Curriculum Vitae

Name: Bothina Hamad Manasreh
Sex: Female
Citizen: USA

Education:
1997-2001 : Ph.D. in Physics, University of Jordan .
1992-1995 : M. Sc. In Physics, University of Jordan.
1984-1988: B. Sc. in Physics, Kuwait University.

Languages:
1. Arabic (native).
2. English (excellent speaking, reading and writing).
3. German (Fair speaking, reading and writing).

Positions:
2015- : Research professor, University of Arkansas
2013-2014: Chair of the physics department, University of Jordan.
2012-psesent: Professor, Physics Department, University of Jordan.
2010-2011: Fulbright fellow (Sabbatical leave) at Central Michigan University, MI, USA.
2008-2012: Associate Professor at the University of Jordan.
2005-2008: Assistant Professor at the University of Jordan.
2004-2005: Lecturer at the University of Jordan.
2003-2004: Research fellow of Alexander von Humboldt foundation at Fritz-Haber Institute, Berlin (Germany).
2001-2003: Assistant Professor at the University of Applied Science, Amman-Jordan.
1996-2001: Lab. Instructor at Philadelphia University, Jordan.
1995-1996: Teacher in a high school, Ministry of Education-Jordan.
1992-1995: Lab. Instructor at Jordan University. 1991-1992: Teacher in a high school, Kuwait. 1988-1990: Lab. Instructor at Kuwait University.

Teaching experience at the University of Jordan:

A. Undergraduate Classes:

The following subjects are taught in the Applied science University, Jordan and The University of Jordan:

1. General physics I.
2. General physics II.
3. Mathematical physics I and II.
4. Quantum Mechanics I and II.
5. Classical Mechanics.
6. Electromagnetic theory I and II.

B. Graduate Classes:

The following subjects are taught in the The University of Jordan:

1. Advanced Mathematical physics
2. Theoretical Methods of Physics
3. Quantum Mechanics I and II
4. Special Topics
5. Group Theory
6. Condensed matter
7. Quantum Chemistry

Teaching experience at the University of Arkansas:

A. Undergraduate Classes:
Modern Physics

B. Graduate Classes:
Condensed Matter Physics I

C. Advanced Quantum Mechanics

Supervised Graduate Students and their current positions:

1. Belal Al-Qassem : PhD. Thesis: Investigation of Interlayer Exchange Coupling Across Metallic Spacer Layers (2006). Assistant professor in the physics department at King Fahad University (Saudi Arabia).

2. Hanan Al-Sa'adi: M.Sc. Thesis: A Theoretical study of the Structural and Dynamical properties of metal surfaces (2007). High school teacher (Jordan).

3. Hashem Al-Yamani : M.Sc. Thesis: Ab-initio investigations of the structure and energetics of metal oxide surfaces (2008).

4. Ahmad Mousa: PhD. Thesis: Structure, electronic and elastic properties of the shape memory alloys (2009). Associate professor in basic science at the Middle East University (Jordan).

5. Ahmad Mubarak: PhD. Thesis: The influence of hydrogen on the electronic and magnetic structures of transition metal surfaces and interfaces (2009). Assistant professor in the physics department at King Abdul Aziz University (Saudi Arabia).

6. Ihsan Erikat: Ph.D. Thesis: Ab initio study of CO oxidation reaction on Transition-metal catalysts (2011). Associate professor in the physics department at Jerash University (Jordan).

7. Yasmeen Qawasmeh: M.Sc. Thesis: Theoretical study of the electronic and magnetic properties of full Heusler alloys from first principles (2010). PhD student at Free University of Berlin (Germany).

8. Ameena Haidary: M.Sc. Thesis: First principles investigation of oxygen adsorption on FCC (110) transition-metal surfaces (2011). High school teacher (Yemen).

9. Saed Alazar: PhD. Thesis: Structural, electronic and magnetic properties of $Fe_{3-x}Mn_xZ$ (Z=Al, Ge, Sb) Heusler Alloys (2013). Assistant professor in the physics department at Dar Al Uloom University (Saudi Arabia).

10. Bedor Abualhaj: M. Sc. Thesis: First principles investigations of the magnetic and electronic properties of Co_2CrAl-Heusler alloy (2013). PhD student at Heidelberg University (Germany).
11. Sanaa Al-Rjoub: M. Sc. Thesis: Theoretical study of the relativistic effect on the structural, electronic, and optical properties of HgX (X=S, Se, Te) binary and ternary alloys: first principles calculations (2014). High school teacher (Jordan).
12. Hadeel Abu Sammour: **M. Sc.** Thesis: Ab-initio study of electrical and thermal transport properties of thermoelectrical materials PbX (X=S ,Se ,Te) (2014). A researcher at the German Jordan University (Jordan).
13. Reem Shadeed: M. Sc. Thesis: Theoretical Study of the Structural, Electronic, Electrical and Mechanical Properties of Carbon Nano Ribbons and Nanotubes (2015). PhD student at the University of North Dakoda (USA).
14. Hashem Al-Yamany: PhD. Thesis: First principles investigations of the structural, energetics and thermoelectric properties of doped Fe_2VAl Heusler alloys (2015). Principal of a high school (Jordan).
15. Sajeda Kassab: M. Sc. Investigations of the energetic, structural, electronic, and magnetic properties of M/Ir (100) [M=Fe,Co,Ni] systems :First Principle Calculations (to complete her thesis by spring 2017).
16. Raad Haleoot: PhD. Theoretical investigations of the theomoelectric properties of Heusler alloys (Ph.D. candidate)
17. Abhiyan Pandit: PhD. Theoretical investigations of the theomoelectric properties of monochalcogenides and their low-dimensional systems (Ph.D. candidate).
18. Aida Sheibani: M.Sc. Theoretical investigations of the theomoelectric properties of mono- and di-chalcogenides (Ph.D. candidate).
19. Hind Alqurashi: PhD. Theoretical investigations of the theomoelectric properties of transition-metal oxides (Ph.D. candidate).
20. Eesha Sanjay Andharia: (Ph.D. candidate).
21. Abdullah Hzzazi: (M.Sc. candidate).
22. Shuruq Alsayegh: (M.Sc. candidate).

Research Interests:

1. **Magnetism:** The theme of this research is to predict the magnetic structure of surfaces and interfaces from first principles using the state-of-the art density functional theory to tackle the many-body problem in solving Schrödinger's equation for solids. The exciting aspects of such low-dimensional systems are the discovery of unexpected magnetic behavior at surfaces and ultra-thin films such as the magnetocrystalline anisotropy. The interlayer exchange coupling is also investigated in superlattice structures composed of ferromagnetic materials mediated by non-magnetic spacers such as Co_n/Ir_m, Fe_n/Ir_m and Fe_n/W_m superlattices that are promising for applications in spintronic devices.

2. **Catalysis:** In this branch, the oxidation of carbon monoxide is investigated using transition-metal catalytic surfaces. The study of CO oxidation reaction is of a practical importance for the control of the environmental pollution that results from combustion processes. In general, the catalytic activity for the CO oxidation over transition metal surfaces is determined by the propensity of the metal surface to dissociate oxygen molecules and counter balanced by the bond strength of the active oxygen species on the metal surface. We analyze the adsorption of O and CO on transition-metal surfaces such as Ir(100) using the electronic structure interpretations to provide a deep understanding of

the site preference for different coverages. The pathway and transition state are then determined using constrained minimization and nudge elastic band methods. The key event of such reactions is the movement of both CO and O to a site with less stability. The energy barrier is then determined, which is the energy needed for the diffusion of the species to activated sites and weakening for species bonds with metal surface.

3. **Thermoelectrics:** Thermoelectric (TE) materials are solid state devices that could be designed using two dissimilar materials such as n-and p-type semiconductors, connected electrically in series and thermally in parallel. Thermoelectric devices are double functional devices that can be used for power generation or refrigeration. They can be designed to convert thermal energy from a temperature gradient into electrical energy (Seebeck effect), where carriers diffuse from the hot to the cold side creating a voltage drop and a current flow. However, if a voltage drop is applied to the TE ends, a current flows from one end carrying heat to the other creating a temperature gradient (Peltier effect). Te-based alloys are known to have the highest figure-of-merit (ZT) value, which is a measure of TE performance. However, these materials are not very promising for functional applications due to their high costs, low natural abundance, instability at high temperatures, and toxicity. Therefore, oxides appear to be a better alternative as they are of low cost, more abundance and stable against decomposition at high temperatures, the fact that makes them more appropriate for applications, especially in power generation. In this branch of research, we calculate the transport properties (Seebeck coefficient, electrical and thermal conductivities) of tungsten bronze oxides to predict materials of high figure-of-merit.

Honors and Grants:

1. NASA RID ESPSCOR grant (2017).
2. Higher council of higher education grant of 38000 JD: 2014
3. Fulbright fellowship (2010 – 2011).
4. Max-Planck fellowship (Max-Planck institute for complex systems, Dresden):20092010.
5. Higher council of higher education grant of 77000 JD: 2009
6. Deanship of scientific research grant of 10000 JD: 2008
7. Deanship of scientific research grant of 15,000 JD: 2006
8. Humboldt Foundation grant of 18,000 Euro for a dual core Opteron linux (10 cpus) : 2006.
9. Humboldt Foundation fellowship for research: 2003-2004.
10. Kuwait University Fellowship for graduate studies: 1988-1990.
11. Kuwait University Fellowship for undergraduate studies: 1984-1988.

Conferences and activities:

1. Visiting research fellow (Alexander von Humboldt fellowship at Free University of Berlin, Germany, (January, 2016).
2. Visiting research fellow (DFG grant at Free University of Berlin, Germany, (January, 2016).
3. TMS 2014*:* Annual Meeting & Exhibition, San Diageo, California, 2014.
4. Visiting research scientist (Free university of Berlin, Germany, (June-July, 2014).
5. TMS 2013*:* Annual Meeting & Exhibition, San Antonio, Texas.
6. Visiting research fellow (Alexander von Humboldt fellowship Free University of Berlin, Germany, (January, 2013).

7. Visiting research fellow (Alexander von Humboldt fellowship Free university of Berlin, Germany, (30 June – 30 August, 2012).
8. Psi-k conference: Berlin 2010.
9. Visiting research fellow (Alexander von Humboldt fellowship) at Institute of theoretical solid state, Technical university of Freiberg, Germany, (18 June – 1 September, 2009).
10. International conference of nanotechnology and materials; May 4-7, 2009, Bahrain.
11. The International Conf. for Materials in Jordan; March 4-6 , 2009, Jordan.
12. Advanced School in High Performance and Grid Computing (3 -14 November 2008), Trieste, Italy.
13. DFT meets Experiment & 7th Tutorial Hands-on-FPLO, August 25 -28, 2008, Dresden, Germany.
14. Visiting research fellow (Max-Planch fellowship) at Max Planck Institute for the Physics of Complex Systems (July, August, 2008)**.**
15. Visiting research fellow (DFG) at Institute of theoretical solid state (IFW), Dresden, Germany, (June, 2008).
16. Nanotechnology and Nanomaterials conference, Sharm-El Sheikh, Egypt, 11-13 January (2008).
17. Visiting research fellow (Alexander von Humboldt fellowship) at Institute of theoretical solid state (IFW), Dresden, Germany, (14 June -4 September, 2007).
18. Scientific visit to Talat's Rahman group at the physics department, University of Central Florida, Orlando, Florida, USA, February 2007.
19. SUMMER SCHOOL ON COMPUTATIONAL MATERIALS SCIENCE, July 31-August 11, 2006, University of Illinois at Urbana-Champaign.
20. Visiting research fellow (DFG) at Fritz-Haber Institute-Max-Planck Institute, Berlin, Germany, (17 July-15 September, 2006).
21. Scientific visit to Talat's Rahman group at the physics department, Kansas State university, USA, February 2006.
22. Twenty Third European Conference on Surface Science (ECOSS-23),4 -9 September 2005 (FU Berlin; Henry-Ford-Bau and Harnack House , Germany).
23. Visiting research fellow (Alexander von Humboldt fellowship) at Fritz- Haber Institute-Max-Planck institute, Berlin, Germany, (6 June-16 September, 2005).
24. Workshop on Electronic structure of materials, Isfahan University of Technology, Isfahan (26 April -6 May, 2005).
25. Internal Workshop Stralsund – Germany, September 2003.
26. Workshop on Application of Density-Functional Theory in condensed-Matter Physics, Surface Physics, Chemistry, Engineering, and Biology, Berlin, 21-30 July 2003 .
27. Scientific visit to Fritz-Haber Institute-Max-Planck institute, Berlin, Germany, June-2002.
28. Second regional conference on magnetic and superconducting materials at Yarmouk University, 2001.
29. Seventh Petra School of Physics at the University of Jordan, 2000.
30. Forth-Conference in Condensed Matter Physics at the University of Jordan. May, 2000.
31. Sixth Petra School of Physics at Yarmouk University, 1998.

Community service, departmental committees, and outside memberships:

1. Committee of development.
2. Scientific Committee.
3. Seminars Committee

4. Committee of scientific research.
5. Committee of Jordanian physical society.
6. Member of Alexander von Humboldt club in Jordan.

Publications:

1. Abhiyan Pandit and **Bothina Hamad**. "Anharmonic lattice dynamics and thermal conductivity of ZrS_2 monolayer from first principles", *Submitted*.
2. Abhiyan Pandit, Raad Haleoot and **Bothina Hamad**. "Thermal conductivity and enhanced thermoelectric performance of SnTe bilayer", accepted in *Journal of Material Science*.
3. Aida Sheibani Gunder, Charles Paillard, Abhyian Pandit, Raad Haleoot, Laurent Bellaiche, and **Bothina Hamad**. "Effect of the polar distortion on the thermoelectric properties of GeTe", *Eur. Phys. J. B* **94,** 11 (2021). https://doi.org/10.1140/epjb/s10051-020-00019-1.
4. Abhiyan Pandit and **Bothina Hamad**. "Thermoelectric and lattice dynamics properties of layered MX (M = Sn, Pb; X = S, Te) compounds", *Applied Surface Science* **538**, 147911(2020). DOI: 10.1016/j.apsusc.2020.147911
5. Raad Haleoot and **Bothina Hamad**. "Thermoelectric properties of doped β-InSe by Bi: First Principle Calculations." *Physica B* **587**, 412105 (2020). doi.org/10.1016/j.physb.2020.412105
6. Haleoot, Raad and **Bothina Hamad**. "Thermodynamic and Thermoelectric Properties of CoFeYGe (Y= Ti, Cr) Quaternary Heusler Alloys: First Principle Calculations." *Journal of Physics: Condensed Matter* 32, no. 7 (2020): 075402. DOI: 0.1088/1361-648X/ab5321.
7. Mohammad Obeid, Ihsan Erikat, Bothina Hamad and Jamil Khalifeh, "Ab initio study of the adsorption of 3d transition metals on Ni(100) surface", SN Applied Sciences **2**, 637 (2020) https://doi.org/10.1007/s42452-020-2373-4
8. Sajeda Kassab, Ihsan Erikat, **Bothina Hamad**, and Jamil Khalifeh, "First Principles Calculations of the Energetic, Structural, Electronic, and Magnetic Properties of Fe/Ir(100) System", *Journal of Electronic materials* **48**, 6932 (2019). https://doi.org/10.1007/s11664-019-07509-8.
9. Zuheir El-bayyari and **Bothina Hamad**, "Embryonic Iridium nanoclusters (n =3–13): A molecular dynamics computer simulation", *International Journal of Modern Physics C* **30**, **2050002** (2019). https://doi.org/10.1142/S0129183120500023
10. Pandit, Abhiyan, Raad Haleoot, and **Bothina Hamad**. "Structural, Electronic and Thermoelectric Properties of $Pb_{1-x}Sn_xTe$ Alloys." *Journal of Electronic Materials*: 1-7 (2019). DOI: 10.1007/s11664-019-07715-4
11. R. Haleoot and **B. Hamad**, "Ab Initio Investigations of the Structural, Electronic, Magnetic, and Thermoelectric Properties of CoFeCuZ (Z = Al, As, Ga, In, Pb, Sb, Si, Sn) Quaternary Heusler Alloys", Journal of Electronic Materials 48, 1164-1173 (2019). DOI: 10.1007/s11664-018-6833-1
12. F Soltani, H Baaziz, Z Charifi, F. El Haj Hassan and B. Hamad, "*Ab initio* study of the fundamental properties of $Zn1-xTMxSe$(TM=Mn, Co and Fe)", Pramana – J. Phys.93, 18 (2019). https://doi.org/10.1007/s12043-019-1775-6

13. Bothina Hamad, "Electronic and Thermoelectric Properties of SnSe1-xSx (x = 0, 0.25, 0.5, 0.75, and 1) Alloys: First-Principles Calculations", Journal of Electronic Materials 47, 4047-4055 (2018).DOI: 10.1007/s11664-018-6291-9
14. Z. Charifi, G. djamaa, H. Baaziz, F. Soyalp, and **B. Hamad**, "Ab-initio investigations of the structural, electronic, magnetic and mechanical properties of CrX (X=As, Sb, Se, and Te) transition metal pnictides and chalcogenides" , Physica Scripta 94, 015701 (2018). https://doi.org/10.1088/1402-4896/aaece3
15. T. Ghellab, Z. Charifi, | H. Baaziz, K. Bouferrache, and **B. Hamad**, **"**Electronic structure and optical properties of complex hydrides LiBH4 and NaAlH4 compounds", International Journal of Energy Research 43, 3653-3667 (2018). https://doi.org/10.1002/er.4517
16. Dj Mokhtari, H. Baaziz, Dj Guendouz, Z. Charifi, and **B. Hamad**, "Theoretical Investigation of Structural, Electronic, Magnetic, and Mechanical Properties of Quaternary Heusler Alloys CoVTiX (X = As, Si)", J, Supercond. Nov. Magn.31, 3625–3636 (2018). DOI: 10.1007/s10948-018-4614-y
17. Y. Al-Khatatbeh1, K. Tarawneh and **B. Hamad**, "The prediction of a new high-pressure phase of hafnia using first-principles computations", Mat. Sci. Eng. **305**, 012006 (2018). https://doi:10.1088/1757-899X/305/1/012006
18. H. Al-Taani, K. Tarawneh , Y. Al-Khatatbeh and **B. Hamad**, "The high-pressure stability of Ni2In-type structure of ZrO2 with respect to OII and Fe_2P-type phases: A first-principles study", Mat. Sci. Eng. **305**, 012016 (2018).https://doi:10.1088/1757-899X/305/1/012016
19. **B. Hamad**, "*Theoretical Investigations of the Thermoelectric Properties of* $Fe_2NbGa_{1-x}Al_x$ *(x = 0, 0.25, 0.5) Alloys*", J Elect. Mater. DOI: 10.1007/s11664-017-5721-4
20. M. Tayyem, **B. Hamad**, and Beate Paulus, "*Adsorption of O,* O_2 *and CO on iridium clusters and the investigations of their stability*", Chem. Phys. **495**, 10 (2017). https://doi.org/10.1016/j.chemphys.2017.08.008
21. **B. Hamad**, "*Ab-initio investigations of the structural, electronic and thermoelectric properties of* Fe_2NbAl*-based alloy",* J. Mater. Sci. **51**, 10887 (2016). doi: 10.1007/s10853-016-0300-2
22. Al-rajoub and **B. Hamad**, "*Ab-initio investigations of the electronic and optical properties of Hg1-xCdxSe alloys*", Modern Physics Letters B **30**, 1650173 (2016). http://dx.doi.org/10.1142/S0217984916501736
23. H. Al-Yamani and **B. Hamad**, "*Ab-initio investigations of the structural, energetic and thermoelectric properties of* Fe_2VAl *Heusler alloy",* Journal of Electronic Materials **45**, 1101 (2016).doi:10.1007/s11664-015-4265-8
24. S. Al-rajoub and B. Hamad, "*Theoretical investigations of the structural, electronic, and optical properties of Hg1-xCdxTe alloys*", Phil. Mag. **95**, 2466 (2015). http://dx.doi.org/10.1080/14786435.2015.1061219
25. Z. Charifi, **B.Hamad**, H.Baaziz and F.Soyalp, "*Theoretical investigations of Co2Mn1-xCrxSn and Co2MnSn1-ySiy pseudo-ternary alloys: First principles calculations*", J. Magn. Magn. Mater. **393**, 139-145 (2015). doi:10.1016/j.jmmm.2015.05.054
26. N. Mecholsky, **B. Hamad** and M. Fornari, "*Anisotropy effects on the thermoelectric electronic transport coefficients*" Energy Harvesting and Systems 2, 15 (2015).
27. **B. Hamad**; A. Marashdeh; Z. El-Bayyari, "*Investigation of the stability of platinum clusters and the adsorption of nitrogen monoxide: Ab-initio calculations*," Chemical Physics 443, 26 (2014). http://dx.doi.org/10.1016/j.chemphys.2014.07.004

28. M. Debbichi and **B. Hamad**, *" Impact of excess iron on the calculated electronic and magnetic properties of $Co_{3-x}Fe_xSi$ Heusler compounds*," J. Appl. Phys. **116**, 103902 (2014). http://dx.doi.org/10.1063/1.4895127
29. **B. Hamad**, "*Magnetic structure calculations of Ir0.5Mn0.5 over-and sublayer at Co(001) surface*," J. Magn. Mag. Mater. **369**, 1 (2014). http://dx.doi.org/10.1016/j.jmmm.2014.05.049
30. **B. A. Hamad**, "*Investigations of the electronic and magnetic structures of Co2YGa (Cr, Mn) Heusler alloys and their (100) surfaces*," J. App. Phys. **115**, 113905 (2014). http://dx.doi.org/10.1063/1.4868469
31. R. Shaltaf, H. K. Juwhari,**B. Hamad**, J. Khalifeh, G.-M. Rignanese, X. Gonze "*Structural, electronic, vibrational and dielectric properties of $LaBGeO_5$ from first principles*," J. App. Phys.**115**, 074103 (2014). http://dx.doi.org/10.1063/1.4866357
32. I. A. Erikat and B. A. Hamad, and J.M. Khalifeh, "*First-principles study of molecular NO dissociation on Ir(100) surface*," Eur. Phys. J. **B87**, 48 (2014). http://dx.doi.org/10.1140/epjb/e2014-40566-x
33. I. A. Erikat and **B. A. Hamad**, "*A first principle study for the adsorption and absorption of carbon atom and the CO dissociation on Ir(100) surface*,"J. Chem. Phys. 139, 174703 (2013). http://dx.doi.org/10.1063/1.4827516
34. N. T. Mahmoud, .M. Khalifeh. , A. A. Mousa, H. K. Juwhari, **B. A. Hamad** , "*The energetic, electronic and magnetic structures of $Fe_{2-x}Co_xVSn$ alloys: Ab-initio calculations*,"Physica B **430**, 58 (2013). http://dx.doi.org/10.1016/j.physb.2013.08.022
35. B. Abu Alhaj and **B. A. Hamad, "***Electronic and magnetic properties of $Co_{2x}Fe_xCrAl$ alloys: ab-initio calculations,"* Phys. Status Solidi B **251**, 184 (2014). http://dx.doi.org/10.1002/pssb.201349215
36. S. Ikhmaies, B. Hamad, and J. Khalifeh, " *Ab-initio calculations of the optical properties of Δ-NbN single crystal*," Characterization of Minerals, Metals and Materials 2013, Proceedings of TMS 2013, 142th Annual Meeting & Exhibition which was held at San Antonio, Texas, USA, March 3-7 , 2013, 267-274.
37. B. Abu Alhaj and **B. A. Hamad,** J.M. Khalifeh and R. Shaltaf, **"***Ab-initio calculations of the electronic and magnetic structures of Co2Cr1-xMnxSi alloys***,"**J. Mag. Man. Mater. **336**, 37 (2013). http://dx.doi.org/10.1016/j.jmmm.2013.02.026
38. A.A. Mousa, J.M. Khalifeh and **B. A. Hamad, "***Electronic, Elastic structure and phase stability of TaRu shape memory alloy,*" American Journal of condensed matter physics 3, 1-8 (2013). http://dx.doi.org/10.1002/9781118659045.ch28
39. N.T. Mahmoud, J. M. Khalifeh, **B. A. Hamad** and A. A. Mousa," *The effect of defects on the electronic and magnetic properties of the Co2VSn full Heusler alloy: ab-initio calculations*,"Intermetallics**33**, 33 (2013). http://dx.doi.org/10.1016/j.intermet.2012.09.012
40. B. Abu Alhaj and **B. A. Hamad**, " *The effect of defects on the electronic and magnetic properties of Co_2CrAl Heusler alloy*," J. Phys. Chem. Solids, **74**,265 (2013). http://dx.doi.org/10.1016/j.jpcs.2012.09.017
41. S.M. Azar, **B. A. Hamad**, J. M. Khalifeh, "*Structural, electronic and magnetic properties of (Z=Al, Ge, Sb) Heusler alloys*," J. Mag. Mag. Mater.**324**, 1776 (2012). http://dx.doi.org/10.1016/j.jmmm.2011.12.037

42. B. Abu Alhaj and **B. A. Hamad**, "*Ab-initio calculations of the electronic and magnetic structures of Co2Cr1-xMnxAl alloys*," J. Appl. Phys. **112**, 123904 (2012). http://dx.doi.org/10.1063/1.4768906
43. I. Erikat, **B. Hamad** and J. Khalifeh, "*A density functional study for adsorption and oxidation of NO on Ir(1 0 0) surface*," Applied Catalysis A **449**, 9 (2012). http://dx.doi.org/10.1016/j.apcata.2012.09.042
44. **B. Hamad**, Z. Charifi, H. Baaziz, and F. Soyalp, "*A DFT study of the electronic and magnetic properties of $Fe_2MnSi_{1-x}Ge_x$ alloys*,"J. Magn and Magn Mater.**324**, 3345 (2012). http://dx.doi.org/10.1016/j.jmmm.2012.05.052
45. Y. Qawasmeh and **B. Hamad**, "*Investigation of the structural, electronic and magnetic properties of Ni-based Heusler alloys from first principles*," J. Appl. Phys. **111**, 033905 (2012). http://dx.doi.org/10.1063/1.3681286
46. H. Baaziz , Z. Charifi , Ali Hussain Reshak, **B. Hamad** and Y. Al-Douri, "*Structural and electronic properties of GaN_xAs_{1-x}alloys*," Appl. Phys. A **106**, 687 (2012). http://dx.doi.org/10.1007/s00339-011-6666-8
47. I. Erikat, **B. Hamad** and J. Khalifeh, " *Coadsorption of CO and O on Ir(100): First Principles Calculations*," Physica B **407**, 468 (2012). http://dx.doi.org/10.1016/j.physb.2011.11.016
48. **B. Hamad**, J. Khalifeh, Q-M Hu, and C. Demangeat, "*Electronic and magnetic properties of Fe3-xCrxSi ordered alloys from first principles*," J. Material Science **47**,797 (2012). http://dx.doi.org/10.1007/s10853-011-5857-1
49. **B. Hamad** and Q-M Hu, "*The effect of defects on the electronic and magnetic properties of Fe2MnSi Heusler alloy*," Phy.Stat. Solidi. B, **248**, 2893 (2011). http://dx.doi.org/10.1002/pssb.201147305
50. **B. Hamad** and M. Richter, "*Exchange coupling and magnetocrystalline anisotropy of Fe/W superlattices*," Phys. Rev. B **83**, 245135 (2011). http://dx.doi.org/10.1103/PhysRevB.83.245135
51. I. Erikat, **B. Hamad** and J. Khalifeh, "*A density functional study on adsorption and dissociation of O_2 on Ir(100) surface*," Chemical Physics **385**, 35 (2011). http://dx.doi.org/10.1016/j.chemphys.2011.05.015
52. A. Ramanathan, J. Khalifeh and **B. Hamad**, "*A DFT study of substrate effect on the magnetism of the V(001) surface*," Surface Science **605**,1074(2011). http://dx.doi.org/10.1016/j.susc.2011.03.007
53. **B. Hamad**, "*The effect of defects on the electronic structure and magnetic map of the Fe_2CrSi Heusler alloy: Ab-initio calculations*," Eur. Phys. J. B **80**, 11-18 (2011). http://dx.doi.org/10.1140/epjb/e2011-10605-5
54. I. Erikat, **B. Hamad** and J. Khalifeh, " *Catalytic oxidation of CO on Ir(100)*," Physica status solidi B **248**, 1425 (2011). http://dx.doi.org/10.1002/pssb.201046578
55. A. Mubarak, **B. Hamad** and J. Khalifeh, "*Energetics, structural and magnetic ordering of H/Fe/M(001), (M= Cu, Ag) systems*," Journal of Magnetism and Magnetic Materials **323**, 383 (2011). http://dx.doi.org/10.1016/j.jmmm.2010.08.041
56. **B. A. Hamad** and J. Kortus, "*Magnetic properties of X0.5Mn0.5/Cu(001) overlayers, X = Fe, Mn, and Ir: ab-initio calculations*," Eur. Phys. J. B **76**, 373 (2010). http://dx.doi.org/10.1140/epjb/e2010-00237-8

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