Khenata , Masood Yousaf , S.Bin Omran : **Structural, elastic, electronic, bonding, and optical properties of BeAZ2 (A= Si, Ge, Sn; Z= P, As) chalcopyrites.** Journal of Alloys and Compounds 06/2015; 646., DOI:10.1016/j.jallcom.2015.06.026
115. Sandeep, D P Rai, A Shankar, M P Ghimire, R Khenata, R K Thapa: **Study of electronic and magnetic properties in 4f electron based cubic EuAlO<sub>3</sub>: A first-principles calculation.** Physica Scripta 06/2015; 90(6)., DOI:10.1088/0031-8949/90/6/065803
116. Fahad Ali Shah, Saleem Ayaz Khan, Suneela Arif, Sikander Azam, R. Khenata, S. Bin Omran: **Theoretical investigation of electronic structure and optical response and their interrelation with the transport properties of Ga<sub>1-x</sub>In<sub>x</sub>N (x=0, 0.25, 0.50, 0.75).** Current Applied Physics 05/2015; 15(5)., DOI:10.1016/j.cap.2015.02.014
117. R. Arar, T. Ouahrani, D. Varshney, R. Khenata, G. Murtaza, D. Rached, A. Bouhemadou, Y. Al-Douri, S. Bin Omran, A.H. Reshak: **Structural, mechanical and electronic properties of sodium based fluoroperovskites NaXF<sub>3</sub> (X=Mg, Zn) from first-principle calculations.** Materials Science in Semiconductor Processing 05/2015; 33., DOI:10.1016/j.mssp.2015.01.040
118. M. El Amine Monir, R. Khenata, G. Murtaza, H. Baltache, A. Bouhemadou, Y. Al-Douri, S. Azam, S. Bin Omran, H. Ud Din: **Half-metallic ferromagnetism in Be<sub>1-x</sub>V<sub>x</sub>Te alloys: an Ab-initio study.** Indian Journal of Physics 05/2015; 89(12)., DOI:10.1007/s12648-015-0696-6
119. Sikander Azam, Saleem Ayaz Khan, Jan Minar, Wilayat Khan, Haleem Ud Din, R Khenata, G Murtaza, S Bin-Omran, Souraya Goumri-Said: **Coulomb interaction and Spin-orbit coupling calculations of thermoelectric properties of the quaternary chalcogenides Tl<sub>2</sub>PbXY<sub>4</sub> (X=Zr, Hf and Y=S, Se).** Semiconductor Science and Technology 05/2015;, DOI:10.1088/0268-1242/30/10/105018
120. Bakhtiar Ul Haq, A. Afaq, Galila Abdellatif, R. Ahmed, S. Naseem, R. Khenata: **First Principles Study of Scandium Nitride and Yttrium Nitride Alloy System: prospective material for optoelectronics.** Superlattices and Microstructures 05/2015; 85., DOI:10.1016/j.spmi.2015.04.018
121. Y. Al-Douri, U. Hashim, R. Khenata, A.H. Reshak, M. Ameri, A. Bouhemadou, A. Rahim Ruslinda, M. K. Md Arshad: **Ab initio method of optical**

**investigations of CdS<sub>1-x</sub>Tex alloys under quantum dots diameter effect.**  
Solar Energy 05/2015; 15., DOI:10.1016/j.solener.2015.02.024

122. Malak Azmat Ali, Afzal Khan, Shah Haider Khan, T. Ouahrani, G. Murtaza, R. Khenata, S. Bin Omran: **First principles study of Cu based Delafossite Transparent Conducting Oxides CuXO<sub>2</sub> (X=Al, Ga, In, B, La, Sc, Y).** Materials Science in Semiconductor Processing 04/2015; 38., DOI:10.1016/j.mssp.2015.03.038
123. Sikander Azam, Saleem Ayaz Khan, R. Khenata, G. Murtaza, S. Bin Omran, Saleh Muhammad: **Optoelectronic and Magnetic Properties of Eu<sub>2</sub>Si<sub>5</sub>N<sub>8</sub>: An Ab-initio Study.** Zeitschrift fur Naturforschung a 04/2015;, DOI:10.1515/zna-2015-0187
124. A. Shankar, D. P. Rai, Sandeep, J. Maibam, R. Khenata, R. K. Thapa: **Elastic and Optical Properties of Filled Skutterudite EuRu<sub>4</sub>P<sub>12</sub>.** Chinese Journal of Physics- Taipei- 04/2015; 53(2), DOI:10.6122/CJP.20141004
125. A. Bouhemadou, R. Khenata, S. Bin-Omran, G. Murtaza, Y. Al-Douri: **Structural, elastic, electronic and optical properties of new layered semiconductor BaGa<sub>2</sub>P<sub>2</sub>.** Optical Materials 04/2015; 46., DOI:10.1016/j.optmat.2015.03.059
126. A. Bouhemadou, S. Bin-Omran, D. Allali, S.M. Al-Otaibi, R. Khenata, Y. Al-Douri, M. Chegaar, A.H. Reshak: **Electronic and optical properties of the LiCdX (X=N, P, As and Sb) filled-tetrahedral compounds with the Tran-Blaha modified Becke-Johnson density functional.** Materials Research Bulletin 04/2015; 64., DOI:10.1016/j.materresbull.2015.01.003
127. H. Rached, D. Rached, R. Khenata, B. Abidri, M. Rabah, N. Benkhettou, S. Bin Omran: **A first principle study of phase stability, electronic structure and magnetic properties for Co<sub>2-x</sub>CrxMnAl Heusler alloys.** Journal of Magnetism and Magnetic Materials 04/2015; 379., DOI:10.1016/j.jmmm.2014.12.013
128. M. Sajjad, Sadia Manzoor, H.X. Zhang, N.A. Noor, S.M. Alay-e-Abbas, A. Shaukat, R. Khenata: **The half-metallic ferromagnetism character in Be<sub>1-x</sub>V<sub>x</sub>Y (Y=Se and Te) alloys: An ab-initio study.** Journal of Magnetism and Magnetic Materials 04/2015; 379., DOI:10.1016/j.jmmm.2014.11.004
129. A. Abdiche, R. Riane, M. Guemou, R. Khenata, R. Moussa, G. Murtaza, S. Bin Omran: **First principle study of structural and electronic properties of cubic quaternary B<sub>x</sub>Ga<sub>1-x</sub>As<sub>1-y</sub>N<sub>y</sub> alloys.** Solid State Communications 03/2015; 206., DOI:10.1016/j.ssc.2015.01.011
130. Masood Yousaf, S.A. Dalhatu, G. Murtaza , R. Khenata , M. Sajjad , A. Musa : **Optoelectronic properties of XIn<sub>2</sub>S<sub>4</sub> (X = Cd, Mg) thiospinels through**

**highly accurate all-electron FP-LAPW method coupled with modified approximations.** Journal of Alloys and Compounds 03/2015; 625., DOI:10.1016/j.jallcom.2014.11.104

131. M. El Amine Monir, H. Baltache, R. Khenata, G. Murtaza, Sikander Azam, A. Bouhemadou, Y. Al-Douri, S. Bin Omran, Roshan Ali: **First-principles calculations of a half-metallic ferromagnet zinc blende  $Zn_{1-x}V_xTe$ .** Journal of Magnetism and Magnetic Materials 03/2015; 378., DOI:10.1016/j.jmmm.2014.10.070
132. R. Hafeez, G. Murtaza, R. Khenata, Kin Mun Wong, S. Naeem, M.N. Khalid: **Structural, Chemical Bonding, Electronic and Magnetic Properties of  $XY_3$  ( $X = Al, Ga$  and  $Y = V, Nb, Cr, Mo$ ) Compounds.** Acta Physica Polonica Series a 03/2015; 127(3).
133. R. Hafeez, G. Murtaza, R. Khenata, Kin Mun Wong, S. Naeem, M.N. Khalid, Z.A. Alahmed, S. Bin Omran: **Structural, Chemical Bonding, Electronic and Magnetic Properties of  $XY_3$  ( $X = Al, Ga$  and  $Y = V, Nb, Cr, Mo$ ) Compounds.** Acta Physica Polonica Series a 03/2015; 127(3)., DOI:10.12693/APhysPolA.127.770
134. S.Benalia, M.Merabet, D.Rached, Y.Al-Douri, B.Abidri, R.Khenata, M.Labair: **Band gap behavior of scandium aluminum phosphide and scandium gallium phosphide ternary alloys and superlattices.** Materials Science in Semiconductor Processing 03/2015; 31., DOI:10.1016/j.mssp.2014.12.021
135. Mukhtar Ahmad, Naeemullah, G. Murtaza, R. Khenata, S. Bin Omran, A. Bouhmadiou: **Structural, elastic, electronic, magnetic and optical properties of  $RbSrX$  ( $C, Si, Ge$ ) half-Heusler compounds.** Journal of Magnetism and Magnetic Materials 03/2015; 377., DOI:10.1016/j.jmmm.2014.10.108
136. M. Belkhouane, S. Amari, A. Yakoubi, A.Tadjer, S. Méçabih, G. Murtaza, S. Bin Omran, R. Khenata: **First-principles study of the electronic and magnetic properties of  $Fe_2MnAl$ ,  $Fe_2MnSi$  and  $Fe_2MnSi0.5Al0.5$ .** Journal of Magnetism and Magnetic Materials 02/2015; 377., DOI:10.1016/j.jmmm.2014.10.094
137. Mazhar Ullah, Saleem Ayaz Khan, G. Murtaza, R. Khenata, Naeem Ullah, S. Bin Omran: **Electronic, thermoelectric and magnetic properties of  $La_2NiMnO_6$  and  $La_2CoMnO_6$ .** Journal of Magnetism and Magnetic Materials 02/2015; 377., DOI:10.1016/j.jmmm.2014.10.069
138. G. Murtaza, Naeem Ullah, Abdur Rauf, R. Khenata, S. Bin Omran, A. Waheed: **First-principles study of structural, optical and electronic properties of zinc mercury chalcogenides.** Materials Science in Semiconductor Processing 02/2015; 30(2015)., DOI:10.1016/j.mssp.2014.10.048

139. S. Bouras, B. Ghebouli, M. Benkerri, M.A. Ghebouli, H. Choutri, L. Louail, T. Chihi, M. Fatmi, A. Bouhemadou, R. Khenata, H. Khachai: **Theoretical characterization of quaternary iridium based hydrides NaAeIrH<sub>6</sub> (Ae = Ca, Ba and Sr)**. Materials Chemistry and Physics 01/2015; 149-150., DOI:10.1016/j.matchemphys.2014.09.040
140. A. Shankar, D. P. Rai, R. Khenata, J. Maibam, Sandeep, R. K. Thapa: **Study of 5f electron based filled skutterudite compound EuFe<sub>4</sub>Sb<sub>12</sub>, a thermoelectric (TE) material: FP-LAPW method.** Journal of Alloys and Compounds 01/2015; 619., DOI:10.1016/j.jallcom.2014.09.086
141. M. El Amine. Monir, H. Baltache, G. Murtaza, R. Khenata, Waleed K. Ahmed, A. Bouhemadou, S. Bin Omran, T. Seddik: **Spin-polarized structural, elastic, electronic and magnetic properties of half-metallic ferromagnetism in V-doped ZnSe.** Journal of Magnetism and Magnetic Materials 01/2015; 374., DOI:10.1016/j.jmmm.2014.08.014
142. O. Boudrifa, A. Bouhemadou, N. Guechi, S. Bin-Omran, Y. Al-Douri, R. Khenata: **First-principles prediction of the structural, elastic, thermodynamic, electronic and optical properties of Li<sub>4</sub>Sr<sub>3</sub>Ge<sub>2</sub>N<sub>6</sub> quaternary nitride.** Journal of Alloys and Compounds 01/2015; 618(1)., DOI:10.1016/j.jallcom.2014.08.143
143. K. Haddadi, A. Bouhemadou, S. Bin-Omran, S. Maabed, R. Khenata: **An ab initio study of the structural, elastic, electronic and optical properties of the newly synthesized nitridoaluminate LiCaAlN<sub>2</sub>.** Philosophical Magazine 01/2015; 95(1)., DOI:10.1080/14786435.2014.992490
144. Sandeep Chettri, D. P. Rai, A. Shankar, M. P. Ghimire, R. Khenata, R. K. Thapa: **A systematic study of LaAlO<sub>3</sub> with variation of Nd doping, case of bandgap tuning: A first principles method.** Modern Physics Letters B 01/2015; 29(4)., DOI:10.1142/S0217984916500287.
145. A. Djied, T. Seddik, O. Merabiha, G. Murtaza, R. Khenata, R. Ahmed, S. Bin-Omran, S. Uğur, A. Bouhemadou: **Structural phase transition and opto-electronic properties of NaZnAs.** Journal of Alloys and Compounds 11/2014; 622., DOI:10.1016/j.jallcom.2014.10.173
146. F. Litimein, R. Khenata, Sanjeev K. Gupta, G. Murtaza, Ali. H. Reshak, A. Bouhemadou, S. Bin Omran, Masood Yousaf, Prafulla K. Jha: **Structural, electronic, and optical properties of orthorhombic and triclinic BiNbO<sub>4</sub> determined via DFT calculations.** Journal of Materials Science 11/2014; 49(22)., DOI:10.1007/s10853-014-8491-x
147. Dinesh Varshney, Swarna Shriya, Meenu Varshney, R. Khenata: **Pressure-induced structural phase transition and elastic properties of rare earth**

**Pr chalcogenides and pnictides.** Phase Transitions 10/2014; 88(1)., DOI:10.1080/01411594.2014.974601

148. K. Hacini, Z. Chouahda, A. Djedid, H. Meradji, S. Ghemid, F. El Haj Hassan, R. Khenata: ***Ab initio study of the structural, electronic, phase diagram, and thermal properties of cadmium beryllium selenide mixed crystals.*** Materials Science in Semiconductor Processing 10/2014; 26(1)., DOI:10.1016/j.mssp.2014.06.
149. Naeem Ullah, G. Murtaza, R. Khenata, Jan Rehman, Haleem Ud Din, S. Bin Omran: ***Structural, chemical bonding and optoelectronic properties of Mg doped zinc chalcogenides: A first principle study.*** Materials Science in Semiconductor Processing 10/2014; 26(2014)., DOI:10.1016/j.mssp.2014.09.016
150. A. Kourdassi, N. Benkhetou, M. Labair, M. Benkabou, S. Benalia, R. Khenata, H. Baltache, Djamel Rached: ***FP-LMTO calculations of the structural, elastic, thermodynamic, and electronic properties of the ideal-cubic perovskite BiGaO<sub>3</sub>.*** Brazilian Journal of Physics 10/2014; 44(6)., DOI:10.1007/s13538-014-0262-2
151. Sibghat-ullah, G. Murtaza, R. Khenata, A.H. Reshak: ***Electronic, optical and bonding properties of MgYZ<sub>2</sub> (Y=Si, Ge; Z=N, P) chalcopyrites from first principles.*** Materials Science in Semiconductor Processing 10/2014; 26(1)., DOI:10.1016/j.mssp.2014.03.053
152. Naeemullah, G. Murtaza , R. Khenata , Mazharullah , S. Bin Omran : ***Phase transition, electronic and optical properties of III-Sb compounds under pressure.*** Phase Transitions 09/2014; 87(9)., DOI:10.1080/01411594.2014.925557
153. Saeed Ullah, Haleem Ud Din, G. Murtaza, T. Ouahrani, R. Khenata, Naeemullah, S. Bin Omran: ***Structural, electronic and optical properties of AgXY<sub>2</sub>(X = Al, Ga, In and Y = S, Se, Te).*** Journal of Alloys and Compounds 08/2014; 617., DOI:10.1016/j.jallcom.2014.08.058
154. Sikander Azam, Saleem Ayaz Khan, Fahad Ali Shah, Saleh Muhammad, Haleem Ud Din, R. Khenata: ***Electronic, optical and thermoelectric properties of Ce<sub>3</sub>PdIn<sub>11</sub> and Ce<sub>5</sub>Pd<sub>2</sub>In<sub>19</sub>: An ab initio study.*** Intermetallics 08/2014; 55., DOI:10.1016/j.intermet.2014.08.001
155. T. Djaafri, A. Djaafri, A. Elias, G. Murtaza, R. Khenata, R. Ahmed, S. Bin Omran, D. Rached: ***Investigations of the half-metallic behavior and the magnetic and thermodynamic properties of half-Heusler CoMnTe and RuMnTe compounds: A first-principles study.*** Chinese Physics B 08/2014; 23(8)., DOI:10.1088/1674-1056/23/8/087103

156. Muhammad Rashid, N.A. Noor, Bushra Sabir, S. Ali, M. Sajjad, F. Hussain, N.U. Khan, B. Amin, R. Khenata: ***Ab-initio study of fundamental properties of ternary ZnO<sub>1-x</sub>S<sub>x</sub> alloys by using special quasi-random structures.*** Computational Materials Science 08/2014; 91., DOI:10.1016/j.commatsci.2014.04.032
157. Naeemullah, G. Murtaza, R. Khenata, A. Safeer, Z.A. Alahmed, S. Bin Omran: ***Shift of band gap from indirect to direct and optical response of CaO by doping S, Se, Te.*** Computational Materials Science 08/2014; 91., DOI:10.1016/j.commatsci.2014.04.039
158. A.H. Reshak, Y. Al-Douri, R. Khenata, Wilayat Khan, Saleem Ayaz Khan, Sikander Azam: ***Electronic structure, Fermi surface topology and spectroscopic optical properties of LaBaCo<sub>2</sub>O<sub>5.5</sub> compound.*** Journal of Magnetism and Magnetic Materials 08/2014; 363., DOI:10.1016/j.jmmm.2014.03.069
159. O. Miloud Abid, A. Yakoubi, A. Tadjer, R. Khenata, R. Ahmed, G. Murtaza, S. Bin Omran, Sikander Azam: ***Ab initio study of the structural, electronic, elastic and thermal properties of RMn<sub>2</sub>Ge<sub>2</sub> (R = Ca, Nd and Y) intermetallic compounds.*** Journal of Alloys and Compounds 07/2014; 616., DOI:10.1016/j.jallcom.2014.07.14613
160. Haleem Ud Din , Sikander Azam , Saleem Ayaz Khan , R. Khenata: ***Optoelectronic behavior of Quaternary Uranium Chalcogenides Rb<sub>2</sub>Pd<sub>3</sub>UM<sub>6</sub> (M = S, Se): A first principle study.*** Journal of Alloys and Compounds 06/2014; 615., DOI:10.1016/j.jallcom.2014.06.180
161. A. Manzar, G. Murtaza, R. Khenata, Masood Yousaf, S. Muhammad, Hayatullah: ***Electronic and Optic Properties of Cubic Spinel CdX<sub>2</sub>O<sub>4</sub> (X=In, Ga, Al) through Modified Becke—Johnson Potential.*** Chinese Physics Letters 06/2014; 31(6)., DOI:10.1088/0256-307X/31/6/067401
162. Y. Al-Douri, Q. Khasawneh, S. Kiwan, U. Hashim, S.B. Abd Hamid, A.H. Reshak, A. Bouhemadou, M. Ameri, R. Khenata: ***Structural and optical insights to enhance solar cell performance of CdS nanostructures.*** Energy Conversion and Management 06/2014; 82., DOI:10.1016/j.enconman.2014.03.020
163. D. Allali, A. Bouhemadou, E. Muhammad Abud Al Safi, S. Bin-Omran, M. Chegaar, R. Khenata, A.H. Reshak: ***Electronic and optical properties of the SiB<sub>2</sub>O<sub>4</sub> (B=Mg, Zn, and Cd) spinel oxides: An ab initio study with the Tran-Blaha-modified Becke-Johnson density functional.*** Physica B Condensed Matter 06/2014; 443., DOI:10.1016/j.physb.2014.02.053

164. G. Murtaza, S.K. Gupta, T. Seddik, R. Khenata, Z.A. Alahmed, R. Ahmed, H. Khachai, P.K. Jha, S. Bin Omran: ***Structural, electronic, optical and thermodynamic properties of cubic REGa<sub>3</sub> (RE = Sc or Lu) compounds: Ab initio study.*** Journal of Alloys and Compounds 06/2014; 597., DOI:10.1016/j.jallcom.2014.01.203
165. N. Guechi, A. Bouhemadou, R. Khenata, S. Bin-Omran, M. Chegaar, Y. Al-Douri, A. Bourzami: *Chem Inform Abstract: Structural, Elastic, Electronic and Optical Properties of the Newly Synthesized Monoclinic Zintl Phase BaIn 2 P 2* .. ChemInform 05/2014; 45(18)., DOI:10.1002/chin.201418001
166. Sibghat ullah, G. Murtaza, R. Khenata, A.H. Reshak, S.S. Hayat, S. Bin Omran: ***Towards from indirect to direct band gap and optical properties of XY<sub>2</sub> (X=Zn, Cd; Y=Si, Ge, Sn).*** Physica B Condensed Matter 05/2014; 441., DOI:10.1016/j.physb.2014.02.021
167. M. El Amine Monir, H. Baltache, G. Murtaza, R. Khenata, S. Bin Omran, S. Uğur, S. Benalia, D. Rached: ***Ab initio study of structural, electronic, magnetic and optical properties of Ti-doped ZnTe and CdTe.*** International Journal of Modern Physics B 04/2014; 28(11)., DOI:10.1142/S0217979214500805
168. Hayatullah, G. Murtaza, R. Khenata, S. Muhammad, A.H. Reshak, Kin Mun Wong, S. Bin Omran, Z.A. Alahmed: ***Structural, chemical bonding, electronic and magnetic properties of KMF<sub>3</sub> (M=Mn, Fe, Co, Ni) compounds.*** Computational Materials Science 04/2014; 85., DOI:10.1016/j.commatsci.2013.12.054
169. Bakhtiar Ul Haq, R. Ahmed, A. Shaari, A. Afaq, B.A. Tahir, R. Khenata: ***First-principles investigations of Mn doped zinc-blende ZnO based magnetic semiconductors: Materials for spintronic applications.*** Materials Science in Semiconductor Processing 04/2014; 29., DOI:10.1016/j.mssp.2014.04.004
170. Roshan Ali, G. Murtaza, Y. Takagiwa, R. Khenata, Haleem Uddin, H.Ullah, S. A. Khan: ***Optoelectronic Properties, Elastic Moduli and Thermoelectricity of SrAlGa: An Ab Initio Study.*** Chinese Physics Letters 04/2014; 30(4)., DOI:10.1088/0256-307X/31/4/047102
171. Naeemullah, G. Murtaza, R. Khenata, Z. A. Alahmed, A. H. Reshak: ***Phase transition, electronic and optical properties of NaCl under pressure 15:4 WSPC/147-MPLB.*** Modern Physics Letters B 03/2014; 25(28)., DOI:10.1142/S0217984914500626
172. Naeemullah, G. Murtaza, R. Khenata, A. H. Reshak, S. Naeem, M. N. Khalid: ***Insulator to metal transition and optical response of CsCl under pressure.*** International Journal of Modern Physics B 03/2014; 28(6)., DOI:10.1142/S0217979214500477

173. M. Guemou, A. Abdiche, R. Riane, R. Khenata: ***Ab initio study of the structural, electronic and optical properties of BAs and BN compounds and BN<sub>x</sub>As<sub>1-x</sub> alloys.*** Physica B Condensed Matter 03/2014; 436., DOI:10.1016/j.physb.2013.11.030
174. Masood Yousaf, F. Inam, R. Khenata, G. Murtaza, A.R.M. Isa, M.A. Saeed: ***Prediction study of structural, electronic and optical properties of XIn<sub>2</sub>S<sub>4</sub> (X = Hg, Zn) thiospinels under pressure effect.*** Journal of Alloys and Compounds 03/2014; 589., DOI:10.1016/j.jallcom.2013.11.186
175. Naeem Ullah, G. Murtaza, R. Khenata, Kin Mun Wong, Z.A. Alahmed: ***Phase transition, electronic and optical properties of mercury chalcogenides under pressure.*** Phase Transitions 02/2014; 87(6)., DOI:10.1080/01411594.2014.886110
176. Bakhtiar Ul Haq, R. Ahmed, F. El Haj Hassan, R. Khenata, Mohd Khalid Kasmin, Souraya Goumri-Said: ***Mutual alloying of XAs (X = Ga, In, Al) materials: Tuning the optoelectronic and thermodynamic properties for solar energy applications.*** Solar Energy 02/2014; 100., DOI:10.1016/j.solener.2013.11.020
177. A. Missoum, T. Seddik, G. Murtaza, R. Khenata, A. Bouhemadou, Y. Al-Douri, A. Abdiche, H. Meradji, H. Baltache: ***Ab initio study of the structural and optoelectronic properties of the Half-Heusler CoCrZ (Z= Al and Ga).*** Canadian Journal of Physics 01/2014; 92(10)., DOI:10.1139/cjp-2013-0474
178. D. P. Rai, A. Shankar, Sandeep, Madhav Prasad Ghimire, Rabah Khenata, R. K. Thapa: ***Half-metallic behavior in non-transition metal based binary compounds XC (X = Be, Mg, Ca, Sr, Ba, and Ra): a first principles study.***
179. R. Boulechfar, H. Meradji, Z. Chouahda, S. Ghemid, S. Drablia, R. Khenata: ***FP-LAPW investigation of the structural, electronic and thermodynamic properties of Al<sub>3</sub>Ta compound.*** International Journal of Modern Physics B 01/2014; 28(2)., DOI:10.1142/S0217979214502440
180. A. Manzar, G. Murtaza, R. Khenata, Masood Yousaf, S. Muhammad, Hayatullah: ***Electronic and Optic Properties of Cubic Spinel CdX<sub>2</sub>O<sub>4</sub> (X=In, Ga, Al) through Modified Becke-Johnson Potential.*** Chinese Physics Letters 01/2014; 31.
181. A. SAJID, SIBGHAT-ULLAH, G. MURTAZA, R. KHENATA, A. MANZAR, S. BIN OMRAN: ***Electronic structure and optical properties of chalcopyrite CuYZ<sub>2</sub> (Y=Al, Ga, In; Z=S, Se): An ab initio study.*** Journal of Optoelectronics and Advanced Materials 01/2014; 16(1).

182. G. MURTAZA, SIBGHAT-ULLAH, R. KHENATA, A. H. RESHAK, S.S. HAYAT: ***Optoelectronic properties of XYAs<sub>2</sub> (X=Zn, Cd; Y=Si, Sn) chalcopyrite compounds.*** Journal of Optoelectronics and Advanced Materials 01/2014; 16(1).
183. Naeemullah, G. Murtaza, R. Khenata, N. Hassan, S. Naeem, M.N. Khalid, S. Bin Omran: ***Structural and optoelectronic properties of PbS<sub>x</sub>Se<sub>1-x</sub>, PbS<sub>x</sub>Te<sub>1-x</sub> and PbSexTe<sub>1-x</sub> via first-principles calculations.*** Computational Materials Science 11/2013;, DOI:10.1016/j.commatsci.2013.10.033
184. A Djied, H Khachai, T Seddik, R Khenata, A Bouhemadou, N Guechi, G Murtaza, S Bin-Omran, Z A Alahmed, M Ameri: ***Structural phase transition, mechanical and optoelectronic properties of the tetragonal NaZnP: Ab-initio study.*** Computational Materials Science 12/2013; 84., DOI:10.1016/j.commatsci.2013.11.041
185. N. ARIKAN, M. ERSEN, H. Y. OCAK, A. İYIGÖR, A. CANDAN, Ş UGUR, G. UGUR, R. KHENATA, D. VARSHNEY: ***Ab initio study of phonon dispersion and elastic properties of L1 2 intermetallics Ti<sub>3</sub>Al and Y<sub>3</sub>Al.*** Modern Physics Letters B 12/2013; 27(30)., DOI:10.1142/S0217984913502242
186. ROSHAN ALI, R. KHANATA, BIN AMIN, G. MURTAZA, S. BIN OMRAN: ***Structural, elastic, electronic, chemical bonding and optical properties of M<sub>2</sub>Se (M = Li, Na, K, Rb) through first principle study.*** International Journal of Modern Physics B 12/2013; 27(30)., DOI:10.1142/S0217979213501701
187. A. Manzar, G. Murtaza, R. Khenata, S. Muhammad, Hayatullah: ***Electronic and Optical Properties of Spinel GeMg<sub>2</sub>O<sub>4</sub> and GeCd<sub>2</sub>O<sub>4</sub>.*** Chinese Physics Letters 12/2013; 30(12)., DOI:10.1088/0256-307X/30/12/127401
188. H. Rached, D. Rached, S. Benalia, A.H. Reshak, M. Rabah, R. Khenata: ***First-principles study of structural stabilities, elastic and electronic properties of transition metal monocarbides (TMCs) and mononitrides (TMNs).*** Materials Chemistry and Physics 12/2013; 143(1)., DOI:10.1016/j.matchemphys.2013.08.020
189. Haddou, H. Khachai, R. Khenata, F. Litimein, A. Bouhemadou, G. Murtaza, Z. A. Alahmed, S. Bin-Omran, B. Abbar: ***Elastic, optoelectronic, and thermal properties of cubic CSi 2N4: An ab initio study.*** Journal of Materials Science 12/2013; 48(23)., DOI:10.1007/s10853-013-7636-7
190. M. Ameri, K. Boudia, R. Khenata, B. Bouhafs, A. Rais, S. Bin Omran, B. Abidri, Y. Al-Douri: ***Structural, elastic, electronic and thermodynamic properties of the filled skutterudite CeOs<sub>4</sub>Sb<sub>12</sub> determined by density***

**functional theory.** Materials Science in Semiconductor Processing 12/2013; 16(6)., DOI:10.1016/j.mssp.2013.05.003

191. M. Ameri, N. Bouzouira, R. Khenata, Y Al-Douri, B. Bouhafs, S. Bin-Omran: **FP-LMTO method to calculate the structural, thermodynamic and optoelectronic properties of SixGe<sub>1-x</sub>C alloys.** Molecular Physics 11/2013; 111(21-21)., DOI:10.1080/00268976.2013.775517
192. M. Shoaib, G. Murtaza, R. Khenata, M. Farooq, Roshan Ali: **Structural, elastic, electronic and chemical bonding properties of AB (A=Sc,Y,La;B=N,P,As,Sb,Bi) from first principles.** Computational Materials Science 11/2013; 79., DOI:10.1016/j.commatsci.2013.06.015
193. F. Mekkaoui, F. Litimein, R. Khenata, O. Merabiha, A. Bouhemadou, Dinesh Varshney, F. Soyalp, S. Uğur, S. Bin-Omran, D. Rached: **Prediction Study of the Mechanical and Thermodynamic Properties of the RBRh<sub>3</sub> (R = Sm, Eu, Gd, and Tb) Compounds.** International Journal of Thermophysics 11/2013; 34(11)., DOI:10.1007/s10765-013-1525-9
194. Y. Al-Douri, R. Khenata: **Structural investigation of Si0.5Ge0.5 alloy for optoelectronic applications: Ab initio study.** Optik - International Journal for Light and Electron Optics 11/2013; 124(22)., DOI:10.1016/j.ijleo.2013.04.092
195. T. Seddik, R. Khenata, A. Bouhemadou, N. Guechi, A. Sayede, D. Varshney, Y. Al-Douri, A.H. Reshak, S. Bin-Omran: **External temperature and pressure effects on thermodynamic properties and mechanical stability of yttrium chalcogenides YX (X=S, Se and Te).** Physica B Condensed Matter 11/2013; 428., DOI:10.1016/j.physb.2013.07.014
196. O. Merabiha, T. Seddik, R. Khenata, G. Murtaza, A. Bouhemadou, Y. Takagiwa, S. Bin Omran, D. Rached: **The effects of 5f localization on the electronic and magnetic properties of the hexagonal U<sub>3</sub>ZrSb<sub>5</sub>.** Journal of Alloys and Compounds 10/2013; 586., DOI:10.1016/j.jallcom.2013.10.120
197. Mohammed Ameri, Belfedhal Abdelmounaim, Mokhtar Sebane, Rabah Khenata, Dinesh: **First-principles investigation on structural, elastic, electronic and thermodynamic properties of filled skutterudite PrFe<sub>4</sub>P<sub>12</sub> compound for thermoelectric applications.** Molecular Simulation 09/2013; 40(15)., DOI:10.1080/08927022.2013.854898
198. Hayatullah, G. Murtaza, R. Khenata, S. Naeem, M. N. Khalid, S. Mohammad: **First Principle Calculations of Ground and Excited States' Properties of RbPbF<sub>3</sub>.** Chinese Physics Letters 09/2013; 30(9)., DOI:10.1088/0256-307X/30/9/097101

199. N Chouit, S Amara Korba, M Slimani, H Meradji, S Ghemid, R Khenata: ***First-principles study of the structural, electronic and thermal properties of CaLiF<sub>3</sub>.*** Physica Scripta 09/2013; 88(3)., DOI:10.1088/0031-8949/88/03/035702
200. Y. Al-Douri, Jamal H. Waheb, M. Ameri, R. Khenata, A. Bouhemadou, A. H. Reshak: ***Morphology, Analysis and Properties Studies of CdS Nanostructures under Thiourea Concentration Effect for Photovoltaic Applications.*** International journal of electrochemical science 08/2013; 8(8).
201. U1 Haq Bakhtiar, R. Ahmed, R. Khenata, M. Ahmed, R. Hussain: ***A first-principles comparative study of exchange and correlation potentials for ZnO.*** Materials Science in Semiconductor Processing 08/2013; 16(4)., DOI:10.1016/j.mssp.2012.11.012
202. Hayatullah, G. Murtaza, R. Khenata, S. Muhammad, S. Naeem, M.N. Khalid, M. Manzar: ***Structural, elastic, electronic and optical properties of CsMCl<sub>3</sub> (M=Zn, Cd).*** Physica B Condensed Matter 07/2013; 420., DOI:10.1016/j.physb.2013.03.011
203. F. SEMARI, T. OUAHRANI, H. KHACHAI, R. KHENATA, M. RABAH, A. BOUHEMADOU, G. MURTAZA, B. AMIN, D. RACHED: ***Electronic band structure, optical, thermal and bonding properties of XMg<sub>2</sub>O<sub>4</sub> (X = Si, Ge) spinel compounds.*** International Journal of Modern Physics B 06/2013; 27(18)., DOI:10.1142/S0217979213500823
204. A. Manzar, G. Murtaza, R. Khenata, S. Muhammad, Hayatullah: ***Electronic Band Profile and Optical Response of Spinel MgIn<sub>2</sub>O<sub>4</sub> through Modied Becke-Johnson Potential.*** Chinese Physics Letters 06/2013;, DOI:10.1088/0256-307X/30/6/067401
205. A. Sayede, R. Khenata, A. Chahed, O. Benhelal: ***Electronic and Optical Properties of Layered RE<sub>2</sub>Ti<sub>2</sub>O<sub>7</sub> (RE=Ce and Pr) from First Principles.*** Journal of Applied Physics 05/2013; 113(17)., DOI:10.1063/1.4803124
206. A. Manzar, G. Murtaza, R. Khenata, S. Muhammad, Hayatullah: ***Electronic Band Structure and Optical Response of Spinel SnX<sub>2</sub>O<sub>4</sub> (X=Mg, Zn) through Modified Becke-Johnson Potential.*** Chinese Physics Letters 04/2013; 30(4)., DOI:10.1088/0256-307X/30/4/047401
207. Hayatullah, S. Naeem, G. Murtaza, R. Khenata, M. N. Khalid: ***First principle study of CsSrM<sub>3</sub> (M=F, Cl).*** Physica B Condensed Matter 04/2013; 414., DOI:10.1016/j.physb.2013.01.009
208. A. Bouhemadou, G. Uğur, Ş. Uğur, S. Al-Essa, M.A. Ghebouli, R. Khenata, S. Bin-Omran, Y. Al-Douri: ***Elastic and thermodynamic properties of***

**ZnSc<sub>2</sub>S<sub>4</sub> and CdSc<sub>2</sub>S<sub>4</sub> compounds under pressure and temperature effects.** Computational Materials Science 04/2013; 70., DOI:10.1016/j.commatsci.2013.01.004

209. N. Bettahar, D. Nasri, S. Benalia, M. Merabet, B. Abidri, N. Benkhetou, R. Khenata, D. Rached, M. Rabah: **Electronic Structure and Thermodynamic Properties of the Cubic Antiperovskite Compound InNCe<sub>3</sub> via First-Principles Calculations.** International Journal of Thermophysics 03/2013; 34(3), DOI:10.1007/s10765-013-1434-y
210. G. Murtaza, Hayatullah, R. Khenata, M.N. Khalid, S. Naeem: **Elastic and optoelectronic properties of RbMF<sub>3</sub> (M = Zn, Cd, Hg): A mBJ density functional calculation.** Physica B Condensed Matter 02/2013; 410(1), DOI:10.1016/j.physb.2012.10.024
211. Ghassan E. Arif, Y. Al-Douri, Farah Aini Abdullah, R. Khenata: **Differential equations to calculate the ionicity factor of hexagonal structure semiconductors.** Superlattices and Microstructures 01/2013; Volume 53(1), DOI:10.1016/j.spmi.2012.09.006
212. M. Harmel, H. Khachai, M. Ameri, N. Baki, A. Haddou, M. Khalfa, B. Abbar, S.B. Omran, G. Uğur, Ş. Uğur, R. Khenata: **Erratum: Full-potential calculation of structural, electronic, and thermodynamic properties of fluoroperovskite CsMF<sub>3</sub>(M = Be and Mg) (International Journal of Thermophysics (2012) 33 (2339-2350) DOI:10.1007/s10765-012-1353-3).** DOI:10.1007/s10765-012-1374-y
213. M. Ould Kada, T. SEDDIK, A. SAYEDE, R. KHENATA, A. BOUHEMADOU, E. DELIGOZ, Z. A. ALAHMED, S. BIN OMRAN, D. RACHED: **Elastic, electronic and thermodynamic properties of rh3x (x = zr, nb and ta) intermetallic compounds.** International Journal of Modern Physics B 01/2013; 28(3), DOI:10.1142/S0217979214500064
214. M. Jibran, G. Murtaza, M.A. Khan, R. Khenata, S. Muhammad, Roshan Ali: **First principle study of MF<sub>2</sub> (M = Mg, Ca, Sr, Ba, Ra) compounds.** Computational Materials Science 01/2013; 81., DOI:10.1016/j.commatsci.2013.09.010
- 215.** A. Bouhemadou, O. Boudrifia, N. Guechi, R. Khenata, Y. Al-Douri, Ş. Uğur, B. Ghebouli, S. Bin-Omran: **Structural, elastic, electronic, chemical bonding and optical properties of Cu-based oxides ACuO (A = Li, Na, K and Rb): An ab initio study.** Computational Materials Science 01/2013; 81., DOI:10.1016/j.commatsci.2013.09.011
216. B. Ghebouli, M.A. Ghebouli, M. Fatmi, A. Bouhemadou, R. Khenata, D. Rashed: **Spin-polarized structural, electronic and magnetic properties of**

**diluted magnetic semiconductors  $\text{Ca}0.75\text{TM}0.25\text{O}$  ( $\text{TM} = \text{Fe, Co and Ni}$ ) in the rock salt (B1) phase.**

217. A. Abdiche Abdiche, R. Riane, M. Guemou, Y. Al-Douri, R. Baghdad, R. Khenata: **Pressure Effect on Structural, Electronic and Optical Properties of Zinc Blend Mgo Solid Solution.** 12/2012; 1(1)., DOI:10.5963/AMSA0101002
218. M. Harmel, H. Khachai, M. Ameri, R. Khenata, N. Baki, A. Haddou, B. Abbar, S. Uğur, S. Bin Omran, F. Soyalp: **DFT-based ab initio study of the electronic and optical properties of cesium based fluoro-perovskite  $\text{CsMF}_3$  ( $\text{M}=\text{Ca and Sr}$ ).** International Journal of Modern Physics B 12/2012; 26(32)., DOI:10.1142/S0217979212501998
219. M. Harmel, H. Khachai, A. Ameri, N. Baki, A. Haddou, M. Khalfa, B. Abbar, S. Bin Omran, G. Uğur, S. Uğur, R. Khenata: **Full-Potential Calculation of Structural, Electronic, and Thermodynamic Properties of Fluoroperovskite  $\text{CsMF}_3$  ( $\text{M} = \text{Be and Mg}$ ).** International Journal of Thermophysics 12/2012; 33(1)., DOI:10.1007/s10765-012-1353-3
220. Y. Al-Douri, H. Baaziz, Z. Charifi, R. Khenata, U. Hashim, M. Al-Jassim: **Further optical properties of  $\text{CdX}$  ( $\text{X} = \text{S, Te}$ ) compounds under quantum dot diameter effect: Ab initio method.** Renewable Energy 09/2012; 45., DOI:10.1016/j.renene.2012.02.020
221. N. Mehtougui, D. Rached, R. Khenata, H. Rached, M. Rabah, S. Bin-Omran: **Structural, Electronic and Mechanical Properties of  $\text{RuO}_2$  from First-Principles Calculations.** Materials Science in Semiconductor Processing 08/2012; 15(4)., DOI:10.1016/j.mssp.2012.02.001
222. Dinesh Varshney, Swarna Shriya, M. Varshney, R. Khenata: **Pressure dependent mechanical properties of europium mono chalcogenides under high pressure.** Computational Materials Science 08/2012; 61., DOI:10.1016/j.commatsci.2012.04.009
223. M. Hichour, D. Rached, R. Khenata, M. Rabah, M. Merabet, Ali H. Reshak, S. Bin Omran, R. Ahmed: **Theoretical investigations of  $\text{NiTiSn}$  and  $\text{CoVSn}$  compounds.** Physics and Chemistry of Minerals 08/2012; 73(8)., DOI:10.1016/j.jpcs.2012.03.014
224. Dinesh Varshney, S. Shriya, R. Khenata: **Structural phase transition and elastic properties of mercury chalcogenides.** Materials Chemistry and Physics 08/2012; 135(2-3)., DOI:10.1016/j.matchemphys.2012.04.060
225. T. Seddik, R. Khenata, A. Bouhemadou, D. Rached, Dinesh Varshney, S. Bin-Omran: **Structural, electronic and elastic properties of the new ternary**

**alkali metal chalcogenides  $KLiX$  ( $X = S, Se$  and  $Te$ )**. Computational Materials Science 08/2012; 61., DOI:10.1016/j.commatsci.2012.04.020

226. Tarik Ouahrani, R Khenata, B Lasri, Ali H Reshak, A Bouhemadou, S Bin-Omran: **First and second harmonic generation of the  $XAl_2Se_4$  ( $X \frac{1}{4} Zn, Cd, Hg$ ) defect chalcopyrite compounds**. Physica B Condensed Matter 07/2012; 407(18)., DOI:10.1016/j.physb.2012.05.057
227. B. Amin, R. Khenata, A. Bouhemadou, Iftikhar Ahmad, M. Maqbool: **Opto-electronic response of spinels  $MgAl_2O_4$  and  $MgGa_2O_4$  through modified Becke-Johnson exchange potential**. Physica B Condensed Matter 07/2012; 407(13)., DOI:10.1016/j.physb.2012.03.075
228. Ghebouli, M.A, Bouhemadou, Fatmi, Khenata, Rached, Ouahrani, Bin-Omran: **Theoretical prediction of the structural, elastic, electronic, optical and thermal properties of the cubic perovskites  $CsXF_3$  ( $X = Ca, Sr$  and  $Hg$ ) under pressure effect**. Solid State Sciences 07/2012; 14(7)., DOI:10.1016/j.solidstatesciences.2012.04.019
229. A. Bouhemadou, K. Haddadi, R. Khenata, D. Rached, S. Bin-Omran: **Structural, elastic and thermodynamic properties under pressure and temperature effects of  $MgIn_2S_4$  and  $CdIn_2S_4$** . Physica B Condensed Matter 06/2012; 407(12)., DOI:10.1016/j.physb.2012.03.017
230. Bouhemadou, M.A. Ghebouli, G. Uğur, Ş. Uğur, B. Ghebouli, R. Khenata, S. Bin-Omran: **Ab initio study of some fundamental physical properties of the cubic inverse-perovskite  $Mn_3ZnC$  and  $Mn_3GeC$** . Computational Materials Science 06/2012; 58., DOI:10.1016/j.commatsci.2012.01.030
231. M Hichour, D Rached, R Khenata, M Rabah, M Merabet, Ali H Reshak, S Bin Omran, R Ahmed: **Theoretical investigations of  $NiTiSn$  and  $CoVSn$  compounds**. Journal of Physics and Chemistry of Solids 05/2012;
232. Ali H Reshak, I.V. Kityk, R Khenata, Y Al-Douri, S Auluck: **An ab initio density functional study of the optical functions of 9-Methyl-3-Thiophen-2-YI-Thieno [3,2e] [1,2,4] Thriazolo [4,3c] Pyrimidine-8-Carboxylic Acid Ethyl Ester crystals**. Spectrochimica Acta Part A Molecular and Biomolecular Spectroscopy 04/2012; 95., DOI:10.1016/j.saa.2012.04.055
233. M Arbi, N Benramdane, Z Kebbab, R Miloua, F Chiker, R Khenata: **First principles calculations of structural, electronic and optical properties of zinc aluminum oxide**. Materials Science in Semiconductor Processing 04/2012; 15(3)., DOI:10.1016/j.mssp.2012.03.010
234. M. Guemou, B. Bouhafs, A. Abdiche, R. Khenata, Y. Al Douri, S. Bin Omran: **First-principles calculations of the structural, electronic and optical**

**properties of cubic  $BxGa1-xAs$  alloys.** Physica B Condensed Matter 04/2012; 407(8)., DOI:10.1016/j.physb.2012.01.132

235. H. Righi, D. Rached, S. Benalia, R. Khenata, S. Bin Omran, Ali H. Reshak: **Theoretical investigation of the elastic, thermodynamic, electronic and magnetic properties of  $PrNi2Si2$  and  $PrNi2Ge2$ .** Computational Materials Science 03/2012; 54(1)., DOI:10.1016/j.commatsci.2011.10.001
236. T. Seddik, R. Khenata, O. Merabha, A. Bouhemadou, S. Bin-Omran, D. Rached: **Elastic, electronic and thermodynamic properties of fluoro-perovskite  $KZnF3$  via first-principles calculations.** Applied Physics A 03/2012; 106(3)., DOI:10.1007/s00339-011-6643-2
237. Y. Al-Douri, B. Merabet, H. Abid, R. Khenata: **First-principles calculations to investigate optical properties of  $ByAlxIn1-x-yN$  alloys for optoelectronic device.** Superlattices and Microstructures 03/2012; 51(3)., DOI:10.1016/j.spmi.2012.01.004
238. A. Bouhemadou, G. Uğur, Ş. Uğur, F. Soyalp, R. Khenata, S. Bin-Omran: **Theory study of structural parameters, elastic stiffness, electronic structures and lattice dynamics of  $RBRh3$  ( $R = Sc, Y, La$  and  $Lu$ ).** Computational Materials Science 03/2012; 54(1)., DOI:10.1016/j.commatsci.2011.10.029
239. A. Abdiche, R. Baghdad, R. Khenata, R. Riane, Y. Al-Douri, M. Guemou, S. Bin-Omran: **Structural and electronic properties of zinc blende  $B_xAl_1-xN_yP_{1-y}$  quaternary alloys via first-principle calculations.** Physica B Condensed Matter 02/2012; 47(3)., DOI:10.1016/j.physb.2011.10.056
240. F. Litimein, R. Khenata, A. Bouhemadou, Y. Al-Douri and S. Bin Omran: **First-principle calculations to investigate the elastic and thermodynamic properties of  $RBRh3$  ( $R=Sc, Y$  and  $La$ ) perovskite compounds.** Molecular Physics 01/2012; 110(2)., DOI:10.1080/00268976.2011.635607
241. M. Ameri, A. Touia, R. Khenata, Y. Al-Douri, H. Baltache: **Structural and optoelectronic properties of  $NiTix$  and  $CoVx$  ( $X = Sb$  and  $Sn$ ) half-Heusler compounds: An ab initio study.** Optik - International Journal for Light and Electron Optics 01/2012; 124(7)., DOI:10.1016/j.ijleo.2011.12.052
242. K. Bougerara, F. Litimein, R. Khenata, E. Uçgun, H. Y. Ocak, S. Ugur, G. Uğur, Ali H. Reshak, F. Soyalp, and S. Bin Omran: **Structural, Elastic, Electronic and Optical Properties of  $Cu3TMSe4$  ( $TM = V, Nb$  and  $Ta$ ) Sulfanite Compounds via First-Principles Calculations.** Science of Advanced Materials 01/2012; 5(1)., DOI:10.1166/sam.2013.1435

243. Ali Hussain Reshak, H. Kamarudin, R. Khenata, I. V. Kityk, S. Auluck: *ChemInform : Electronic Band Structure and Optical Propertis of Titanium Oxyphosphates Li<sub>0.50</sub>Co<sub>0.25</sub>TiO(PO<sub>4</sub>) Single Crystals: An ab initio Calculations.*. ChemInform 11/2011; 42(45)., DOI:10.1002/chin.201145001
244. A. Maachou, H. Aboura, B. Amrani, R. Khenata, S. Bin Omran, Dinesh Varshney: *Structural stabilities, elastic and thermodynamic properties of Scandium Chalcogenides via first-principles calculations.* Computational Materials Science 10/2011; 50(11)., DOI:10.1016/j.commatsci.2011.05.038
245. M. Merabet, D. Rached, R. Khenata, S. Benalia, B. Abidri, N. Bettahar, S. Bin Omran: *Electronic structure of (BP)<sub>n</sub>/(BAs)<sub>n</sub> (0 0 1) superlattices.* Physica B Condensed Matter 09/2011; 406(17)., DOI:10.1016/j.physb.2011.05.034
246. Y. Al-Douri, R. Khenata, A.H. Reshak: *Investigated optical studies of Si quantum dot.* Solar Energy 09/2011; 85(9)., DOI:10.1016/j.solener.2011.06.017
247. F. Zerarga, A. Bouhemadou, R. Khenata, S. Bin-Omran: *Structural, Electronic and Optical Properties of Spinel Oxides ZnAl<sub>2</sub>O<sub>4</sub>, ZnGa<sub>2</sub>O<sub>4</sub> and ZnIn<sub>2</sub>O<sub>4</sub>.* ChemInform 08/2011; 13(8)., DOI:10.1016/j.solidstatesciences.2011.06.016
248. Ali Hussain Reshak, H. Kamarudin, I.V. Kityk, R. Khenata, S. Auluck: *Electronic band structure and optical properties of titanium oxyphosphates Li<sub>0.50</sub>Co<sub>0.25</sub>TiO(PO<sub>4</sub>) single crystals: An ab-initio calculations.* Journal of Solid State Chemistry 08/2011; 184(8)., DOI:10.1016/j.jssc.2011.06.010
249. Tarik Ouahrani, I. Merad-Boudia, H. Baltache, R. Khenata, Z. Bentalha: *Effect of pressure on the global and local properties of cubic perovskite crystals.* Physica Scripta 07/2011; 84(2)., DOI:10.1088/0031-8949/84/02/025704
250. F. Zerarga, A. Bouhemadou, R. Khenata, S. Binomran: *FP-LAPW study of the structural, elastic and thermodynamic properties of spinel oxides ZnX<sub>2</sub>O<sub>4</sub> (X = Al, Ga, In).* Computational Materials Science 07/2011; 50(9)., DOI:10.1016/j.commatsci.2011.04.013
251. A. Bouhemadou, R. Khenata, S. Binomran: *Structural parameters, electronic structures, elastic stiffness and thermal properties of M<sub>2</sub>PC (M=V, Nb, Ta).* Physica B Condensed Matter 07/2011; 406(14)., DOI:10.1016/j.physb.2011.04.047

- 252.** Ali Hussain Reshak, I. V. Kityk, R. Khenata, S. Auluck: ***Effect of increasing tellurium content on the electronic and optical properties of cadmium selenide telluride alloys CdSe 1-x Te x : An ab initio study.*** Journal of Alloys and Compounds 06/2011; 509(24)., DOI:10.1016/j.jallcom.2011.03.029
- 253.** Mohammed Ameri, Noureddine Bouzouira, Mohammed Doui-Aici, Rabah Khenata, Abdelkader Yakoubi, Boualem Abidri, Nouredinne Moulay, Mohammed Maachou: ***FP-LMTO Investigation of the Structural and Electronic Properties of Cu<sub>x</sub>Ag<sub>1-x</sub>I Alloys.*** Materials Sciences and Applications 05/2011; 2(07)., DOI:10.4236/msa.2011.27103
- 254.** Mohammed Ameri, Ali Bentouaf, Mohammed Doui-Aici, Rabah Khenata, Fatima Boufadi, Amina Touia: ***Structural and Electronic Properties Calculations of Al x In 1-x P Alloy.*** Materials Sciences and Applications 05/2011; 2(07)., DOI:10.4236/msa.2011.27101
- 255.** N Benayad, D Rached, R Khenata, F Litimein, Ali H Reshak, M Rabah, H Baltache: ***First principles study of the structural, elastic and electronic properties of Ti<sub>2</sub>InC and Ti<sub>2</sub>InN.*** Modern Physics Letters B 04/2011; 1720(25)., DOI:10.1142/S021798491102605X
- 256.** H. Rached, D. Rached, R. Khenata, S. Benalia, M. Rabah, F. Semari, H. Righi: ***Structural stabilities, elastic, and electronic properties of iridium mononitride: A first-principles study.*** Phase Transitions 03/2011; 84(3)., DOI:10.1080/01411594.2010.530483
- 257.** Tarik Ouahrani, Ali H. Reshak, R. Khenata, H. Baltache, B. Amrani, A. Bouhemadou: ***Structural, electronic, linear, and nonlinear optical properties of ZnCdTe<sub>2</sub> chalcopyrite.*** physica status solidi (b) 03/2011; 248(3)., DOI:10.1002/pssb.200945463
- 258.** M. Merabet, S. Benalia, D. Rached, R. Khenata, A. Bouhemadou, S. Bin Omran, Ali H. Reshak, M. Rabah: ***Structural and electronic properties of bulk GaP and AlP and their (GaP)<sub>n</sub>/(AlP)<sub>n</sub> superlattices.*** Superlattices and Microstructures 02/2011; 49(2)., DOI:10.1016/j.spmi.2010.11.012
- 259.** Ali H. Reshak, T. Ouahrani, R. Khenata, A. Otero-de-la-Roza, V. Luaña, H. Baltache: ***Density functional calculation for the first and second harmonic generation of the chalcopyrite Ga<sub>2</sub>AsSb.*** Computational Materials Science 01/2011; 50(3)., DOI:10.1016/j.commatsci.2010.10.026
- 260.** F. Boukabrine, F. Chiker, H. Khachai, A. Haddou, N. Baki, R. Khenata, B. Abbar, A. Khalfi: ***Ab initio calculation of ZnSiAs<sub>2</sub> and CdSiAs<sub>2</sub> semiconductor compounds.*** Physica B Condensed Matter 01/2011; 406(2)., DOI:10.1016/j.physb.2010.10.024

261. Ali H Reshak, T Ouahrani, R Khenata, A Otero-De-La-Roza, V Luaña, H Baltache: **Density functional calculation for the first and second harmonic generation of the chalcopyrite Ga<sub>2</sub>AsSb**. Computational Materials Science 01/2011;
262. F. Semari, R. Khenata, M. Rabah, A. Bouhemadou, S. Bin Omran, Ali H. Reshak, D. Rached: **Full potential study of the elastic, electronic, and optical properties of spinels MgIn<sub>2</sub>S<sub>4</sub> and CdIn<sub>2</sub>S<sub>4</sub> under pressure effect**. Journal of Solid State Chemistry 12/2010; 183(12)., DOI:10.1016/j.jssc.2010.09.022
263. Y Al-Douri, Ali Hussain Reshak, H Baaziz, Z Charifi, R Khenata, S Ahmad, U Hashim: **An ab initio study of the electronic structure and optical properties of CdS 1Åx Te x alloys**. Solar Energy 11/2010; 84(12)., DOI:10.1016/j.solener.2010.10.006
264. Y Ayeb, T Ouahrani, R Khenata, Ali H Reshak, D Rached, A Bouhemadou, R Arrar: **FP-LAPW investigation of structural, electronic, linear and nonlinear optical properties of ZnIn<sub>2</sub>Te<sub>4</sub> defect-chalcopyrite**. Computational Materials Science 11/2010; 50(2)., DOI:10.1016/j.commatsci.2010.09.030
265. F Semari, R Khenata, M Rabah, A Bouhemadou, S Bin Omran, Ali H Reshak, D Rached: **Full potential study of the elastic, electronic, and optical properties of spinels MgIn<sub>2</sub>S<sub>4</sub> and CdIn<sub>2</sub>S<sub>4</sub> under pressure effect**. Journal of Solid State Chemistry 10/2010;
266. M. Hachemaoui, R. Khenata, A. Bouhemadou, S. Bin-Omran, Ali H. Reshak, F. Semari, D. Rached: **Prediction study of the structural and elastic properties for the cubic skutterudites LaFe<sub>4</sub>A<sub>12</sub> (A = P, As and Sb) under pressure effect**. Solid State Communications 10/2010; 150(s 39–40)., DOI:10.1016/j.ssc.2010.07.048
267. Tarik Ouahrani, Alberto Otero-de-La-Roza, A. H. Reshak, R. Khenata, H. I. Faraoun, B. Amrani, M. Mebrouki, Víctor Luaña: **Elastic properties and bonding of the AgGaSe<sub>2</sub> chalcopyrite**. Physica B Condensed Matter 09/2010; 405(17)., DOI:10.1016/j.physb.2010.05.061
268. H. Rached, D. Rached, M. Rabah, R. Khenata, Ali H. Reshak: **Full-potential calculation of the structural, elastic, electronic and magnetic properties of XFeO<sub>3</sub> (X=Sr and Ba) perovskite**. Physica B Condensed Matter 09/2010; 405(17-405)., DOI:10.1016/j.physb.2010.05.060
269. M. Reffas, A. Bouhemadou, R. Khenata, T. Ouahrani, S. Bin-Omran: **Ab initio study of structural, elastic, electronic and optical properties of spinel**

**SnMg2O4.** Physica B Condensed Matter 09/2010; 405(18-405).,, DOI:10.1016/j.physb.2010.06.058

270. T. Seddik, R. Khenata, A. Bouhemadou, Ali H. Reshak, F. Semari, B. Amrani: **Prediction study of the structural, elastic and high pressure properties of Yttrium chalcogenide.** Computational Materials Science 07/2010; 49(2).,, DOI:10.1016/j.commatsci.2010.05.024
271. A. Bouhemadou, R. Khenata, D. Rached, B. Amrani: **Theoretical prediction of the elastic, electronic and optical properties of the filled tetrahedral semiconductor  $a\text{-LiMgSb}$ .** Computational Materials Science 06/2010; 49(1).,, DOI:10.1016/j.commatsci.2010.04.021
272. T. Ouahrani, Ali H. Reshak, R. Khenata, B. Amrani, M. Mebrouki, A. Otero-de-la-Roza, V. Luana: *ChemInform Abstract: Ab initio Study of the Structural, Linear and Nonlinear Optical Properties of CdAl<sub>2</sub>Se<sub>4</sub> Defect-Chalcopyrite.* ChemInform 04/2010; 41(15).,, DOI:10.1002/chin.201015002
273. M. Hichour, R. Khenata, D. Rached, M. Hachemaoui, A. Bouhemadou, Ali. H. Reshak, F. Semari: **FP-APW+lo study of the elastic, electronic and optical properties for the cubic antiperovskite ANSr<sub>3</sub> (A=As, Sb and Bi) under pressure effect.** Physica B Condensed Matter 04/2010; 405(7).,, DOI:10.1016/j.physb.2010.01.069
274. F. Litimein, D. Rached, R. Khenata, H. Baltache: *ChemInform Abstract: FPLAPW Study of the Structural, Electronic, and Optical Properties of Ga<sub>2</sub>O<sub>3</sub>: Monoclinic and Hexagonal Phases.* ChemInform 03/2010; 41(10).,, DOI:10.1002/chin.201010003
275. T. Ouahrani, A. Otero-de-la-Roza, R. Khenata, V. Luña, B. Amrani: **Structural and thermodynamic properties of SbAsGa<sub>2</sub> and SbPGa<sub>2</sub> chalcopyrites.** Computational Materials Science 01/2010; 47(3).,, DOI:10.1016/j.commatsci.2009.10.001
276. T. Ouahrani, Ali H. Reshak, R. Khenata, B. Amrani, M. Mebrouki, A. Otero-de-la-Roza, V. Luña: **Ab-initio study of the structural, linear and nonlinear optical properties of CdAl<sub>2</sub>Se<sub>4</sub> defect-chalcopyrite.** Journal of Solid State Chemistry 01/2010; 183(1).,, DOI:10.1016/j.jssc.2009.09.034
277. M. Hachemaoui, F. Semari, R. Khenata, A. Bouhemadou, M. Rabah: **Structural, Elastic and Electronic Properties of XAl<sub>2</sub>O<sub>4</sub> (X=Mg, Zn) Compounds.** European Journal of Scientific Research 01/2010; 1.
278. T. Seddik, F. Semari, R. Khenata, A. Bouhemadou, B. Amrani: **High pressure phase transition and elastic properties of Lutetium chalcogenide.** Physica B Condensed Matter 01/2010; 405(1).,, DOI:10.1016/j.physb.2009.08.113

279. D. Rached, M. Hichour, M. Rabah, S. Benalia, H. Rached, R. Khenata: ***Prediction study of the structural, elastic, electronic and optical properties of the antiperovskite BiNBa 3***. Solid State Communications 12/2009; 149(45)., DOI:10.1016/j.ssc.2009.08.033
280. T. Ouahrani, A. H. Reshak, A. Otero de la Roza, M. Mebrouki, V. Lúaña, R. Khenata, B. Amrani: ***First-principles study of structural, electronic, linear and nonlinear optical properties of Ga 2 PSb ternary chalcopyrite***. Physics of Condensed Matter 12/2009; 72(3)., DOI:10.1140/epjb/e2009-00345-6
281. T Ouahrani, Ali H Reshak, R Khenata, B Amrani, M Mebrouki, A Otero-De-La-Roza, V Lúañ: ***Ab-initio study of the structural, linear and nonlinear optical properties of CdAl 2 Se 4 defect-chalcopyrite***. Journal of Solid State Chemistry 11/2009;
282. H. Khachai, R. Khenata, A. Haddou, A. Bouhemadou, A. Boukortt, B. Soudini, F. Boukabrine, H. Abid: ***First-principles study of structural, electronic and elastic properties under pressure of calcium chalcogenides***. Physics Procedia 11/2009; 2(3)., DOI:10.1016/j.phpro.2009.11.044
283. M. Hichour, D. Rached, M. Rabah, S. Benalia, R. Khenata, F. Semari: ***Structural and elastic properties of antiperovskites XNBa 3 (X=As, Sb) under pressure effect***. Physica B Condensed Matter 11/2009; 404(21)., DOI:10.1016/j.physb.2009.07.154
284. A. Bouhemadou, R. Khenata, B. Amrani: ***Structural and thermodynamic properties of the cubic perovskite BiAlO 3***. Physica B Condensed Matter 11/2009; 404(20)., DOI:10.1016/j.physb.2009.05.052
285. D. Rached, M. Rabah, R. Khenata, B. Abidri, S. Benalia: ***Structural phase transition and elastic properties of Curium and Uranium monobismuthides under pressure effect***. Solid State Communications 11/2009; 149(41-42)., DOI:10.1016/j.ssc.2009.07.033
286. F. Litimein, D. Rached, R. Khenata, H. Baltache: ***FPLAPW study of the structural, electronic, and optical properties of Ga2O3: Monoclinic and hexagonal phases***. Journal of Alloys and Compounds 11/2009; 488(1-488)., DOI:10.1016/j.jallcom.2009.08.092
287. Ali Hussain Reshak, M Piasecki, S Auluck, I V Kityk, R Khenata, B Andriyevsky, C Cobet, N Esser, A Majchrowski, M Swirkowicz, R Diduszko, W Szyski: ***Effect of U on the Electronic Properties of Neodymium Gallate (NdGaO3): Theoretical and Experimental Studies***. The Journal of Physical Chemistry B 11/2009; 113(46)., DOI:10.1021/jp908025p

288. M. Moakafi, R. Khenata, A. Bouhemadou, F. Semari, Ali H. Reshak, M. Rabah: ***Elastic, Electronic and Optical Properties of Cubic Antiperovskites SbNCa3 and BiNCa3***. Computational Materials Science 10/2009; 46(4)., DOI:10.1016/j.commatsci.2009.05.011
289. M. Hachemaoui, R. Khenata, A. Bouhemadou, Ali H. Reshak, D. Rached, F. Semari: ***FP-APW+lo study of the elastic, electronic and optical properties of the filled skutterudites CeFe4As12 and CeFe4Sb12***. Current Opinion in Solid State and Materials Science 10/2009; 13(5-6-13)., DOI:10.1016/j.cossms.2009.04.004
290. A. Bouhemadou, Y. Al-Douri, R. Khenata, K. Haddadi: ***Structural, elastic, electronic, optical and thermal properties of c-SiGe 2 N 4***. Physics of Condensed Matter 09/2009; 71(2)., DOI:10.1140/epjb/e2009-00272-6
291. B Amrani, F El, Haj Hassan, R Khenata, H Akbarzadeh: ***Theoretical study of Cu x Ag 1Åx I alloys***. Journal of Physics and Chemistry of Solids 07/2009; 6615(47)., DOI:10.1016/j.jpcs.2009.05.003
292. H. Rached, D. Rached, R. Khenata, Ali H. Reshak, M. Rabah: ***First-principles calculations of structural, elastic and electronic properties of Ni<sub>2</sub>MnZ (Z = Al, Ga and In) Heusler alloys***. physica status solidi (b) 07/2009; 246(7)., DOI:10.1002/pssb.200844400
293. M. Moakafi, R. Khenata, A. Bouhemadou, N. Benkhettou, D. Rached, Ali H. Reshak: ***Elastic, electronic and optical properties of SiGe2N4 under pressure: An ab initio study***. Physics Letters A 06/2009; 373(27)., DOI:10.1016/j.physleta.2009.05.004
294. M. Rabah, D. Rached, R. Khenata, N. Moulay, A. Zenati: ***FP-LMTO investigations of mechanical stability and high pressure of platinum nitride compounds***. Solid State Communications 06/2009; 149(23-149)., DOI:10.1016/j.ssc.2009.03.023
295. N. Bettahar, S. Benalia, D. Rached, M. Ameri, R. Khenata, H. Baltache, H. Rached: ***Elastic stability, electronic structure and optical properties of PtN2 with pyrite and fluorite structures***. Journal of Alloys and Compounds 06/2009; 478(1-2-478)., DOI:10.1016/j.jallcom.2008.11.125
296. Ali Hussain Reshak, R Khenata, I V Kityk, K J Plucinski, S Auluck: ***X-ray Photoelectron Spectrum and Electronic Properties of a Noncentrosymmetric Chalcopyrite Compound HgGa<sub>2</sub>S<sub>4</sub>: LDA, GGA, and EV-GGA***. The Journal of Physical Chemistry B 05/2009; 113(17)., DOI:10.1021/jp901142q
297. H Khachai, R Khenata, A Bouhemadou, A Haddou, Ali H Reshak, B Amrani, D Rached, B Soudini: ***FP-APW+lo calculations of the electronic and optical***

**properties of alkali metal sulfides under pressure.** Journal of Physics Condensed Matter 03/2009; 21(9)., DOI:10.1088/0953-8984/21/9/095404

298. S. Benalia, M. Hachemaoui, D. Rached, R. Khenata, N. Bettahar, M. Benyahia: **FP-LMTO calculations of elastic and electronic properties of the filled skutterudite CeRu 4P 12.** Journal of Physics and Chemistry of Solids 03/2009; 70(3)., DOI:10.1016/j.jpcs.2009.01.006
299. A. Bouhemadou, R. Khenata, F. Djabi: **Structural, elastic, electronic and optical properties of the cubic perovskite BiAlO 3. Solid State Sciences 02/2009;** 11(2)., DOI:10.1016/j.solidstatesciences.2008.08.006
300. Ali H Reshak, · S Auluck, · I V Kityk, · Y Al-Douri, · R Khenata, · A Bouhemadou: **Electronic properties of orthorhombic LiGaS 2 and LiGaSe 2. Applied Physics A 02/2009;** 94(2)., DOI:10.1007/s00339-008-4794-6
301. A Bouhemadou, R Khenata, M Kharoubi, T Seddik, Ali H Reshak, Y Al-Douri: **FP-APW + lo Calculations of the Elastic Properties in Zinc-Blende III-P Compounds Under Pressure Effects.** Computational Materials Science 01/2009; 45(2)., DOI:10.1016/j.commatsci.2008.11.013
302. Bouhemadou, R. Khenata: **Structural, electronic and elastic properties of M 2SC ( $M = Ti, Zr, Hf$ ) compounds. Physics Letters A** 01/2009; 372(42)., DOI:10.1016/j.physleta.2008.08.066
- 303.** A. Bouhemadou, Y. Al-Douri, R. Khenata and K. Haddadi: **Structurl, elastic, electronic and thermal properties of C-SiGe<sub>2</sub>Sn4.**
- 304.** D. Rached. M. Hichour, M. Rabah, S. Benalia, R. Khenata: **Prediction study of structural, elastic, electronic and optical properties of BiNBa3.** Solid State Communications 01/2009; 149.
305. H. Khachai, R. Khenata, A. Haddou, A. Bouhemadou, A. Bokkort, B. Soudini, F. Boukabrine, H. Abid: **First principle study of structural, electronic and elastic properties of calcium chacogenides.** Physics procedia 01/2009; 2.
306. S. Benalia, M. Hachemaoui, D. Rached, R. Khenata, N. Bettahar and M. Benyahia: **FP-LMTO calculations of elastic and electronic properties of the filled skutterudite CeRu4P12.** Journal of Physics and Chemistry of Solids 01/2009; 70.
- 307.** A. Bouhemaou, R. Khenata, F. Djabi: *Structural, elastic and optical properties of the cubic BiAlO<sub>3</sub>.*
308. M. Hachemaoui, R. Khenata, M. D.Khodja, B. Belgoumène: **L'étude de l'effet de pression sur les propriétés structurales, élastiques, électroniques et optiques de Si,Ge et ZnSe.**

309. M Hachemaoui, R Khenata, A Bouhemadou, Ali H Reshak, D Rached, F Semari: ***FP-APW + lo study of the elastic, electronic and optical properties of the filled skutterudites CeFe 4 As 12 and CeFe 4 Sb 12.*** Current Opinion in Solid State and Materials Science 01/2009;
310. Ali Hussain Reshak, Xuean Chen, I V Kityk, S Auluck, K Iliopoulos, S Couris, R Khenata: ***X-ray photoelectron spectra and the electronic band structure for non-centrosymmetric Bi 2 ZnB 2 O 7 nonlinear single crystal.*** Current Opinion in Solid State and Materials Science 01/2009;
311. M. Rabah, D. Rached, M. Ameri, R. Khenata, A. Zenati, N. Moulay: ***Theoretical study of ground state and high-pressure phase of platinum carbide.*** Journal of Physics and Chemistry of Solids 11/2008; 69(11)., DOI:10.1016/j.jpcs.2008.08.005
312. S. Benalia, M. Ameri, D. Rached, R. Khenata, M. Rabah, A. Bouhemadou: ***First-principle calculations of elastic and electronic properties of the filled skutterudite CeFe 4P 12.*** Computational Materials Science 10/2008; 43(4)., DOI:10.1016/j.commatsci.2008.02.018
313. A Bouhemadou, R Khenata: ***Elastic, electronic and optical properties of the filled tetrahedral semiconductor LiCdP.*** Semiconductor Science and Technology 09/2008; 23(10)., DOI:10.1088/0268-1242/23/10/105024
314. H. Khachai, R. Khenata, A. Bouhemadou, Ali.H. Reshak, A. Haddou, M. Rabah, B. Soudini: ***First principles study of the elastic properties in X<sub>2</sub>S (X=Li, Na, K and Rb) compounds under pressure effect.*** Solid State Communications 08/2008; 147(5-6)., DOI:10.1016/j.ssc.2008.05.028
315. M. Moakafi, R. Khenata, A. Bouhemadou, H. Khachai, B. Amrani, D. Rached, M. Rérat: ***Electronic and optical properties under pressure effect of alkali metal oxides. Physics of Condensed Matter 07/2008;*** 64(1)., DOI:10.1140/epjb/e2008-00286-6
316. M. Dine El Hannani, D. Rached, M. Rabah, R. Khenata, N. Benayad, M. Hichour, A. Bouhemadou: ***First-principles investigations of structural, electronic and magnetic properties of cubic LaMnO<sub>3</sub>.*** Materials Science in Semiconductor Processing 06/2008; 11(3)., DOI:10.1016/j.mssp.2009.04.002
317. A. Bouhemadou, F. Djabi, R. Khenata: ***First principles study of structural, elastic, electronic and optical properties of the cubic perovskite BaHfO<sub>3</sub>.*** Physics Letters A 06/2008; 372(24-372)., DOI:10.1016/j.physleta.2008.04.015
318. Ali Hussain Reshak, Xuean Chen, I.V. Kityk, S. Auluck, K. Iliopoulos, S. Couris, R. Khenata: ***X-ray photoelectron spectra and the electronic band structure for non-centrosymmetric Bi<sub>2</sub>ZnB<sub>2</sub>O<sub>7</sub> nonlinear single crystal.***

319. A. Bouhemadou, R. Khenata, M. Kharoubi, Y. Medkour: ***First-principles study of structural and elastic properties of Sc<sub>2</sub>AC (A=Al, Ga, In, Tl).*** Solid State Communications 04/2008; 146(3-4)., DOI:10.1016/j.ssc.2008.01.033
320. M. Ameri, D. Rached, M. Rabah, F. El Haj Hassan, R. Khenata, M. Doui-Aici: ***First principles study of structural and electronic properties of B<sub>x</sub>Zn<sub>1-x</sub>S and B<sub>x</sub>Zn<sub>1-x</sub>Te alloys.*** physica status solidi (b) 01/2008; 245(1)., DOI:10.1002/pssb.200743128
321. M. Ameri, D. Rached, M. Rabah, F. El Haj Hassan, R. Khenata, M. Doui-Aici: ***First principle study of structural and electronic properties of B<sub>x</sub>Zn<sub>1-x</sub>S and B<sub>x</sub>Zn<sub>1-x</sub>Te alloys.*** physica status solidi (b) 01/2008; 244.
- 322.** M. Hichour, D. Rached, M. Rabah, S. Benalia, R. Khenata, F. Semari: ***Structural and elastic properties of antiperovskites XNb<sub>3</sub>(X=As, Sb) under pressure effect.*** Physica B Condensed Matter 01/2008; 404.
323. R. Khenata, M. Moakafi, A. Bouhemadou, M. Hachemaoui, H. Khacah: ***First principle study of electronic and optical properties of some alkali metal oxides under pressure effect.***
324. Y. Benmimoun, A. Bouhemadou, R. Khenata, A. H. Reshak, B. Amrani, M. Ameri, H. Baltache: ***Structural, electronic and optical properties of SrCl<sub>2</sub> under hydrostatic stress.*** Physics of Condensed Matter 01/2008; 61(2)., DOI:10.1140/epjb/e2008-00064-6
325. A. Bouhemadou, R. Khenata, M. Chegaar, S. Maabed: ***First-Principles Calculations of Structural, Elastic, Electronic and Optical Properties of the Antiperovskite AsNMg<sub>3</sub>.*** Physics Letters A 11/2007; 371(4)., DOI:10.1016/j.physleta.2007.06.030
326. A Bouhemadou, R Khenata: ***Calculated structural, elastic and electronic properties of SiX<sub>2</sub>O<sub>4</sub> (X = Mg, Zn, Cd) compounds under pressure. Modelling and Simulation*** in Materials Science and Engineering 10/2007; 15(7)., DOI:10.1088/0965-0393/15/7/006
327. A. Bouhemadou, R. Khenata: ***Prediction study of structural and elastic properties under the pressure effect of M<sub>2</sub>GaC (M=Ti,V,Nb,Ta).*** Journal of Applied Physics 09/2007; 102(4-102)., DOI:10.1063/1.2773634
328. A Bouhemadou, R.Khenata, D.Rached, F.Zerarga, M. Maamache: ***Structural, electronic and optical properties of spinel oxides: Cadmium gallate and***

**cadmium indate.** The European Physical Journal Applied Physics 06/2007; 38(3)., DOI:10.1051/epjap:2007094

329. D. Rached, M. Ameri, M. Rabah, R. Khenata, A. Bouhemadou, N. Benkhettou, M. Dine el Hannani: ***Electronic structure calculations of europium chalcogenides EuS and EuSe***. physica status solidi (b) 06/2007; 244(6)., DOI:10.1002/pssb.200642450
330. A. Bouhemadou, R. Khenata: ***Ab initio study of the structural, elastic, electronic and optical properties of the antiperovskite SbNMg3***. Computational Materials Science 06/2007; 39(4)., DOI:10.1016/j.commatsci.2006.10.003
331. R. Khenata, A. Bouhemadou, Ali. H. Reshak, R. Ahmed, B. Bouhafs, D. Rached, Y. Al-Douri, M. Rérat: ***First-principles calculations of the elastic, electronic, and optical properties of the filled skutterudites CeFe4P12 and ThFe4P12***. Physical Review B 05/2007; 75(19)., DOI:10.1103/PhysRevB.75.195131
332. A. Bouhemadou, R. Khenata and F. Zerarga: ***Prediction study of structural and elastic properties under pressure effect of CdX<sub>2</sub>O<sub>4</sub> (X = Al, Ga, In) spinel oxides***. Computational Materials Science 05/2007; 39(3)., DOI:10.1016/j.commatsci.2006.09.002
333. A. Bouhemadou, R. Khenata: ***First-principles studies of pressure dependence of elastic and electronic properties in filled tetrahedral semiconductors LiMgX (X=N, P, and As)***. Journal of Physics and Chemistry of Solids 04/2007; 68(4)., DOI:10.1016/j.jpcs.2007.01.022
334. A. Bouhemadou, R. Khenata, M. Chegaar: ***Structural and elastic properties of Zr 2 AlX and Ti 2 AlX (X=C and N) under pressure effect***. Physics of Condensed Matter 04/2007; 56(3)., DOI:10.1140/epjb/e2007-00115-6
335. A. Bouhemadou, R. Khenata: ***Ab initio study of structural phase stability and elastic properties of ScSb and YSb under pressure effect***. Physics Letters A 03/2007; 362(s 5–6)., DOI:10.1016/j.physleta.2006.10.054
336. A. Bouhemadou, R. Khenata, F. Zerarga: ***Ab initio study of the structural and elastic properties of spinels MgX<sub>2</sub>O<sub>4</sub> (X = Al, Ga, In) under pressure***. Physics of Condensed Matter 03/2007; 56(1)., DOI:10.1140/epjb/e2007-00003-1
337. A. Bouhemadou, R. Khenata and F. Zerarga: ***Prediction study of elastic properties under pressure effect for filled tetrahedral semiconductors LiZnN, LiZnP and LiZnAs***. Solid State Communications 02/2007; 141(5)., DOI:10.1016/j.ssc.2006.10.0343

338. M. Ameri, D. Rached, Mr. Rabah, R. Khenata, N. Benkhettou, B. Bouhafs, Mr. Maachou: ***Structural and electronic properties calculations of  $BxZn1-xSe$  alloy. Materials Science in Semiconductor Processing*** 02/2007; 10(1)., DOI:10.1016/j.mssp.2007.01.003
339. A. Bouhemadou, R. Khenata, M. Chegaar: *Structural and elastic properties of  $Zr_2AlX$  and  $Ti_2AlX$  ( $X = C$  and  $N$ ) under pressure effect.*
340. A. Bouhemadou, R. Khenata, D. Rached, F. Zerarga, M. Maamache: ***Structural, electronic and optical properties of spinel oxides: Cadmium gallate and cadmium indate.***
341. A. Bouhemadou, R. Khenata: ***Pseudo-potential calculations of structural and elastic properties of spinel oxides  $ZnX_2O_4$  ( $X = Al, Ga, In$ ) under pressure effect.*** Physics Letters A 12/2006; 360(2)., DOI:10.1016/j.physleta.2006.08.008
342. A. Bouhemadou, R. Khenata, F. Zegrar, M. Sahnoun, H. Baltache, A.H. Reshak: ***Ab Initio Study of Structural, Electronic, Elastic and High Pressure Properties of Barium Chalcogenides.*** Computational Materials Science 12/2006; 38(2-38)., DOI:10.1016/j.commatsci.2006.03.001
343. A. Bouhemadou, R. Khenata, M. Maamache: ***Structural phase stability and elastic properties of lanthanum monochalcogenides at high pressure.*** Journal of Molecular Structure THEOCHEM 11/2006; 777(1)., DOI:10.1016/j.theochem.2006.08.031
344. R Khenata, A Bouhemadou, M Sahnoun, Ali H Reshak, H Baltache, M Rabah: ***Elastic, electronic and optical properties of  $ZnS$ ,  $ZnSe$  and  $ZnTe$  under pressure.*** Computational Materials Science 11/2006; 7820(1)., DOI:10.1016/j.commatsci.2006.01.013
345. M. Rabah, D. Rached, N. Benkhettou, R. Khenata, H. Baltache, B. Soudini, M. Ameri and H. Abid: ***First-principles calculations of ground-state and high-pressure phase of magnesium telluride.*** Computational Materials Science 10/2006; 37(4)., DOI:10.1016/j.commatsci.2005.12.022
346. D. Rached, M. Rabah, N. Benkhettou, R. Khenata, B. Soudini, Y. Al-Douri, H. Baltache: ***First-principle study of structural, electronic and elastic properties of beryllium chalcogenides  $BeS$ ,  $BeSe$  and  $BeTe$ .*** Computational Materials Science 09/2006; 37(3-37)., DOI:10.1016/j.commatsci.2005.08.005
347. D. Rached, M. Rabah, R. Khenata, N. Benkhettou, H. Baltache, M. Maachou and M. Ameri: ***High pressure study of structural and electronic properties of magnesium telluride.*** Journal of Physics and Chemistry of Solids 08/2006; 67(8)., DOI:10.1016/j.jpcs.2006.02.017

348. R. Khenata, A. Bouhemadou, M. Hichour, H. Baltache, D. Rached, M. Rérat: ***Elastic and optical properties of BeS, BeSe and BeTe under pressure.*** Solid-State Electronics 07/2006; 50., DOI:10.1016/j.sse.2006.06.019
349. R. Khenata, M. Sahnoun, H. Baltache, M. Rérat, D. Rached, M. Driz, B. Bouhafs: ***Structural, electronic, elastic and high-pressure properties of some alkaline-earth chalcogenides: An ab initio study.*** Physica B Condensed Matter 01/2006; 371., DOI:10.1016/j.physb.2005.08.046
350. R. Khenata, H. Baltache, M. Sahnoun, A. Bouhemadou, B. Bouhafs, M. Rérat: ***Optical properties of spinel oxides: MgAl<sub>2</sub>O<sub>4</sub> and ZnAl<sub>2</sub>O<sub>4</sub> under hydrostatic pressure.***
351. R. Khenata, M. Sahnoun, H. Baltache, M. Rérat, A. H. Reshak, N. Illes, B. Bouhafs: ***First-principle calculations of structural, electronic and optical properties of BaTiO<sub>3</sub> and BaZrO<sub>3</sub> under hydrostatic pressure.*** Solid State Communications 10/2005; 136(2)., DOI:10.1016/j.ssc.2005.04.004
352. R. Khenata, M. Sahnoun, H. Baltache, M. Rérat, Ali H. Reshak, Y. Al-Douri, B. Bouhafs: ***Full-Potential Calculations of Structural, Elastic and Electronic Properties of MgAl<sub>2</sub>O<sub>4</sub> and ZnAl<sub>2</sub>O<sub>4</sub> Compounds.*** Physics Letters A 09/2005; 344(2-4)., DOI:10.1016/j.physleta.2005.06.043
353. R. Khenata, B. Daoudi, M. Sahnoun, H. Baltache, M. Rérat, AH Reshak, B. Bouhafs, H. Abid, M. Driz: ***Structural, electronic and optical properties of fluorite-type compounds.*** Physics of Condensed Matter 09/2005; 47(1)., DOI:10.1140/epjb/e2005-00301-6
354. A. Bouhemadou, R. Khenata, M. Sahnoun, H. Baltache and M. Kharoubi: ***First-principles study of structural, elastic and high-pressure properties of cerium chalcogenides.*** Physica B Condensed Matter 06/2005; 363(1-4)., DOI:10.1016/j.physb.2005.03.029
355. Mohammed Sahnoun, Mohamed Zbiri, Claude A. Daul, R. Khenata, H. Baltache, M. Driz: ***Full potential calculation of structural, electronic and optical properties of KMgF<sub>3</sub>.*** Materials Chemistry and Physics 05/2005; 91(1)., DOI:10.1016/j.matchemphys.2004.11.019
356. M. Sahnoun, R. Khenata, H. Baltache, M. Rérat, M. Driz, B. Bouhafs, B. Abbar: ***First-principles calculations of optical properties of GeC, SnC and GeSn under hydrostatic pressure.*** Physica B Condensed Matter 01/2005; 355., DOI:10.1016/j.physb.2004.11.067
357. Mohammed Sahnoun, Claude A. Daul, R. Khenata, H. Baltache: ***Optical Properties of Germanium Dioxide in the Rutile Structure.*** Physics of Condensed Matter 01/2005; 45(4)., DOI:10.1140/epjb/e2005-00219-y

358. H. Baltache, R. Khenata, M. Sahnoun, M. Driz, B. Abbar, B. Bouhafs: ***Full potential calculation of structural, electronic and elastic properties of alkaline earth oxides MgO, CaO and SrO.*** Physica B Condensed Matter 02/2004; 344(1-4-344)., DOI:10.1016/j.physb.2003.09.274
359. R. Khenata, H. Baltache, M. Rérat, M. Driz, M. Sahnoun, B. Bouhafs, B. Abbar: ***First-principle study of structural, electronic and elastic properties of SrS, SrSe and SrTe under pressure.*** Physica B Condensed Matter 12/2003; 339(4)., DOI:10.1016/j.physb.2003.07.003
360. Y. Al-Douri, R. Khenata, Z. Chelahi-Chikr, M. Driz, H. Aourag: ***Effect of spin orbit on the electronic properties of zinc-blende compounds.*** Journal of Applied Physics 10/2003; 94(7)., DOI:10.1063/1.1607516
361. R. Khenata, H. Baltache, M. Sahnoun, M. Driz, M. Rérat, B. Abbar: ***Full potential Linearized Augmented Plane wave calculations of structural and electronic properties of GeC, SnC and GeSn.*** Physica B Condensed Matter 08/2003; 336(3-4)., DOI:10.1016/S0921-4526(03)00298-9

## 5. 2- CHAPTER IN BOOKS:

**Advances in Condensed Matter Physics; Ed. By Ali Hussain Reshak, Signpost - India (2008).**

**Chapter 6:** High pressure structural (B1-B2) phase transition and elastic properties of thorium chalcogenides and pnictides.

A. Aid , R. Khenata , A Bouhemadou ,T. Seddik , A. H. Reshak

**Chapter 4:** Calculated structural and elastic properties of  $M_2GeC$  ( $M = Ti, V, Cr, Zr, Nb, Mo, Hf, Ta, W$ )

A. Bouhemadou, R. Khenata, M. Chegaar, A. H. Reshak

B.

## 5.3-CONFERENCES:

### 5.3.1: NATIONAL

- **4<sup>th</sup> National Days in Physics and its Application CNPA'2000. 21-23 November 2000. Sidi-Fredj, Algeria;**"Linearized augmented plane wave calculation of the electronic structure and total energy of Tungsten",R. Khenata, B. Baltache, H. Aourag
  
- **4<sup>th</sup> National Days in Physics and its Application CNPA'2000. 21-23 November 2000. Sidi-Fredj, Algeria.**"Electronic structure of PbSe and PbTe band structure and densities of states".H. Baltache, M. Sahnoun, R. Khenata, H. Aourag

- **4<sup>th</sup> National Days in Physics and its Application CNPA'2000. 21-23 November 2000. Sidi-Fredj, Algeria.** "Electronic charge densities in PbS and PbTe ". M. Sahnoun , R. Khenata, H. Baltache, H. Aourag
  
- **5<sup>th</sup> Days on Chemical Theory -Mostaganem-Algeria 5 – 7 Mai 2001.** "Electronic properties of bcc, fcc, and hcp Cr crystal"; "Electronic structures and optical properties of ZnO", M. Sahnoun, R. Khenata
  
- **5<sup>th</sup> Days on Chemical theory -Mostaganem-Algeria 5 – 7 Mai 2001.** "Local-density and generalized-gradient calculations of the structural properties; of semiconductors", "Structural and electronic properties of SrX(X=S,Se,Te) R. Khenata , M. Sahnoun , H. Baltache
  
- **5<sup>th</sup> Days on Chemical theory -Mostaganem-Algeria 5 – 7 Mai 2001.** "Electronic and optical properties of boron compounds BaS, and BSb" H. Baltache, R. Khenata
  
- **1<sup>st</sup> congress on the Physic and its Applications (JPA-01),16-18 Mai 2004, Tiaret University (Algeria).** "Trends in band gap pressure coefficients in IV-IV compound" R. Khenata, H. Baltache, M. Rérat.
  
- **1<sup>st</sup> Congress on Physic and its Application (JPA-01),16-18 Mai 2004, Tiaret University (Algeria).** "ab initio calculations of structural, electronic and elastic properties of CaO, SrO and MgO". H. Baltache, R. Khenata A. Maachou, A. Aid.
  
- **Mascara Numerical Simulation Days (JSNM-06-25-27 Mars 2006),** "Effect of pressure on electronic and optical properties of PbTiO<sub>2</sub> and PbZrO<sub>3</sub>"H. Baltache, R. Khenata, A. Bouhemadou, M. Rérat.
  
- **Mascara Numerical Simulation Days (JSNM-06-25-27 Mars 2006)** "Structural phase stability and elastic properties of lanthanummonochalcogenides at high pressure"A. Bouhemadou, R. Khenata, B. Bennecer.
  
- **Mascara Numerical Simulation days - Mascara (JSNM-06-25-27 Mars 2006)** "Structural phase transformation and elastic constants of barium chalcogenides at high pressure" A. Bouhemmadou, R. Khenata, F.Zegrar, A. H. Reskak.

### **5.3.2: INTERNATIONAL**

- **International Conference on Materials Science and Applications Development and Innovation. Taif University - Saudi Arabia.** Theoretical study of structural, electronic, elastic and vibrational properties of

quaternary Heusler type CuCoMnG. Gökay Uğur, Abdelmadjid Bouhemadou, Şule Uğur, Abdullah Candan, Fethi Soyalp & Rabah Khenata.

- **International Conference on Materials Science and Applications Development and Innovation. Taif University - Saudi Arabia.** First-principles investigation on the elastic, magnetic, electronic and phonon properties of NiFeMnGa and NiCoMnGa half-metallic alloys. Şule Uğur, Rabah Khenata, Gökay Uğur, Ahmet İyigör, Fethi Soyalp & , Abdelmadjid Bouhemadou,
- **International Conference on Materials Science and Applications Development and Innovation. Taif University - Saudi Arabia.** Ab initio structural, electronic, elastic and phonon calculations for B2 NiAl and NiGa. Fethi Soyalp, Gökay Uğur, Şule Uğur, Rabah Khenata & Abdelmadjid Bouhemadou,
- **Fifth Saudi Conference (SSC'5-2012)-Oum El Qurra University-Mekka 2012- Saudi Arabia** "Elastic, electronic and thermodynamic properties of KZnF<sub>3</sub> via first-principles". R. Khenata, A. Bouhemadou, S. Bin Omran, T. Seddik.
- **First International Conference on Innovative Materials and Techniques-GIMT-2012-Tunisia, 2012.** "Calculation of structural, elastic magnetic and electronic properties of ferromagnetic CnP under pressure"; H. Baltache, A. Bendjdid, R. Khenata, T.Ouahrani, D. Rached.
- **6<sup>th</sup> Morocco Days on Materials Science. 9-11 November 1998. Annaba University-Algeria,**"Spin-orbit splittings of II-VI and III-V semiconductor bands at  $\Gamma$ , L and X". R. Khenata, B. Belgoumene, M. Driz, H. Aourag.
- **International Congress on Materials Science and Engenniring.27-30 November 1999. University-U.S.T.H.B- Algeria.**"Empirical pseudo-potential calculations of ternary semimagnetic semiconductors Cd Mn Te".R. Khenata, B. Belgoumene, H. Khachai, S. Brahou.
- **International Congress on Materials Science and Engenniring.27-30 November 1999. University-U.S.T.H.B- Algeria.**"The modification of the spin-orbit interaction in the zinc-blende binary II-VI and III-V Semiconductors".R. Khenata, B. Belgoumene, M. Driz, H. Khachai, S. Brahou.
- **International Congress on Materials Science and Engenniring.27-30 November 1999. University-U.S.T.H.B- Algeria.**"The model dielectric function for semiconductors" H. Baltache, R. Khenata, M. Driz.
- **Maghreb Conferences in engineering Sciences- CMGE'99.4-6 December1999. Constantine University** "Band structure study of ternary diluted magnetic semiconductor ZnMnTe".R. Khenata, H. Baltache, M. Sahnoun, B. Belgoumene, M. Driz
- **The International Conferences in Materials Science,3-5 April 2000, M'sila- University-Algeria.**"The calculation of the static dielectric function and the plasmon energy" H. Baltache, R. Khenata, M. Driz, H. Aourag

- **5<sup>th</sup> International Day on Marine Sciences, J'NESMA2001, Mai2001, Borg-el Bahi, Temenfost, Alger-Algeria.**" Infrared Rayon and useful in electronic applications"R. Khenata, M. Sahnoun, H. Baltache
- **5<sup>th</sup> International Workshop on Computational Condensed Matter Physics: Total energy and force methods.11-13 January 2001.** Trieste, Italie."Full-LAPW Calculations of electronic structure of beryllium chalcogenides of BeS, BeSe and BeTe" R. Khenata, M. Sahnoun, H. Baltache, H. Aourag
- **5<sup>th</sup> International Workshop on Computational Condensed Matter Physics :Total energy and force methods.11-13 January 2001.** Trieste, Italie. "Full-Potential LAPW study of MgO using different exchange-correlation functionals".M. Sahnoun , R. Khenata, H. Baltache, B. Bouhafs, M. Driz, H. Aourag
- **International Conference in Materials Science, Tlemcen-University-Algeria, November-2003.**"Structural phase transformation and equation of states of Strontium chalcogenides at high pressure". R. Khenata, H. Baltache, M. Driz, B. Abbar.
- **International Conference on Electrical Engineering, Communication & Physical Systems. Saida University- Algeria-** Mai -2004. "First principle calculation of optical properties of GeC, SnC and GeSn under hydrostatic pressure".M. Driz, R. Khenata, M. Sahnoun, M. Rérat.
- **Scientific Days- Franco-Algerian - Ourgla – University-November-2004.**" FP-LAPW calculations of grounds states properties for the cubic zinc-blende-like AlN, GaN and InN compounds".B. Daoudi, R. Khenata, O. Boukraa, H. Abid
- **Scientific Days- Franco-Algerian - Ourgla – University-November-2004.**" Ab initio study of the phase transformations under high pressure and elastic properties of cerium chalcogenides".Bouhamadou, R. Khenata, M. Kharoubi.
- **4<sup>th</sup> International Congress in Materials Sciences -2-4 Mai 2006 : Tlemcen-University - Algeria.**"First principle study of optical properties of MgAl<sub>2</sub>O<sub>4</sub> and ZnAl<sub>2</sub>O<sub>4</sub> compounds" R. Khenata, H. Baltache, B. Bouhafs, B. Bouhemadou, M. Rérat.
- **5<sup>th</sup> International Congress on Materials Science and Engineering CISGM-5-22-24- Novemeber-2008-Gulma** University-Algeria "Electronic band structure and optical properties of ZnIn<sub>2</sub>Te<sub>4</sub> with FP-LAPW approach" Y. Ayeb, R. Arrar. M. Halit, M. Hachemaoui, R. Khenata
- **5<sup>th</sup> International Congress on Materials Science and Engineering CISGM-5-22-24- Novemeber-2008-Gulma University-Algeria**"First principle study f electronic and optical properties of alkali metal oxides under pressure effects" R. Khenata, M.Moakafi, A.Bouhemadou, M.Hachemaoui, H. Khachai

- **6<sup>th</sup> International Conferences on the Materials Science(CSM6), Beirut-Lebanon(2008).** “ Structural , Electronic and optical properties of X<sub>2</sub>S compounds”,“Theoretical Study of the mechanical and electronic properties of some spinel compounds”“FP calculations of high pressure properties of ThX (X=S,Se and Te)”R. Khenata, A.Bouhemadou and H. Balatche
- **10<sup>th</sup> International Conferences on the Materials Science(CIPMCPS), Beni Mellal- Morocco.25-26 Mars-2010** “First principle study of eleatsic, electronic and optical properties of some spinel compounds”.
- **10<sup>th</sup> International Conferences on the Materials Science(CIPMCPS), Beni Mellal- Morocco.25-26 Mars-2010** “Structural phase transformation and elastic properties of GdN” H. Baltache and R. Khenata

### **5.3.3. INVITED PLENARY CONFERENCE:**

Plinary conference titled: **First principle studies of the mechanical, electronic and optical properties of some spinel sulphides under pressure effects**. Department of Physics and Astronomy- King Saud university- Saudi Arabia- March 2012.

## **6. RESEARCH AND PROJECTS:**

I was president (of) and member (in) more than 12 projects in different fields (Physics, Mechanics). Eight of them are completed.

- I was member in more than 10 CNEPRU Projects: Algérien CNEPRU projects : N° D01220060041 (2007) ; N° D01220080007 (2009) ; N° D01220090033 (2010) ; N° E03720090011(2010) ; N° D02120100026 (2011) ;.....
- I was responsible (Chief) of the CNEPRU Project number D03720060004 (for three years starting from January 2006)
- I was member in one PNR project number: In fundamental Sciences.

## **7- RESEARCH SUPERVISION:**

### **7-1: TWELVE MAGITER THESIS COMPLTED**

- 1. Hichour Malika, Mascara University
- 2. Sedik Tayeb, Mascara University
- 3. Missoun Adda, Mascara University
- 4. Djiad Abdelhamid, Mascara University
- 5. Ougad Sofiane, Mascara University

- 6. Boubker Nacéra, Mascara University
- 7. Moutassem Mohamed, Mascara University
- 8. Bendjedid Aicha, Mascara University
- 9. Zerrouki Tayeb, Mascara University
- 10. Meziane Ouda, Mascara University
- 11. Amriche Oumria, Mascara University
- 12 Belkacemi benyamina, Mascara University

## **7-2: FOURTEEN (14) DOCTORATE (PHD) THESIS COMPLTED**

### **1- Moakafi Mohamed**

**Title :** Contribution à l'étude des propriétés structurales, électroniques et optiques sous l'effet de pression des oxydes alcalin:  $X_2O$  ( $X=Li, Na, K, Rb$ ) par la méthode FP-LAPW

**Date of presentation:** **March 2010** at Sidi Bel-Abbès university.

### **2- Hichour Malika**

**Title:** Etude des propriétés structurales, élastiques, électroniques et optiques des antipérovskites  $ANSr_3$  ( $A=AS, Sb$  et  $Bi$ ).

**Date of presentation:** **May 2010** at Sidi Bel-Abbès University.

### **3- Benalia Salah Eddine**

**Title:** Etude des propriétés structurales, électroniques et optiques des Skutterudites remplis  $CeTr_4P_{12}$  ( $Tr=Fe, Ru$  et  $Os$ ) par la méthode FP-LMTO. **Date of presentation:** **November 2009** at Sidi Bel-Abbès university.

### **4- Ayeb Yakob**

**Title:** Etude des propriétés structurales, électroniques et optiques du  $ZnIn_2Te_4$  chalcopyrites

**Date of presentation:** **June 2012** at Sidi Bel-Abbès University.

### **5- Ouahrani Tarik**

**Title:** Calcul des propriétés structurales, thermiques et optiques des composées chacopyrites par la méthode FP-(L)APW.

**Date of presentation:** **February 2011**, at Abou Bekr Belkaid University - Tlemcen.

### **6- Hachemaoui Malika**

**Title:** Etude de l'effet de pression sur des propriétés structurales, élastiques électroniques et optiques des matériaux de type skutturidites par la méthode FP-LAPW : Cas du  $XFe_4Y_{12}$  ( $X=La, Ce; Y=P, As, Sb$ ).

**Date of presentation:** **June 2012** at Sidi Bel-Abbès university

### **7- Seddik Tayeb**

**Title:** Contribution à l'étude des propriétés structurales, élastiques, optoélectroniques et thermodynamiques des matériaux à base de ( $K, Y$  et  $Lu$ ).

**Date of presentation:** **Aprial 2013** at Sidi Bel-Abbès University

**8- Semari Fatiha**

**Title:** Contribution à l'étude des propriétés mécaniques, optoélectroniques et thermophysiques des matériaux de type  $X^{II}Y^{III}Z_4$  et  $X^{IV}Y^{II}Z_4$  ( $Z=O, S$  et  $Se$ ) par la méthode FP-LPAW.

**Date of presentation:** July 2013 at Sidi Bel-Abbès University

**9- Djied Abdelhamid**

**Title:** Contribution à l'étude des propriétés structurales, mécaniques et optoélectroniques des composés ternaires à base sodium  $NaZnX$  ( $X=P, As$  et  $Sb$ ) par la méthode (FP-LAPW).

**Date of presentation:** Juin 2014 at Sidi Bel-Abbès University

**10- Ould Kada Mokhtaria**

**Title:** Contribution à l'étude des propriétés structurales, électroniques et thermodynamiques des matériaux à base de (Rh et de Ce) par la méthode FP-LAPW.

**Date of presentation:** Juin 2014 at Sidi Bel-Abbès University

**11- Mekkaoui Fatiha**

**Title:** Etudes des propriétés structurales, élastiques et électroniques des pérovskites cubic  $RBRh_3$  ( $R=Sm, Eu, Gd$  et  $Tb$ )

**Date of presentation:** Juin 2014 at Sidi Bel-Abbès University

**12- Missoum Adda**

**Title:** Contribution à l'étude des propriétés mécaniques, optoélectroniques et thermodynamiques des alliages Heusler à base de (Al, Ga, Sb et Sn) par la méthode des ondes planes linéairement augmentées

**Date of presentation:** Aprial 2015 at Sidi Bel-Abbès University

**13- Djaafri Tayeb**

**Title:** Full potential calculations of the elastic, magnetic and thermodynamic properties of some metal Heusler alloys

**Date of presentation:** Aprial 2015 at Sidi Bel-Abbès University

**14- Arar Rabie**

**Title:** Etude par la méthode du premier principe des propriétés, structurale, électronique et thermodynamiques de quelques composés ternaires à base de fluor.

**Expected Date of presentation:** June 2015 at Sidi Bel-Abbès University

**7.3. TEACHING EXPEREINCE:**

Twenty two years (22) of teaching

**7.4. SEMINAIR ORGANIZATION:**

- President of the Scientific and organization committies of « Mascara International Numerical Simulation Days” (JSNM1) 25-27 Aprial-2006-Mascara».
- Member in the Scientific and organization committies for more than 15 scientific manifestations

## **8- MEMBER OF THE EDITORIAL BOARDS**

- *Editor: International Journal of Nanoelectronics and Materials (IJNEAM).*  
<http://www.myjurnal.my/public/browse-journal-view.php?id=219>
- *Editorial broad: International Journal of Nano Science and Technology; ISSN: 2328- 5443.*  
<http://www.ijnst.com/Editorial%20Board.php>
- *Editorial broad: Biointerface Research in Applied Chemistry, Open Access Journal (ISSN: 2069-5837)*  
[http://biointerfaceresearch.com/?page\\_id=87](http://biointerfaceresearch.com/?page_id=87)

### **Referee in More than 20 Journals (Elsevier, IOP, Springer and ACS)**

- Referee of the “Computational Materials Science”, Publisher “Elsevier”.
- Referee of the “Journal of Alloys and Compounds”, Publisher “Elsevier”.
- Referee of the Journal Phys. Chem. B. (ASC).
- Referee of the “Physica B”, Publisher “Elsevier”.
- Referee of the “Journal of Molecular Structure”, Publisher “Elsevier”.
- Referee of the “Solid State Communications”, Publisher “Elsevier”.
- Referee of the journal of “Physica Status Solidi b”, Publisher “Wiley”.
- Referee of the journal of “Physics Letters A”, Publisher “Elsevier”.
- Referee of the journal of “Physics Research International”, Publisher “Springer”.
- Referee of the journal of “European Physical Journal B”, Publisher “Springer”.
- Referee of the journal of “Philosophical magazine”, Publisher “Springer”.
- Referee of the journal of “Materials Sciences”, Publisher “Springer”
- Referee of the journal of “Journal of Applied Physics”, Publisher “ACS”

## **9. SCIENTIFIC AND PEDAGOGIC RESPONSABILITIES:**

### **9.1. SCIENTIFIC**

- Responsible (DOMAIN) for field training LMD "Science and Technology" from April 2010 to date "Two contracts", Ministerial Decision, October 2010
- Head of "Semiconductor and numerical simulation" team in the Laboratory of Quantum Physics and Mathematical Modeling of the Material (LPQ3M).
- Head of LPQ3M-Laboratory. Ministerial Decision, Febr. 2014
- Member in the National Scientific Comity for the Evaluation of National and International Journals of Physics in Algeria. Ministerial Decision, July 2014
- Member in National Comity of university for evaluating the associate professors for promotion to full professor rank (CUN).
- Founding Member of Academy of Science and Technology in Algeria, Presidential Decree number 49 of au 16 sept. 2015.

### **9.2. PEDAGOGIC**

- Responsible on the Magister formation titled " Physics of nanomaterials" Ministerial Decision, 26 Aout 2006.
- Local coordinator of the Doctoral school in physics titled "Physics and Chemistry of Materials " Ministerial Decisions, N° 224 and 225 July 2009 and N° 257 du Juillet 2010

## **10. HONOURS AND AWARDS**

- National Award : President of the Algerian republic- Laghouat University , November 2011
- International Award: Scopus award –November 2013.

## **11. SCIENTIFIC VISITS**

1. Invitation from Prof. Gerard Vorgoten- Department of Physics-Chemical laboratory-Lille University-France (2003 for one month).

2. Invitation from Prof. Michel Rérat- Physical Chemistry Group (IPREM-UMR) - Pau University- France.( 2004;2005,2007; 2008 for one month in each year).
3. Invitation from Prof. Claude Daul - Physics Department- Fribourg University-Suisse(2006 for one month)
4. Invitation from Prof. Claude Demenegeat- Institute of Physical and Chemistry of Materials of Strasbourg (IPCMS) Strasbourg University- France (2007 for one month).
5. Invitation from Prof. Fouad El Haj Hassan- Physics Department-El Hadeth University Beirut-Lebanon (2009for one month)
6. Invitation from Prof. Fethi Soyal and Gokay Ugur ( Ghazi university- Turkey)
7. Invitation from Prof. AbdelAziz Zugbi- Physics Department- DAMAS- University- Syria (2009 for one month)
8. Invitatation from Prof. A. Munoz, Terinife-Spain (2013 for one month) Inviataion from prof. Dinesh Varshney- Devi Ahiliya University-India (2014 for one month)