

## Curriculum Vitae

**Dr. Nabil M. Al-Aqtash**

Physics Department  
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### Education:

1/2005-3/2011 PhD, Physics, New Mexico State University, NM, USA.  
1/2005-5/2007 M.Sc., Physics, New Mexico State University, NM, USA.  
8/1998-5/2001 M.Sc., Physics, University of Jordan, Jordan.  
8/1994-8/1997 B.Sc., Physics, Mu'tah University, Jordan.

### Professional Experience:

9/2015-present Assistance Professor, Physics Department, Hashemite University.  
4/2011-8/2015 Research Associate, Physics Department, University of Nebraska at Omaha, Omaha, Nebraska, USA.  
1/2007-3/2011 Graduate Research and Teaching Assistant, Department of physics, New Mexico State University, Las Cruces, NM, USA.  
1/2005-1/2007 Graduate Teaching Assistant, Department of physic, New Mexico State University, Las Cruces, NM, USA.  
2/2002-1/2005 Research and Teaching Assistant, Department of physics, Hashemite University, Jordan.  
9/1998-5/2001 Graduate Teaching Assistant, Department of physic, University of Jordan, Jordan.  
8/1998-1/2002 Teacher of Physics and science, Ministry of Education, Jordan.

### Facilities and Techniques:

An *ab initio* Density functional theory (DFT) techniques.

SIESTA (Spanish Initiative for Electronic Simulations with Thousands of Atoms) code based on DFT.

VASP (Vienna Ab-initio Simulation Package) code based on DFT.

PARSEC (Pseudopotential Algorithm for Real-Space Electronic Calculations) code based on DFT.

GAMESS (General Atomic and Molecular Electronic Structure System) ab initio quantum chemistry package

TranSIESTA electron transport code based on DFT coupled with nonequilibrium Green's function (NEGF) method.

Ab-initio Monte Carlo simulations using Monte Carlo (MC) method with Metropolis algorithm.

### **Professional Associations:**

Member of the American Physical Society (APS)

### **PhD Dissertation**

“First-Principles Studies of Functionalization and Substitutional Doping of Graphene and Carbon Nanotubes” New Mexico State University, 2011.

### **Publication List:**

- 1. N. Al-Aqtash** and I. Vasiliev, Ab Initio Study of Carboxylated Graphene, *The Journal of Physical Chemistry C* 2009 113 (30), 12970-12975.
- 2. N. Al-Aqtash** and I. Vasiliev, Ab Initio Study of Boron- and Nitrogen-Doped Graphene and Carbon Nanotubes Functionalized with Carboxyl Groups, *The Journal of Physical Chemistry C*, 2011, 115 (38), 18500–18510.
- 3. N. Al-Aqtash**, K. Al-Tarawneh, T. Tawalbeh, and Igor Vasiliev, Ab initio study of the interactions between boron and nitrogen dopants in graphene, *Journal of Applied Physics* 2012 112, 034304.
- 4. H. Li, N. Al-Aqtash**, L. Wang, R. Qin, Q. Liu, J. Zheng, W-N. Mei, R. Sabirianov, Z. Gao, J. Lu, Electromechanical switch in metallic graphene nanoribbons via twisting, *Physica E: Low-dimensional Systems and Nanostructures* 2012 44 (10 ), 2021-2026.
- 5. P. Kharel; X.Z. Li; V.R. Shah; N. Al-Aqtash; K. Tarawneh; R.F. Sabirianov; R. Skomski; D.J. Sellmyer**, Structural, magnetic, and electron transport properties of MnBi:Fe thin films, *Journal of Applied Physics* 2012;111(7), 07E326.
- 6. P. Kharel, Y. Huh, V. R. Shah, X. Z. Li, N. Al-Aqtash, K. Tarawneh, E. S. Krage, R. F. Sabirianov, R. Skomski, and D. J. Sellmyer**, Structural and magnetic properties of Mn<sub>2+δ</sub>TiSn, *Journal of Applied Physics* 2012;111(7), 07B101.
- 7. N. Al-Aqtash**, H. Li, L. Wang, W-N. Mei, R. Sabirianov, Electromechanical switching in graphene nanoribbons, *Carbon* 2013 51, 102-109.
- 8. Nabil Al-aqtash; Florin Apostol; Wai-Ning Mei; Renat Sabirianov**, Electronic and Optical Properties of TaO<sub>1-x</sub>N<sub>1+x</sub>-based Alloys, *Journal of Solid State Chemistry* 2012 198, 337–343.
- 9. K. Altarawneh and N. Al-Aqtash** , Boron- and Nitrogen-Doped Carbon Nanotubes with Surface Defects: An *ab initio* study, *Journal of Computational and Theoretical Nanoscience* Vol. 10, 1–7, 2013.
- 10. K. Altarawneh and N. Al-Aqtash**, First-principles Study of Boron- and Nitrogen-Doped Graphene in the Presence of Point Surface Defects, *Journal of Computational and Theoretical Nanoscience* Vol. 10, 1–8, 2013 .

11. P. Kharel<sup>1</sup>, Y. Huh<sup>1</sup>, **N. Al-Aqtash**, V. R. Shah, R. F. Sabirianov, R. Skomski and D. J. Sellmyer, Structural and magnetic transitions in cubic Mn<sub>3</sub>Ga, *J. Phys.: Condens. Matter*, 26 126001 (2013).
12. K. Altarawneh, **N. Al-Aqtash**, Role of Vacancies in Zigzag Graphene Nanoribbons: An Ab Initio Study, *Journal of Nano Research* 27,65-73 (2014).
13. **N. Al-Aqtash** and R. F. Sabirianov, Spin density wave in periodically strained Graphene Nanoribbon, *Nanoscale* 6, 4285-4291 (2014).
14. K. Altarawneh, **N. Al-Aqtash**, and R. F. Sabirianov, Large Magnetoresistance of MnBi/Bi/MnBi Spin Valve, *Journal of Magnetism and Magnetic Materials* 363, 43–48 (2014).
15. **N. Al-Aqtash** and R. F. Sabirianov, Photo-switching of magnetization in iron nanoparticles, *J. Mater. Chem. C*, 2, 6873-6878 (2014).
16. **N. Al-Aqtash**, A. Alsaad and R. F. Sabirianov, Ferroelectric properties of BaZrO<sub>3</sub>/PbZrO<sub>3</sub> and SrZrO<sub>3</sub>/PbZrO<sub>3</sub> superlattices: An ab-initio study, *Journal of Applied Physics*, 116, 074112 (2014).
17. A. Alsaad, **N. Al-Aqtash** and R. F. Sabirianov, Generalized stacking fault in FePt nanoparticles and effects of extended defects on magnetocrystalline anisotropy energy, *Journal of Magnetism and Magnetic Materials*, 374, 525–529 (2015).
18. **N. Al-Aqtash** and I. Vasiliev, Carboxylation of Boron- and Nitrogen-Doped Graphene and Carbon Nanotubes, *NSTI-Nanotech 2010*, ISBN:978-1-4398-3402-2 Vol. 2, 2010.

### **Conferences:**

“Ab Initio Study of Covalent Functionalization of Defective Carbon Nanotubes by Carboxyl Group (COOH),” APS Four –Corners Meeting, Oct. 2007, Flagstaff, Arizona.

“Role of Surface Defects in the Carboxylation of Carbon Nanotubes: An *ab Initio* Study,” APS March Meeting, March 10-14, 2008, New Orleans, Louisiana.

“First-Principles Studies of Metal-Graphene and Metal-Nanotube Heterostructures,” APS March Meeting, March 10-14, 2008, New Orleans, Louisiana.

“First-Principles Studies of Covalent Functionalization of Graphene by Carboxyl Groups” APS March Meeting, March 16-20, 2009; Pittsburgh, Pennsylvania.

“Ab Initio Study of Carboxylated Graphene” APS Four –Corners Meeting, Oct. 23-24, 2009, Golden, Colorado.

“Functionalization of Boron- and Nitrogen-Doped Graphene and Carbon Nanotubes: An *ab Initio* Study” APS March Meeting, March 15–19, 2010, Portland, Oregon.

“Carboxylation of Boron- and Nitrogen-Doped Graphene and Carbon Nanotubes: First Principles Study” Nanotech 2010 Conference and Expo, June 21-24, 2010, Anaheim, California.

“Ab Initio Study of Interaction between Boron and Nitrogen Dopants in Graphene” APS Four –Corners Meeting, October 15-16, 2010, Ogden, Utah.

“First Principles Study of Interactions between Dopant Atoms in Graphene” APS March Meeting, March 21–25, 2011, Dallas, Texas.

“Giant Electromechanical Response in Graphene Nanoribbons” APS March Meeting, February 27–March 2 2012; Boston, Massachusetts.

“Effect of Nitrogen Doping on the Electronic and Optical Properties of TaON” APS March Meeting, February 27–March 2 2012; Boston, Massachusetts.

“Inducing Magnetization by Flexing Graphene Nanoribbon” APS March Meeting, February 27–March 2 2012; Boston, Massachusetts.

“Photo-Switching of Magnetization in Iron Nanoparticles” APS March Meeting, February 27–March 2 2012; Boston, Massachusetts.

**Talks and Poster Presentations:**

“Ab Initio Study of Covalent Functionalization of Carbon Nanotubes by Carboxyl Group (COOH)” Graduate Research and Arts Symposium, March 2008, NMSU, New Mexico.

“An ab initio Study of Covalent Functionalization of Graphene by Carboxyl Groups” Graduate Research and Arts Symposium, March 2009, NMSU, New Mexico.

“Covalent functionalization of Boron/ Nitrogen doped Graphene : an ab Initio Study” Graduate Research and Arts Symposium, March 2010, NMSU, New Mexico.

“First-Principles Studies of Functionalization and Substitutional Doping of Graphene and Carbon Nanotubes” Graduate Research and Arts Symposium, March 2011, NMSU, New Mexico.

“Giant Electromechanical Response in Graphene Nanoribbons” EPSCoR RII Track 2 Workshop, November 7, 2011, San Juan, Puerto Rico.

“Effect of Nitrogen doping on electronic properties of TaON and its effect on photocatalytic properties” EPSCoR RII Track 2 Workshop, November 7, 2011, San Juan, Puerto Rico.

“Photo-Switching of Magnetization in Iron Nanoparticles” Workshop at University of Nebraska at Lincoln, June 15, 2012, Lincoln, NE.

“Mechanism of Photocatalytic Water Splitting in TiO<sub>2</sub> Surface” EPSCoR Track 2 Meeting, October 15, 2012, San Juan, Puerto Rico.

“Electronic and Optical Properties of TaO<sub>1-x</sub>N<sub>1+x</sub>-based Alloys” EPSCoR Track 2 Meeting, October 15, 2012, San Juan, Puerto Rico.

**Summer Schools:**

Summer 2007 summer school on Multiscale Theory, Simulation, and Reality at the Nano-Bio Interface, National Center for Supercomputing Applications (NCSA), and University of Illinois at Urbana-Champaign.

**References:**

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