R. Shaltaf Ph.D

r.shaltaf@ju.edu.jo

Current position

Assistant Professor
Department Of Physics
Faculty of Science
University of Jordan
Amman-Jordan

Education & Qualification

Postdoctoral Fellow — 2005-2009
European Theoretical Spectroscopy Facility (ETSF)
Unité Physico-Chimie et de Physique des Matériaux (PCPM)
Université catholique de Louvain Belgium

Ph.D. in Theoretical Solid State Physics — 1999-2004
Middle East Technical University, Turkey
Thesis title: *"Adsorption and Growth on Si(001) Surface"*

M.Sc. in Atomic and Molecular Physics — 1996-1998
Middle East Technical University, Turkey
Thesis title: *"Geometry Optimization Of Small Copper Clusters: Monte Carlo Simulations Study"*

B.Sc. in Physics — 1991-1995
Yarmouk University, Jordan

List Of Publications & Work In Progress

1. *"Electronic and Structural Properties of GeTe(100) and (110) Surfaces"*
   R. Shaltaf, E. Durgun, J.-Y. Raty, Ph. Ghosez, and X. Gonze,
   in preparation.

2. *"Reliability of Plasmon Pole Models within Many Body Perturbation Theory"*
   R. Shaltaf, M. Giantomassi, G.-M. Rignanese and X. Gonze,
   in preparation.

3. *"Electronic properties of interfaces and defects from Many-Body Perturbation Theory: Recent developments and applications"*
   M. Stankovski, M. Giantomassi, R. Shaltaf, M. Grüning, F. Bruneval, G.-M. Rignanese, submitted.

4. *"Quasiparticle Corrections on the Band Offsets at the HfO_2:Si and ZrO_2:Si Interfaces"*
   M. Grüning, R. Shaltaf, and G.-M. Rignanese,

Phys. Rev. B.**81**, 035330 (2010).

5. *"ABINIT : first-principles approach to material and nanosystem properties"*
X. Gonze , B. Amadon, P.-M. Anglade, J.-M. Beuken, b, F. Bottin, P. Boulanger, F. Bruneval, D. Caliste, b, R. Caracas, M. Ct, T. Deutsch, L. Genoves, Ph. Ghose, h, M. Giantomassi, S. Goedeckerc, D.R. Hamannm, P. Hermet, F. Jolletd, G. Jomard, S. Leroux, M. Mancini , S. Mazevet, M.J.T. Oliveira, G. Onida, Y. Pouillon, T. Rangel, G.-M. Rignanese, D. Sangalli, R. Shaltaf, M. Torrent, M.J. Verstraete, G. Zerah and J.W. Zwanziger
Comp. Phys. Comm.,**180**, 2582 (2009).

6. *"Polarization vortices in germanium tellurite nanoplatelets: A theoretical study "*
E. Durgun, Ph. Ghosez, R. Shaltaf, X. Gonze, and J.-Y. Raty
Phys. Rev. Lett. **103**, 247601 (2009).

7. *Electronic Properties of Zircon and Hafnon from Many-Body Perturbation Theory*
R. Shaltaf, T. Rangel, M. Grüning, X. Gonze, G.-M. Rignanese, and D. R. Hamann
Phys. Rev. B. **79**, 195101 (2009).

8. *"Structure Prediction and Co Oxidation on Alumina Supported PdPt Mono- and Bi-Metallic Catalysts"*
S. Kaya, E. Erunal, R. Shaltaf, S. Ellialtioglu, and D. Uner,
Turk J Chem **33**, 11 (2009).

9. *"Lattice Dynamics and Specific Heat of α-GeTe: a theoretical and experimental study"*
R. Shaltaf, X. Gonze, M. Cardona, R. K. Kremer, and G. Siegle,
Phys. Rev. B. **79**, 075204, (2009).

10. *"Band Offsets at the Si/SiO_2 Interface from Many-Body Perturbation Theory"*
R. Shaltaf, G.-M. Rignanese, X. Gonze, F. Giustino and A. Pasquarello,
Phys. Rev. Lett. **100**, 186401 (2008).

11. *"Dynamical, Dielectric, and Elastic Properties of GeTe Investigated with First-Principles Density Functional Theory"*
R. Shaltaf, E. Durgun, J.-Y. Raty, Ph. Ghosez, and X. Gonze,
Phys. Rev. B **78**, 205203 (2008).

12. *"Hybrid Exchange-Correlation Functional for Accurate Prediction of The Electronic and Structural Properties of Ferroelectric Oxides"*

D. I. Bilc, R. Orlando, R. Shaltaf, G.-M. Rignanese, Jorge Íñiguez and Ph. Ghosez,
Phys. Rev. B **77**, 165107 (2008).

13. *"Cs Adsorption on* Si(001) *(2×1) Surface : an ab initio study"*
R. Shaltaf, E. Mete, and S. Ellialtioglu,
Phys. Rev. B **72**, 205415 (2005).

14. *"DFT Study of Rb Adsorption on* Si(001) *(2×1) Surface"*
E. Mete, R. Shaltaf, and S. Ellialtioglu,
Surf. Sci. **583**, 119 (2005).

15. *"Electronic Structure of a Chain-like Compound:* TlSe*"*
S. Ellialtioglu, E. Mete, R. Shaltaf, K. Allakhverdiev,
F. Gashimzade, M. Nizamettinova, and G. Orudzhev,
Phys. Rev. B **70**, 195118 (2004).

16. *"Mg Adsorption on* Si(001) *Surface From First Principles"*
R. Shaltaf, E. Mete, and S. Ellialtioglu,
Phys. Rev. B **69** , 125417 (2004).

17. *"Ab initio study of the One-Monolayer* Sb/Ge(001) *Interface"*
R. Shaltaf, M. Cakmak, E. Mete, G. P. Srivastava, and S. Ellialtioglu,
Surf. Sci. **566-568**, 956 (2004).

18. *"Electronic and Structural Properties of a 4d-Perovskite: cubic phase of* $SrZrO_3$*"*
E. Mete, R. Shaltaf, and S. Ellialtioglu,
Phys. Rev. B **68**, 035119 (2003).

19. *"Ab initio Study of the One-Monolayer* Sb/Si(001) *Interface"*
M. Cakmak, R. Shaltaf, G. P. Srivastava, and S. Ellialtioglu,
Surf. Sci. **532-535**, 661 (2003).

20. *"Computer Simulation of Small Copper Clusters"*
S. Erkoc and R. Shaltaf,
Phys. Rev. A. **60**, 3053 (1999).

Work & Research Experience

- Assistant Professor — 2009-
  Department Of Physics
  Faculty of Science
  University of Jordan
  Amman-Jordan
- Postdoctoral Fellow — 2005-2009
  European Theoretical Spectroscopy Facility (ETSF)
  Unité Physico-Chimie et de Physique
  des Matériaux (PCPM)
  Université catholique de Louvain Belgium
- Physics Instructor — 2000-2004
  Al Fatih Private School
  Ankara, Turkey

Theory Expertize

- Many body perturbation theory
- Density functional theory methods
- Molecular dynamics and Monte Carlo simulation methods

Computer Expertize

- Programming : Fortran, MPI
- Member of developing team of ABINIT code since 2005
- System : LINUX, UNIX, MS Windows

Invited Talks

1. *"Band Offsets Prediction From Many Body Perturbation Theory."*
   R. Shaltaf,
   13th ETSF/Nanoquanta Conference,
   Theoretical Spectroscopy and Quantum Transport,
   Pugnochiuso, Italy 23-27 September 2008.

2. *" Working with ABINIT."*
   R. Shaltaf,
   Psi-k Training Graduate School,
   Bristol, United Kingdom, March 25-31, 2007.

3. *"Speeding Up the GW Code: Parallelism + PPMs."*
   R. Shaltaf, G.-M. Rignanese and X. Gonze,
   3rd international ABINIT developer workshop,
   Liège Belgium, 29–31 Jan 2007.

4. *"Quasiparticle Calculations of Band Offsets of Different Interfaces with Silicon."*
   R. Shaltaf, G.-M. Rignanese, X. Gonze,
   F. Giustino and A. Pasquarello,
   First-Principles Approaches to Optical and Photoelectron Spectra,
   Munich Germany, 9–12 March 2006.

5. *"Electronic and Dielectric Properties of Group IVB Transition Metal Oxides and Silicates: a first-principles study."*
   G.-M. Rignanese, R. Shaltaf, X. Gonze, F. Bruneval and L. Reining,
   F. Giustino and A. Pasquarello,
   E-MRS spring meeting (E-MRS - IUMRS - ICEM 06),
   Nice France, 29 May–2 June 2006.

6. *"Electronic and Dielectric Properties of Group IVB Transition Metal Oxides and Silicates: a first-principles study."*
   G.-M. Rignanese, R. Shaltaf, X. Gonze, F. Bruneval and L. Reining,
   F. Giustino and A. Pasquarello,
   International Symposium on Structure-Property Relationships in Solid State Materials,
   Pessac, France, 27-30 June, 2006.

Oral & Poster Communications

1. *"Lattice Dynamics and Specific Heat of α-GeTe: a theoretical and experimental study."*
   R. Shaltaf, X. Gonze, M. Cardona, R. K. Kremer, and G. Siegle,
   Poster Presentation,
   14^{th} International Workshop on Computational,
   Physics and Material Science: Total Energy and Force Methods,
   Trieste, Italy, 7-10 January 2009.

2. *"Polarization Patterns in GeTe from Bulk to Ferroelectric Nanoparticles."*
   E. Durgun, R. Shaltaf, J.-Y. Raty, Ph. Ghosez, and X. Gonze,
   Poster Presentation,
   IAP General Meeting,
   K. U. Leuven, Leuven, Belgium , 25 November 2008.

3. *"A new Hybrid Exchange-Correlation Functional for Accurate Prediction of the Electronic and Structural Properties of Ferroelectric Oxide Bulks and Nanostructures."*
   D.I. Bilc, R. Shaltaf, J. Íñiguez, Ph. Ghosez,
   Oral Presentation,

2008 APS March Meeting,
New Orleans, Louisiana, 10-14, March 2008.

4. *"Quasiparticle Calculations of Band Offsets of Silicon with High-κ Dielectrics."*
R. Shaltaf, J. Bouchet, G.-M. Rignanese, X. Gonze,
F. Giustino and A. Pasquarello,
Poster Presentation,
13^{th} International Workshop on Computational,
Physics and Material Science: Total Energy and Force Methods,
Trieste, Italy, 11-13 January 2007.

5. *"First Principle Calculations of Band Offsets of* SiO_2 *and* $ZrSiO_4$ *with Silicon."*
11th Nanoquanta Workshop on Electronic Excitations,
R. Shaltaf, J. Bouchet, G.-M. Rignanese, X. Gonze,
F. Giustino, A. Pasquarello , F. Bruneval and L. Reining,
Oral Presentation,
Houffalize, Belgium, 19-22 September 2006.

6. *"Quasiparticle Calculations of Band Offsets."*
R. Shaltaf, G.-M. Rignanese, X. Gonze, F. Giustino, A. Pasquarello,
F. Bruneval and L. Reining,
Oral Presentation,
Third Nanoquanta Young Researchers Meeting,
Tor Vergata, Rome, Italy, 2-5 May 2006.

7. *"Experimental and Theoretical Studies on* CO *Oxidation Over* $Pt-Pd$ *Bimetallic Catalysts."*
E. Erunal, S. Kaya , R. Shaltaf, S. Ellialtioglu and D. Uner,
Poster Presentation,
24nd European Conference on Surface Science (ECOSS-24),
Paris , France, 3-9 September, 2006.

8. *"Parallelization in GW Part of ABINIT."*
R. Shaltaf,
Oral Presentation,
Parallel workshop of ABINIT,
Louvain La Neuve, Belgium February, 2006.

9. *"The File Format of WFK , KSS, SCR Files in ABINIT."*
R. Shaltaf,
Oral Presentation,
Nanoquanta IT9 meeting,

Louvain La Neuve, Belgium November 2005.

10. *"Quasiparticle Calculations of High-κ-Material band Offsets with Silicon."*
R. Shaltaf, J. Bouchet G.-M. Rignanese,
X. Gonze, F. Giustino and A. Pasquarello,
Poster Presentation,
40 Years of the GW Approximation for the Electronic Self-Energy: Achievements and Challenges,
Bad Honnef, Germany, 12-15 September 2005.

11. *"Activity and Structure Predictions on Mono- and Bimetallic Precious Metal Catalysts."*
E. Erunal, R. Shaltaf, S. Ellialtioglu and D. Uner,
Oral Presentation,
European Congress on Catalysis (EUROPACAT),
Bulgaria, SOFIA, 28 August-1 September 2005.

12. 2nd NANOQUANTA Young Researchers Meeting
Max Blank institute, Berlin Germany 2-5 May 2005

13. *"Monte Carlo Simulations of Pd-Pt Catalysts."*
E. Erunal, S. Ellialtioglu, R. Shaltaf, and D. Uner,
(oral presentation),
NANO-TR ,ODTU, Ankara 2006.

14. *"Bimetalik Pd-Pt Katalizrlerinde Monte Carlo Yontemi ile Yuzey Yapisi Hesaplamalari."*
E. Erunal, S. Ellialtioglu, R. Shaltaf, and D. Uner,
UMMK7,Eskisehir, Universitesi 2006.

15. *"Ab initio Study of Mg Adsorption on Si(001) Surface"*
R. Shaltaf, E. Mete, and S. Ellialtioglu,
Oral Presentation,
10th Ankara Meeting on Condensed Matter Physics (YMP-10),
Ankara, Turkey, 30 November 2003.

16. *"Bir 4d Perovskitin Elektronik ve Yapisalozellikleri : $SrZrO_3$ in Kubik Fazi."*
E. Mete, R. Shaltaf and S. Ellialtioglu,
Oral Presentation,
10th Ankara Meeting on Condensed Matter Physics (YMP-10),
Ankara, Turkey, 30 November 2003.

17. *"Ab initio study of the One-Monolayer Sb/Ge(001) Interface."*
R. Shaltaf, M. Cakmak, E. Mete, G. P. Srivastava, and S. Ellialtioglu,

Poster Presentation,
22nd European Conference on Surface Science (ECOSS-22),
Praha, Czech Republic, 07-12 September 2003.

18. *"Ab initio Study of the One-Monolayer Sb/Si(001) Interface."*
R. Shaltaf, M. Cakmak, E. Mete, G. P. Srivastava, and S. Ellialtioglu,
Poster Presentation,
21st European Conference On Surface Science (ECOSS-21/NANO-7),
Malmo, Sweden, 24 2-8 June 2002.

19. *"Simulation of Amorphous and Crystalline Growth of Tetrahedral Semiconductors."*
R. Shaltaf and S. Ellialtioglu,
Poster Presentation,
20th European Conference On Surface Science (ECOSS-20),
Krakow, Poland, 7-11 September 2001.

Schools & Workshops

1. Third spectroscopy lectures on TDDFT, GW and Bethe-Salpeter Equation
Paris France, 20–24, March 2006
2. Quantum Computation on the Atomic Scale
Istanbul, Turkey, 1–11 June 2003
3. Computer Simulation of Surfaces and Interfaces
NATO-ASI 2002, Albena, Varna, Bulgaria, 9-20 October 2002
4. The Nuts and Bolts of First Principle Simulation
Durham, United Kingdom, 6-13 December 2001

Referee of International Journals

- Physical Review B
- Surface Science
- Physica B

Grants

- TUBITAK (The Scientific and Technical Research Council of Turkey)
Grant No. TBAG-2036 (101T058)
"Structural and electronic properties of low dimensional systems"

- EU's Sixth Framework Program through the Nanoquanta Network of Excellence(NMP4-CT-2004-50019)
Postdoctoral Grant