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Wissam-Helal
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PhD, Physical & Theoretical Chemistry

Associate Professor of Physical and Theoretical Chemistry, Department of Chemistry, The University of Jordan, Amman, Jordan.

Education

PhD, Physical and Theoretical Chemistry, *University of Toulouse (Université Paul Sabatier)*, Toulouse, France. **2005–2009**
Thesis title: Using multi-reference localization methods for quasi-degenerate chemical systems. Thesis supervisors: Stefano Evangelisti and Thierry Leininger.

Master, Physical and Theoretical Chemistry, *University of Toulouse (Université Paul Sabatier)*, Toulouse, France. **2003–2005**
Thesis title: Theoretical study of electron transfer of a bistable system: the spiro molecular cation. Thesis supervisors: Stefano Evangelisti and Thierry Leininger.

Master of Science (MSc) in Chemistry, *Yarmouk University*, Irbid, Jordan. **1997–2001**
Thesis title: Fluorescence probes for polymer rigidity: The case of 10-cyano-9-*tert*-butyl anthracene in polyalkylmethacrylate polymer matrices. Thesis supervisors: Khader Al-Hassan Al-Janaydeh and Yasser Al-Haj.

Bachelor of Science (BSc) in Chemistry, *Applied Science University*, Amman, Jordan. **1993–1997**
I graduated first in my class.

General Secondary Education Certificate, *Ibn Abbas Secondary School, Tlaa' Al-Ali*, Amman, Jordan. **1992–1993**
Scientific section.

Research Interests

- Development of *ab-initio* multi-reference quantum chemical methods for the calculation of the molecular electronic structure and properties.
- Applications of highly correlated *ab-initio* methods to complex chemical systems, such as: organic and inorganic mixed-valence compounds, molecular electronics and devices, and nano-structures (graphenes, nanotubes and fullerenes).
- Theoretical modelling of electronic and vibrational excited states, and intramolecular charge transfer (ICT).
- Linear scaling methods.
- Theoretical modelling of Dye-Sensitized Solae Cells (DSSCs) and Perovskites.
- Benchmarking DFT and wave function based methods for excited states calculations.
- Theoretical modelling of photochemical processes.
- QM/MM and MD methods for large molecules and biomoleclues.

Experience & Work Histroy

Associate Professor of Physical Chemistry, *Department of Chemistry, The University of Jordan*, Amman, Jordan.	**17/08/2020 – up until now**
Assistant Professor of Physical Chemistry, *Department of Chemistry, The University of Jordan*, Amman, Jordan.	**19/03/2018 – 16/08/2020**
Full Time Lecturer of Physical Chemistry, *Department of Chemistry, The University of Jordan*, Amman, Jordan.	**08/09/2013 – 18/03/2018**
Part Time Lecturer, *Department of Chemistry, Tafila Technical University*, Tafila, Jordan.	**03/02/2013 – 15/08/2013**
Researcher, *Laboratory of Quantum Chemistry and Physics, University of Toulouse (Paul Sabatier)*, Toulouse, France.	**01/09/2009 – 31/05/2012**
Research Assistant/Instructor, *Laboratory of Quantum Chemistry and Physics, University of Toulouse (Paul Sabatier)*, Toulouse, France.	**01/10/2005 – 30/06/2009**
Teaching Assistant, *Department of Chemistry, Yarmouk University*, Irbid, Jordan.	**01/09/1999 – 30/05/2000**

Research Publications

1. W. Helal, "Effect of Thermal Fluctuations on the Electronic Excitation Energies of Linear Polyenes: A Combined Molecular Dynamics and TD-DFT Study", *Int. J. Quantum Chem.*, vol. 124, p. e27270, **2024**. doi:10.1002/qua.27270

2. W. Helal, "Double Hybrid Density Functionals for the Electronic Excitaion Energies of Linear Cyanines", *J. Phys. Chem. A*, vol. 127, pp. 131–141, **2023**. doi:10.1021/acs.jpca.2c07192

3. Z. Ishtaiwi, D. Taher, M. Korb, W. Helal, H. K. Juwhari, A. Al-Hunaiti, H. Amarne, K. Assaf, L. Alrawashdeh, M. W. Amer, Y. A. Yousef, and H. Lang, "Luminescent Materials Based on *N*-(3-Nitrophenyl)-*N'*-(4-R-C_6H_4)Oxamato Zincate(II) Complexes," *J. Mol. Struct.*, vol. 1288, p. 135747, **2023**. doi:10.1016/j.molstruc.2023.135747

4. W. Helal, A. Marashdeh, Q. Alkhatib, H. Qashmar, M. Gharaibeh, A. T. Afaneh, "Tuning the Photophysical Properties of BODIPY Dyes Used in DSSCs as Predicted by Double-Hybrid TD-DFT: The Role of the Methyl Substituents", *Int. J. Quantum Chem.*, vol. 122, p. e27000, **2022**. doi:10.1002/qua.27000

5. Q. Alkhatib, W. Helal, and A. T. Afaneh, "Assessment of Time-Dependent Density Functionals for the Electronic Excitation Energies of Organic Dyes Used in DSSCs," *New J. Chem.*, vol. 46, pp. 7682–7694, **2022**. doi:10.1039/D2NJ00210H

6. Q. Alkhatib, W. Helal, and A. Marashdeh, "Accurate Predictions of the Electronic Excited States of BODIPY Based Dye Sensitizers Using Spin-Component-Scaled Double-Hybrid Functionals: A TD-DFT Benchmark Study," *RSC Adv.*, vol. 12, pp. 1704–1717, **2022**. doi:10.1039/D1RA08795A

7. W. Helal, Q. Alkhatib, and M. Gharaibeh, "Can Time-Dependent Double Hybrid Density Functionals Accurately Predict Electronic Excitation Energies of BODIPY Compounds?," *Comput. Theor. Chem.*, vol. 1207, p. 113531, **2022**. doi:10.1016/j.comptc.2021.113531

8. A. Eftaiha, A. K. Qaroush, A. K. Hasan, W. Helal, F. M. Al-Qaisi, "CO_2 Fixation into Cyclic Carbonates Catalyzed by Single-Site Aprotic Organocatalysts: A Benchmark Study", *React. Chem. Eng.*, vol. 7 pp. 1807–1817, **2022**. doi:10.1039/D2RE00157H

9. B. Al Tbakhi, H. Nsairat, W. Alshaer, A. Al-Kadash, W. Helal, L. Alrawashdeh, A. Day, K. I. Assaf, R. Hassouneh, F. Odeh, and A. Al Bawab, "Cinnamaldehyde–Cucurbituril Complex: Investigation of Loading Efficiency and its Role in Enhancing Cinnamaldehyde *in vitro* Anti-Tumor Activity," *RSC Adv.*, vol. 12, pp. 7540–7549, **2022**. doi:10.1039/D2RA00044J

10. A. Ghazzy, D. Taher, M. Korb, K. Al Khalyfeh, W. Helal, H. Amarne, T. Ruffer, Z. Ishtaiwi, H. Lang, "Rearrangement of Diferrocenyl 3,4-Thiophene Dicarboxylate," *Inorganics*, vol. 10, art. no. 96, **2022**. doi:10.3390/inorganics10070096

11. A. Abu-Yamin, D. Taher, M. Korb, K. Al Khalyfeh, Z. Ishtaiwi, H. K. Juwhari, W. Helal, H. Amarne, S. Mahmood, R. Loloee, Y. YouSef, A. Ghazzy, H. Lang, "Synthesis, Chemical and Physical Properties of Lanthanide(III) (Nd, Gd, Tb) Complexes Derived from (E)-Ethyl 4-(2-Hydroxybenzylideneamino)Benzoate," *Polyhedron*, vol. 222, p. 115906, **2022**. doi:10.1016/j.poly.2022.115906

12. Z. Ishtaiwi, D. Taher, M. Korb, W. Helal, A. Al-Hunaiti, H. K. Juwhari, H. Amarne, M. W. Amer, Y. A. Yousef, S. Klaib, and S. T. Abu-Orabi, "Syntheses, Crystal Structures, DFT Calculation and Solid-State Spectroscopic Properties of New Zincate(II) Complexes with N-(4-Substituted Phenyl)-N'-(4-Nitrophenyl)-Oxamate," *Arab. J. Chem.*, vol. 15, no. 12, p. 104349, **2022**. doi:10.1016/j.arabjc.2022.104349

13. H. Amarne, W. Helal, D. Taher, M. Korb, and A. Al-Hunaiti, "Crystal structure, Hirshfeld Surface Analysis and Contact Enrichment Ratios of 5,5-Dimethyl-2-(2,4,6-tris(Trifluoromethyl)Phenyl)-1,3,2-Dioxaborinane," *Mol. Cryst. Liq. Cryst.*, vol. 743, no. 1, pp. 77–88, **2022**. doi:10.1080/15421406.2022.2050981.

14. K. Al Khalyfeh, D. Taher, W. Helal, M. Korb, H. Amarne, and H. Lang, "Crystal Structure and Hirshfeld Surface Analysis of Bis(3-Thienoyl) Disulfide," *J. Chem. Crystallogr.*, vol. 52, pp. 113–121, **2022**. doi:10.1007/s10870-021-00896-z

15. M. Gharaibeh, B. Al-Shami, and W. Helal, "Electronic Spectrum of Boron Dichloride. Theoretical Study of Vibronic Levels of the Ground and First Excited States," *J. Mol. Struct.*, vol. 1224, p. 129206, **2021**. doi:10.1016/j.molstruc.2020.129206

16. K. Al Khalyfeh, D. Taher, W. Helal, M. Korb, I. Hamadneh, A. Al-Dujaili, A. Imraish, H. M. Hammad, R. M. Al-As'ad, S. T. Abu-Orabi, A. Hildebrandt, and H. Lang, "Synthesis and Characterization of 1,4-Chalcogenesters Bearing 5-Membered Heterocycles," *J. Chem. Sci.*, vol. 132, no. 1, p. 117, **2020**. doi:10.1007/s12039-020-01825-x

17. A. Ghazzy, D. Taher, W. Helal, M. Korb, K. Khalyfeh, F. F. Awwadi, R. K. Al-Shewiki, S. Weheabby, N. Al-Said, S. T. Abu-Orabi, and H. Lang, "Aryl Ferrocenylmethylesters: Synthesis, Solid-State Structure and Electrochemical Investigations," *Arab. J. Chem.*, vol. 13, no. 1, pp. 3546–3557, **2020**. doi:10.1016/j.arabjc.2018.12.006

18. H. Amarne, W. Helal, and S. Wang, "Synthesis, Structure and Sensity Functional Theory Calculations of a Novel Photoluminescent Trisarylborane–Bismuth(III) Complex," *Luminescence*, vol. 34, no. 7, pp. 731–738, **2019**. doi:10.1002/bio.3667

19. D. Taher, A. Ghazzy, F. F. Awwadi, W. Helal, K. Al Khalyfeh, M. Korb, A. Hildebrandt, E. Kovalski, and H. Lang, "Ferrocenylmethyl-Functionalized 5-Membered Heterocycles: Synthesis, Solid-State Structure and Electrochemical Investigations," *Polyhedron*, vol. 152, pp. 188–194, **2018**. doi:10.1016/j.poly.2018.06.038

20. D. Taher, S. Klaib, F. F. Awwadi, W. Helal, M. Gharaibeh, G. Rheinwald, T. Rüffer, and H. Lang, "Ti(η^5-1-SiMe3-C9H6)(Cl)2(OR): Structure and Bonding," *Inorganica Chim. Acta*, vol. 477, pp. 270–276, **2018**. doi:10.1016/j.ica.2018.03.003

21. W. Helal, "Tuning Ring Inversion and Internal Rotation in 10-Substituted-9-Tert-Butylanthracenes: A Theoretical Study," *Jordan J. Chem.*, vol. 13, pp. 115–122, **2018**. https://jjc.yu.edu.jo/index.php/jjc/article/view/35

22. M. El Khatib, G. L. Bendazzoli, S. Evangelisti, W. Helal, T. Leininger, L. Tenti, and C. Angeli, "Beryllium Dimer: A Bond Based on Non-Dynamical Correlation," *J. Phys. Chem. A*, vol. 118, no. 33, pp. 6664–6673, **2014**. doi:10.1021/jp503145u

23. W. Helal, S. Evangelisti, T. Leininger, and A. Monari, "A FCI Benchmark on Beryllium Dimer: The Lowest Singlet and Triplet States," *Chem. Phys. Lett.*, vol. 568-569, pp. 49–54, **2013**. doi:10.1016/j.cplett.2013.03.012

24. Y. A. Yousef, K. A. Al-Hassan, and W. Helal, "Excited State Structural Changes of 10-Cyano-9-Tert-Butyl-Anthracene (CTBA) in Polymer Matrices," *J. Fluoresc.*, vol. 23, pp. 957–961, **2013**. doi:10.1007/s10895-013-1221-y

25. W. Helal, A. Monari, S. Evangelisti, and T. Leininger, "Electronic Bistability in Linear Beryllium Chains," *J. Phys. Chem. A*, vol. 113, no. 17, pp. 5240–5245, **2009**. doi:10.1021/jp900663p

26. W. Helal, S. Evangelisti, T. Leininger, and D. Maynau, "*Ab-initio* Multireference Study of an Organic Mixed-Valence Spiro Molecular System," *J. Comput. Chem.*, vol. 30, no. 1, pp. 83–92, **2009**. doi:10.1002/jcc.20982

27. M. Pastore, W. Helal, C. Angeli, S. Evangelisti, T. Leininger, and R. Cimiraglia, "Application of a "Charge-Averaged" Second Order Multireference Perturbation Theory Strategy to the Study of a Model Mixed-Valence Compound," *J. Mol. Struct.: THEOCHEM*, vol. 896, no. 1, pp. 12–17, **2009**. doi:10.1016/j.theochem.2008.10.042

28. M. Pastore, W. Helal, S. Evangelisti, T. Leininger, J.-P. Malrieu, D. Maynau, C. Angeli, and R. Cimiraglia, "Can the Second Order Multireference Perturbation Theory be Considered a Reliable Tool to Study Mixed-Valence Compounds?," *J. Chem. Phys.*, vol. 128, no. 17, p. 174102, **2008**. doi:10.1063/1.2911699

29. W. Helal, S. Evangelisti, T. Leininger, and D. Maynau, "Localized Multi-Reference Approach for Mixed-Valence Systems," *AIP Conf. Proc.*, vol. 1046, no. 1, pp. 3–6, **2008**. doi:10.1063/1.2997308

30. W. Helal, B. Bories, S. Evangelisti, T. Leininger, and D. Maynau, "*Ab-initio* Multi-Reference Study of a Bistable Spiro Molecule," in *Computational Science and Its Applications - ICCSA 2006* (M. Gavrilova *et al.* eds.), (Berlin, Heidelberg), pp. 744–751, Springer Berlin Heidelberg, **2006**. doi:10.1007/11751540_79

Supervisor of Postgraduate Students

1. Qabas Alkhatib, TD-DFT Calculations of Vertical Electronic Excitation Energies for BODIPY and non-BODIPY based DSSCs: A Benchmark Study. Thesis defended at the Department of Chemistry, the University of Jordan, on 12/08/2021.

2. Mohammad Eshtayeh, The Rovibrational *ab-initio* Spectrum of OH Radical in $X^2\Pi$ State. Thesis defended at the Department of Physics, the University of Jordan, on 29/12/2021.

3. Rania Saleh, Rovibrational Spectra for the Ground State of Cyanide Radical. Thesis defended at the Department of Physics, University of Jordan, on 18/08/2022.

4. Barakat Manasrah, Theoretical Stability Study of Halogenated Phosphine Ligands Gold (I) Complexes [X-Au(I)-PX_3] for Focused Electron Beam Induced Deposition (FEBID). Thesis defended at the Department of Chemistry, the University of Jordan, on 01/09/2022.

5. Rahma Al-Sarayra, TD-DFT Predictions of the Vertical Absorption Energies of Porphyrins: A Benchmark Study. Thesis defended at the Department of Chemistry, the University of Jordan, on 05/01/2023.

6. Rozita Alzyoud, Density Functional Theory Calculations for the Stability of Gold(I) N-heterocyclic Triazole Complexes. Thesis defended at the Department of Chemistry, the University of Jordan, on 18/5/2023.

7. Sahar Ferwaneh, Density Functional Theory Calculations for the Stability of Gold(I) N-heterocyclic Carbene Complexes. Thesis defended at the Department of Chemistry, the University of Jordan, on 21/5/2023.

8. Tala Tadrus, TD-DFT Calculations of the Vertical Absorption Energies of Cyanines: A Benchmark Study. Ongoing project.

9. Amani Alshanti, Molecular Dynamics Simulations of Cucurbiturils as Drug Carriers for Selected Drugs Using Extended Tight Binding Quantum Chemistry Based Methods. Ongoing project in collaboration with Al-Balqa' Applied University.

Theses Defence Committees

A) PhD Theses

1. Mahmood Geralleh, A Computational Study on the Catalytic Effect of the Deamination Reaction of Cytidine Monophosphate. Thesis defended at the Department of Chemistry, the University of Jordan, Amman, Jordan, on 30/05/2022.

B) MSc Theses

2. Sufanah Yousef Hasan, Metabolic Pathways of Alcoholic Compounds. Theoretical Studies. Thesis defended at Al-Balqa' Applied University, Salt, Jordan, on 22/07/2019.

3. Bayan Khader Al-Tbakhi, Cinnamaldehyde in Cucurbituril: A Study of Loading Efficiency and Bioavailability and Solubility Enhancement. Thesis defended at the Department of Chemistry, the University of Jordan, Amman, Jordan, on 19/12/2019.

4. Maysa'a Taleb, Thermochemical Parameters of Pyrimidine Chlorinated Compounds. Thesis defended at the Department of Chemistry, the University of Jordan, Amman, Jordan, on 9/12/2020.

5. Mohanad Alshhadat, Density Functional Theory Calculation for Stability of Gold (I) Complexes [X-Au(I)-PR_3] of Phosphine Ligands for Focused Electron Beam Induced Deposition (FEBID). Thesis defended at Al-Balqa' Applied University, Salt, Jordan, on 26/08/2021.

6. Areej Khaled Hasan, CO_2 Fixation into Cyclic Carbonates Catalyzed by Single-Site Ionic Organocatalysts. Thesis defended at the Department of Chemistry, the University of Jordan, Amman, Jordan, 18/05/2022.

7. Amneh H. Smadi, Utilization of CO2/CS2: Synthesis of Heterocyclic Compounds Using Mukaiyama Reagent. Thesis defended at the Hashemite University, Zarqa, Jordan, on 04/08/2022.

8. Sara Alnoaimat, Synthesis of Chloro-Substituted β-ketiminate Palladium Complexes, Spectral and Thermal Investigation of their Structures and Studies of their Biological Activities. Thesis defended at the Department of Chemistry, the University of Jordan, Amman, Jordan, 27/07/2023.

9. Lubna Altarawneh, The Evaluation of Cyclodextrin and Gum Arabic as a Dual Drug Delivery System. Thesis defended at the Department of Chemistry, the University of Jordan, Amman, Jordan, 20/08/2023.

Oral Talks in International Conferences

- W. Helal, B. Bories, S. Evangelisti, T. Leininger, D. Maynau, "Multi-reference localization quantum chemical algorithms for the study of complex organic molecular systems", *ICCSA 2006, International Conference on Computational Science and its Applications*, Glasgow, United Kingdom, 8–11 May 2006.
- W. Helal, B. Bories, S. Evangelisti, T. Leininger, D. Maynau, "Localized Multi-Reference Approach for Mixed-Valence Systems", *ICCMSE 2007, International Conference of Computational Methods in Sciences and Engineering*, Corfu, Greece, 25–30 September 2007.

Summer Schools

- Attending the intensive courses of "*The European Master of Theoretical Chemistry and Computational Modelling*", Department of Chemistry, University of Perugia, Perugia, Italy. (17/07/2006 – 13/08/2006).
- Attending the intensive courses of "*Les Doctoriales*", University of Bordeaux I, Bordeaux, France. (4/4/2008 – 19/4/2008).

Training & Workshops

- Attending the Workshop on "*Access to Technology for Innovation and on Establishing A Technology and Innovation Support Center (TISC) Newtork in Jordan*", Organized by the Wolrd Intellectual Property Organization (WIPO) and the Ministry of Industry, Trade, and Supply of the Hashemite Kingdom of Jordan, Amman, (31/5/2016 – 2/6/2016).
- Attending the Workshop on "*Chemical Security Awareness for Universities in Jordan*", Organized by CRDF Global and Oak Ridge National Laboratory, Amman, (21/08/2022 – 23/08/2022).

Professional Memberships

- Royal Society of Chemistry: Graduateship since 1998.

Awards and Honors

- IRSAMC Scientific research Scholarship, University of Toulouse III, Toulouse, France, 2007.

Administration

- Member of the faculty of science council in the academic year 2021/2022.
- Member of several committees at the the university, faculty, and departmet levels.

Computational Chemistry Skills

Code development: Extensive experience in developing multireference variational and perturbative quantum chemical codes to treat localization of molecular orbitals. These codes were developed by our research group at the University of Toulouse, in collaboration with other research groups.

Computational chemistry packages: Long and extensive working experience with ORCA, Molpro, Molcas, GAMESS, NWChem, Dalton, Gaussian, and other codes.

Computer Skills

Parallel programming: Message Passing Interface (MPI) and OpenMP.

Programming: FORTRAN 77, FORTRAN 90, and C.

Operating systems: UNIX, Linux, and Windows.

Other: LaTeX, MATLAB and other numerical computing platforms, Mathematica and other computer algebra systems.

Miscellaneous Skills

Academic skills: Academic research, teaching, training, consultation, postgradute student supervision, project management and publishing.

Spectroscopic techniques: Time-correlated fluorescence, time resolved spectroscopy, flash photolysis, excited state life time photon counter, femtosecond pulsed lasers of different types for excitation sources, photodiode array multi-channel detectors, and charged-coupled device (CCD) cameras.

Mathematical expertise: Mathematical methods used in theoretical chemistry: Linear algebra, mathematical analysis (differential equations and special functions), numerical methods, abstract algebra, group theory, and statistical methods.

Courses Taught

- General Chemistry I.
- General Chemistry II.
- Physical Chemistry I.
- Physical Chemistry II.
- Physical Chemistry III.
- Quantum Chemistry (*A postgraduate MSc course*).
- Applications in Quantum Chemistry (*A postgraduate PhD course*).
- Experimental General Chemistry.
- Experimental General Chemistry for Non-Chemistry Majors.
- Experimental Physical Chemistry I.
- Experimental Physical Chemistry II.
- Software Packages in Chemistry.

Languages

Arabic: Excellent in writing and oral communication. *Native*

English: Excellent in writing and oral communication. *TOEFL 613*

French: Excellent in writing and oral communication.

Italian: Elementary notions in reading and oral communication.

References

- Available upon request