Department of Physics,
The University of Jordan,
Amman, jordan

(06)5355000–22067
riad-shaltaf
r.shaltaf@ju.edu.jo

RIAD SHALTAF

Appointments

Associate Professor, The University of Jordan, Jordan, 2015–Present.
Visiting Professor, University of Toronto, Canada, 2016–2017.
Assistant Professor, The University of Jordan, Jordan, 2009–2015.
Postdoctoral Fellow, Université Catholique de Louvain, Belgium, 2005-2009.

Education

Ph.D, Theoretical Solid State Physics, Middle East Technical University , Turkey 2005.
M.Sc., Theoretical Condensed Matter Physics, Middle East Technical University , Turkey , 1998.
B.Sc. Physics, Yarmouk University, 1995.

Certificates

Data Analytics, Big Data, and Predictive Analytics, Toronto Metropolitan University, Canada., Oct, 2023.
Neural Networks and Deep Learning, DeepLearning.AI, Nov, 2018.

Research Interests

Structural, electronic, vibrational and optical properties of materials with potential interest using first principle methods which includes: Density Functional Theory, Density Functional Perturbation Theory and Many Body Perturbation Theory.
Scientific coding
Machine learning methods in materials science
Molecular dynamics and Monte Carlo simulations

Publications

Journal Articles

AM Bakeer, NT Mahmoud, R Shaltaf. "Coupled Insights into Structural, Electronic, and Optical Properties of GeTMS3 (TM=Sc, Fe, Zn) Sulfide Perovskite across Different Phases: Ab Initio Study".
International Journal of Energy Research, 2024.

A ALsmadi, N Mahmoud, A Mousa, R Shaltaf. " Multifaceted impact of Ni-ion doping on the structural, electronic, magnetic, and optical properties of CoScO3 compounds: a first-principles study".
Indian Journal of Physics, 1–16, 2024.

S Kassou, A Belaaraj, P Guionneau, R Shaltaf. "Crystal structure, optical and electronic properties studies on an hybrid multifunctional MnCl4-based material".
Advanced Composites and Hybrid Materials, 2, 373–380, 2019.

AA Mousa, MS Abu-Jafar, D Dahliah, RM Shaltaf, JM Khalifeh. "Investigation of the Perovskite KSrX3 (X = Cl and F) Compounds, Examining the Optical, Elastic, Electronic and Structural Properties: FP-LAPW Study".
Journal of Electronic Materials, 47, 641–650, 2018.

R. Shaltaf, J. Khalifeh. "Theoretical investigation of dielectric properties of rare earth stillwellite compounds".
International Journal of Modern Physics B, 29, 1550154, 2015.

R. Shaltaf, B. Hamad, J. Khalifeh, H. Al-Jawheri, G.-M. Rignanese and X. Gonze. "Structural, electronic and dielectric properties of LaBGeO5".
Journal of Applied Physics, 115, 074103, 2014.

B.Abu Alhaj, B. Hamad, J. Khalifeh, R. Shaltaf, "Ab-initio calculations of the electronic and magnetic structures of Co2Cr1-xMnxSi alloys".
Journal of Magnetism and Magnetic Materials, 336, 37, (2013).

M. Stankovski, M. Giantomassi, R. Shaltaf, M. Grüning, F. Bruneval, G.-M. Rignanese, "Electronic properties of interfaces and defects from Many-Body Perturbation Theory: Recent developments and applications".
physica status solidi (b), 248, 275, 2011.

M. Grüning, R. Shaltaf, and G.-M. Rignanese," Quasiparticle calculations of the electronic properties of ZrO2 and HfO2 polymorphs and their interface with Si".
Phys. Rev. B 81, 035330 (2010).

X. Gonze , B. Amadon, P.-M. Anglade, J.-M. Beuken, b, F. Bottin, P. Boulanger, F. Bruneval, D. Caliste, b, R. Caracas, M. Côté, 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 "ABINIT : first-principles approach to material and nanosystem properties".
Comp. Phys. Comm., 180, 2582 (2009).

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

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

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

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

R. Shaltaf, G.-M. Rignanese, X. Gonze, F. Giustino and A. Pasquarello, “Band Offsets at the Si/SiO2 Interface from Many-Body Perturbation Theory”.
Phys. Rev. Lett., 100, 186401 (2008).

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

D. I. Bilc, R. Orlando, R. Shaltaf, G.-M. Rignanese, Jorge Íñiguez and Ph. Ghosez,“Hybrid Exchange-Correlation Functional for Accurate Prediction of The Electronic and Structural Properties of Ferroelectric Oxides”.
Phys. Rev. B 77, 165107 (2008).

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

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

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

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

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

E. Mete, R. Shaltaf, and S. Ellialtioglu, “Electronic and Structural Properties of a 4d-Perovskite: cubic phase of SrZrO3”.
Phys. Rev. B, 68, 035119 (2003).

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

S. Erkoc and R. Shaltaf, “Monte Carlo Computer Simulation of Small Copper Clusters”.
Phys. Rev. A. 60, 3053 (1999).

Book Chapters

Matteo Giantomassi, Martin Stankovski, Riad Shaltaf, et al., "Electronic Properties of Interfaces and Defects from Many-body Perturbation Theory: Recent Developments and Applications".
Advanced Calculations for Defects in Materials: Electronic Structure Methods,
edited by A. Alkauskas, et al., Verlag: Wiley-VCH (2011).

Invited Talks

"DFT Implementation In ABINIT."
R. Shaltaf
The 3rd SESAME-LinkSCEEM Summer School 2013,
Amman-Jordan, 09–15, September 2012.

"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.

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

"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.

"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.

"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.

"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.

Conference Presentations and Posters

"Lattice Dynamics and Specific Heat of -GeTe: a theoretical and experimental study."
Poster Presentation,
14th International Workshop on Computational, Physics and Material Science: Total Energy and Force Methods,
Trieste, Italy, 7-10 January 2009.

"Polarization Patterns in GeTe from Bulk to Ferroelectric Nanoparticles."
Poster Presentation,
IAP General Meeting,
K. U. Leuven, Leuven, Belgium , 25 November 2008.

"A new Hybrid Exchange-Correlation Functional for Accurate Prediction of the Electronic and Structural Properties of Ferroelectric Oxide Bulks and Nanostructures."
Oral Presentation,
2008 APS March Meeting,
New Orleans, Louisiana, 10-14, March 2008.

"Quasiparticle Calculations of Band Offsets of Silicon with High- Dielectrics."
Poster Presentation,
13th International Workshop on Computational, Physics and Material Science: Total Energy and Force Methods,
Trieste, Italy, 11-13 January 2007.

"First Principle Calculations of Band Offsets of SiO2 and ZrSiO4 with Silicon."
11th Nanoquanta Workshop on Electronic Excitations,
Oral Presentation
Houffalize, Belgium, 19-22 September 2006.

"Quasiparticle Calculations of Band Offsets."
Oral Presentation
Third Nanoquanta Young Researchers Meeting,
Tor Vergata, Rome, Italy, 2-5 May 2006.

"Experimental and Theoretical Studies on CO Oxidation Over Pt – Pd Bimetallic Catalysts."
Poster Presentation,
24nd European Conference on Surface Science (ECOSS-24), Paris , France,
3-9 September, 2006.

"Parallelization in GW Part of ABINIT."
Oral Presentation
Parallel workshop of ABINIT
Louvain La Neuve, Belgium February, 2006.
"The File Format of WFK , KSS, SCR Files in ABINIT." Oral Presentation
Nanoquanta IT9 meeting
Louvain La Neuve, Belgium November 2005.
"Quasiparticle Calculations of High- -Material band Offsets with Silicon."
Poster Presentation,
40 Years of the GW Approximation for the Electronic Self-Energy: Achievements and Challenges
Bad Honnef, Germany, 12-15 September 2005.
"Activity and Structure Predictions on Mono- and Bimetallic Precious Metal Catalysts."
Oral Presentation
European Congress on Catalysis (EUROPACAT)
Bulgaria, SOFIA, 28 August-1 September 2005.
2nd NANOQUANTA Young Researchers Meeting
Max Blank institute, Berlin Germany 2-5 May 2005
"Monte Carlo Simulations of Pd-Pt Catalysts."
oral presentation
NANO-TR ,ODTU, Ankara 2006.
"Bimetalik Pd-Pt Katalizrlerinde Monte Carlo Yontemi ile Yuzey Yapisi Hesaplamalari."
UMMK7,Eskisehir, Universitesi 2006.
"Ab initio Study of Mg Adsorption on Si(001) Surface"
Oral Presentation
10th Ankara Meeting on Condensed Matter Physics (YMP-10)
Ankara, Turkey, 30 November 2003.
"Bir 4d Perovskitin Elektronik ve Yapisalozellikleri : SrZrO3 in Kubik Fazi."
Oral Presentation
10th Ankara Meeting on Condensed Matter Physics (YMP-10)
Ankara, Turkey, 30 November 2003.
"Ab initio study of the One-Monolayer Sb/Ge(001) Interface."
Poster Presentation,
22nd European Conference on Surface Science (ECOSS-22)
Praha, Czech Republic, 07-12 September 2003.
"Ab initio Study of the One-Monolayer Sb/Si(001) Interface."
Poster Presentation

21st European Conference On Surface Science (ECOSS-21/NANO-7)
MalmoÙ , Sweden, 24 2-8 June 2002.

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

Schools, & Workshops

4th SESAME-LinkSCEEM summer School on Synchrotron Radiation (SR) and High Performance Computing (HPC) applications
Amman Jordan, 15–17/06/2014

SESAME-JSPS SCHOOL 2011
Amman Jordan, 12–14/11/2011

Third spectroscopy lectures on TDDFT, GW and Bethe-Salpeter Equation Paris France, 20–24, March 2006

Quantum Computation on the Atomic Scale
Istanbul, Turkey, 1–11 June 2003

Computer Simulation of Surfaces and Interfaces NATO-ASI 2002,
Albena, Varna, Bulgaria, 9-20 October 2002

The Nuts and Bolts of First Principle Simulation Durham
United Kingdom, 6-13 December 2001

Grants

Deanship of Scientific Research Fund
"Theoretical investigation of structural, electronic and optical properties of double halide perovskites for photovoltaic applications"

SRF (Scientific Research fund of Higher education Ministry of Jordan)
"Structural and electronic properties of low dimensional systems"

Postdoctoral Grant
EU's Sixth Framework Program through the Nanoquanta Network of Excellence

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

Technical Skills

Programming Languages

Proficient in: Python, TeX, Fortran, MPI.

Theory Expertise

Many body perturbation theory
Density functional theory methods

Density functional Perturbation theory
Molecular dynamics and Monte Carlo simulation methods.

Software

ABINIT, VASP, Castep, FHi98mdPP, OPIUM, AtomPAW, gnuplot, xmgrace, xcrysden, MS Office Suite.
Operating Systems: Windows, Mac OS, UNIX (ATX), and Linux Debian MS Windows.

Teaching Expertise

Graduate level:
Quantum Mechanics
Solid state Physics
Undergraduate level:
Introductory General Physics I, II, III
General physics laboratories I, II
Modern Physics
Optics
Quantum Mechanics
Thermal and Statistical Physics
Mathematical Physics
Solid State Physics