Wissam Faisal Helal, *PhD, Quantum & Theoretical Chemistry*

General and Contact Information

Date and place of birth: 24/09/1974, Algiers, Algeria.
Sex: Male.
Citizenship: Jordan.
Marital status: Single.
Home address: 1, Muhammad Bani Khalaf Street, Al-Rabieh, Amman, Jordan.
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Education

1. PhD in Theoretical and Physical Chemistry: *9/2005 – 5/2009*

- Laboratory of Quantum Chemistry and Physics, University of Toulouse III (Paul Sabatier), Toulouse, France.
- Thesis title: Using multi-reference localization methods for quasi-degenerate chemical systems. (*Thesis written and defended in English*).
- Thesis advisors: Prof. Dr. Stefano Evangelisti and Prof. Dr. Thierry Leininger.

2. Master of Science (M.Sc.) in Theoretical Chemistry: *9/2003 – 9/2005*

- Laboratory of Quantum Chemistry and Physics, University of Toulouse III (Paul Sabatier), Toulouse, France.
- Thesis title: Theoretical study of electron transfer of a bistable system: the Spiro molecular cation. (*Thesis written and defended in English*).
- Thesis advisors: Prof. Dr. Stefano Evangelisti and Prof. Dr. Thierry Leininger.

3. Master of Science (M.Sc.) in Chemistry: *9/1997 – 9/2001*

- Department of Chemistry, Yarmouk University, Irbid, Jordan.
- Rating and cumulative average: Very Good (80.3/100)
- Thesis title: Fluorescence probes for polymer rigidity: The case of 10-*cyano*-9-*tert-butyl* anthracene in polyalkylmethacrylate polymer matrices.
- Thesis advisors: Prof. Dr. Khader Al-Janaydeh and Dr. Yasser Al-Haj.
- Area of Specialization: Physical Chemistry, electronic molecular spectroscopy.

4. Bachelor of Science (B.Sc.) in Chemistry: *9/1993 – 7/1997*

- Department of Chemistry, Applied Science University, Amman, Jordan.
- Rating and cumulative average: Very Good (79.9/100). (*I was graduated first in my class*).

5. General Secondary Education Certificate: *9/1992 – 7/1993*

- Ibn Abbas Secondary School, Tlaa‘ Al-Ali, Amman, Jordan.
- Section: Scientific.

Research Interests

1. Molecular electronic structure theory and computational *ab-initio* quantum chemistry; excited states and intramolecular charge transfer; nanochemistry and nanomaterials.
2. Development of *ab-initio* multi-reference quantum chemical methods for the calculation of the molecular electronic structures and properties.
3. Applications of highly correlated *ab-initio* methods to complex chemical systems, such as: organic and inorganic mixed-valence compounds, molecular electronics and devices, nano-structures (graphenes, nanotubes and fullerenes), and photo-voltaic and solar cells.
4. Linear scaling methods and QM/MM methods for large molecules.

Research Experience

1. **Research Scientist, Laboratory of Quantum Chemistry and Physics, part of the *Center of Research on Complex Atomic and Molecular Systems (IRSAMC)*, University of Toulouse III (Paul Sabatier), Toulouse, France:**
   9/2009 – 5/2012
   Some of my research themes and tasks were:
   - Developing theoretical and computational quantum chemical models and methods: Multi-reference and multi-configurational highly correlated *ab-initio* methods (NEVPT program code), molecular orbital multireference localization methods (CASDI program code), Full Configuration Interaction (FCI) method (NEPTUNUS program code), and linear scaling techniques.
   - Using the above mentioned developed methods to a wide rage of chemical organic and inorganic chemical systems: molecules with near degenerate electronic states and mixed-valence and intramolecular charge-transfer compounds (spiro compounds, *bis*-triarylamines, *bis*-hydrazines, and other small to moderate size organic mixed-valence systems); linear and ring atomic clusters (beryllium and other IIA group clusters); carbon nanotubes and surfaces; organic molecular electronic devices; and photo-voltaic and solar cells.
   - Training of new postgraduate (master and PhD) students in the laboratory with the state of the art computational methods needed to start and conduct their own research projects.
2. **Research assistant, Laboratory of Lasers and Photochemistry, Department of Chemistry, Yarmouk University, Irbid, Jordan:**
   9/2000 – 6/2002
   - Using experimental electronic spectroscopy techniques, mainly fluorescence, to elucidate structural changes in organic excited states.
   - Using photochemical experimental techniques to study photolysis and photodegradation of organic compounds.

Publications

1. Helal, W.; Evangelisti, S.; Leininger, T.; Monari, A. "A FCI benchmark on beryllium dimer: the lowest singlet and triplet states", *Chem. Phys. Lett.* **2013**, *568/569*, 49-54. doi:10.1016/j.cplett.2013.03.012
2. Yousef, Y.; Al-Hassan, K. A.; Helal, W. F., "Excited state structural changes of 10-cyano-9-tert-butyl-anthracene (CTBA) in polymer matrices", *J. Fluoresc.* **2013**, *23*, 957-961. doi:10.1007/s10895-013-1221-y

3. Helal, W.; Monari, A.; Evangelisti, S.; Leininger, T. "Electronic Bistability in Linear Beryllium Chains", *J. Phys. Chem. A* **2009**, *113*, 5240–5245. doi:10.1021/jp900663p

4. Helal, W.; Evangelisti, S.; Leininger, T; Maynau, D. "*Ab-initio* Multireference Study of an Organic Mixed-Valence Spiro Molecular System", *J. Comput. Chem.* **2009**, *30*, 83–92. doi:10.1002/jcc.20982

5. Pastore, M.; Helal, W.; Angeli, C.; Evangelisti, S.; Leininger, T.; Cimiraglia, R. "Application of a charged-averaged second order multireference perturbation theory strategy to the study of a model Mixed-Valence compound", *J. Mol. Struct. (Theochem)* **2009**, *896*, 12–17. doi:10.1016/j.theochem.2008.10.042

6. Pastore, M.; Helal, W.; Evangelisti, S.; Leininger, T.; Malrieu, J.-P.; Maynau, D.; Angeli, C.; Cimiraglia, R. "Can the second order multireference perturbation theory be considered a reliable tool to study mixed-valence compounds?", *J. Chem. Phys.* **2008**, *128*, 174102-(1–9). doi:10.1063/1.2911699

7. Helal, W.; Evangelisti, S.; Leininger, T.; Maynau, D. "Localized Multi-Reference Approach for Mixed-Valence Systems", *AIP Conf. Proc.*, **2008**, *1046*, 3–6. American Institute of Physics. doi:10.1063/1.2997308

8. Helal, W.; Bories, B.; Evangelisti, S.; Leininger, T.; Maynau, D. "*Ab-initio* Multireference Study of a Bistable Spiro Molecule", in Gavrilova, M. et al. (Eds), *Lecture Notes in Computer Science (LNCS)* **2006**, *3980*, 744–751. doi:10.1007/11751540_79

9. Evangelisti, S.; Helal, W.; Angeli, C.; Bendazzoli, G. L.; Leininger, T.; Monari, A. "The electronic structure of Be_2 revisited", submitted to: *J. Am. Chem. Soc.*

10. Verdicchio, M.; Bendazzoli, G. L.; Evangelisti, S.; Helal, W. "A Full CI study of beryllium hydride anion", submitted to: *J. Chem. Phys.*

Oral Talks in International Conferences

1. Helal, W.; Bories, B.; Evangelisti, S.; Leininger, T.; Maynau, D. "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.

2. Helal, W.; Bories, B.; Evangelisti, S.; Leininger, T.; Maynau, D. "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 and Training

1. Attending the intensive course of "The European Master of Theoretical Chemistry and Computational Modelling".
   - Department of Chemistry, University of Perugia, Perugia, Italy.
   - From 17/07/2006 to 13/08/2006.

2. Attending the training course of "Doctoriales".
   - University of Bordeaux I, Bordeaux, France.
   - From 14/4/2008 to 19/4/2008.

3. Attending the training course of "Computational Simulations of Nanomaterials".
   - Institute of Theoretical Chemistry, University of Stuttgart, Stuttgart, Germany.
   - From 9/6/2008 to 20/6/2008.

International Research Cooperation

1. Stefano Evangelisti, Thierry Leininger, Daniel Maynau, and Nadia Ben Amor, Laboratory of Quantum Chemistry and Physics, University of Toulouse III, Toulouse, France.
2. Mariachiara Pastore, Department of Chemistry, University of Perugia, Perugia, Italy.
3. Renzo Cimiraglia and Celestino Angeli, Department of Chemistry, University of Ferrara, Ferrara, Italy.
4. Antonio Monari, Theoretical and Biochemistry Group, Institute Jean Barriol, University of Nancy, Vandoeuvre-lés-Nancy, France.
5. Gian Bendazzoli, Department of Physical and Inorganic Chemistry, University of Bologna, Bologna, Italy.

Awards and Honors

1. Distinguished Paul Sabatier scientific Award of the University of Toulouse, Toulouse, France 2009.
2. IRSAMC Scientific research fellowship, University of Toulouse III, Toulouse, France, 2006.

Professional Memberships

1. American Chemical Society: Member since 1998. Physical Chemistry Division, Theoretical Chemistry Subdivision.
2. Royal Society of Chemistry: Graduateship since 1996, and Membership since 2008 (Faraday Division).
3. Société Chimique de France (France Chemical Society): Member since 2005.

Teaching Experience

1. **Lecturer, Tafila Technical University, Tafila, Jordan:**
   2/2013 – 8/2013
   - Lectured physical chemistry (I & II), experimental physical chemistry (I & II), and quantum chemistry courses for *junior* and *senior* chemistry undergraduates.
2. **Instructor, University of Toulouse III (Paul Sabatier), Toulouse, France:**
   10/2005 – 6/2009
   - Lectured quantum chemistry, computational chemistry, numerical and mathematical methods in chemistry and physics, and molecular orbital theory for *sophomore*, *junior*, and *senior* chemistry and physics undergraduates.
3. **Teaching assistant, Department of Chemistry, Yarmouk Univ., Jordan:**
   9/1999 – 5/2000
   - Lectured general chemistry laboratory courses (general chemstry lab I & II) for *freshman* chemistry and science students.

Relevant Skills

1. **Computational and mathematical chemical modeling:**
   - Theoretical and computational quantum chemical models and computational algorithms with different levels of electronic correlation to describe the structure and the molecular properties of complex chemical compounds: Hartree-Fock Self-Consistent Field (HF-SCF), Configuration Interaction (CI), Many-Body Perturbation Theory (MBPT), Coupled-Cluster (CC), Complete Active Space Self-Consistent Field (CASSCF), Multi-reference Configuration Interaction (MRCI), Multi-reference Perturbation Theory (MRPT), and Full Configuration Interaction (FCI).
   - Other theoretical and computational chemical models: Density Functional Theory (DFT) and Time-Dependent Density Functional Theory (TD-DFT)
2. **Computer literacy:**
   - Programs coding and development: FORTRAN 77, FORTRAN 90, and C. Parallel programming using Message Passing Interface (MPI) and Open Multi-Processing (OpenMP).
   - Operating systems: UNIX, Linux, and Windows.
   - Other: Use and implementation of various general purpose utilities and databases.
3. **Computational chemistry packages:**
   - Molpro, Molcas, GAMESS, NWChem, Dalton, Gaussian, and other universal quantum chemical codes.
   - CASDI and NEVPT (multi-reference variational and perturbative quantum chemical codes to treat localization of molecular orbitals). These two program codes were written and developed by our research group at the University of Toulouse, in collaboration with other research groups.
4. **Spectroscopic and other experimental techniques:**
   - Spectroscopic instruments: Time-correlated fluorescence, time resolved spectroscopy, flash photolysis, excited state life time photon counter, UV-Visible, IR, and Raman spectrometers.
   - Laser excitation sources: Femtosecond pulsed lasers, Nd-YAG, nitrogen laser, dye lasers.
   - Detectors: Photodiode array multi-channel detectors, Charged-Coupled Device (CCD) cameras.
5. **Mathematical expertise:**
   - Mathematical methods used in physical chemistry and quantum mechanics: Linear algebra, abstract algebra, mathematical analysis (differential equations and special functions), numerical methods, group theory, and statistical methods.

Languages

1. Arabic: Excellent in writing and oral communication (native).
2. English: Excellent in writing and oral communication.
3. French: Excellent in writing and oral communication (almost native!).
4. Italian: Elementary notions in reading and oral communication.

References

1. Prof. Dr. Stefano Evangelisti, professor of theoretical and quantum chemistry at the University of Toulouse,
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   - *Fax. (work)*: +33(0)5 61 55 60 65
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2. Prof. Dr. Thierry Leininger, professor of theoretical chemistry at the University of Toulouse,
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3. Prof. Dr. Jean-Paul Malrieu, professor emeritus of quantum chemistry at the University of Toulouse,
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     Université Paul Sabatier (Toulouse III) et CNRS
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   - *Fax. (work)*: +33(0)5 61 55 60 65
   - *email*: malrieu@irsamc.ups-tlse.fr

4. Prof. Dr. Khader Al-Hassan Al-Janaydeh, professor of physical chemistry at Yarmouk University,
   - *Address*: Chemistry Department, Yarmouk University Irbid, 21163 JORDAN
   - *Tel. (work)*: +962 2 721 1111 ext.: 2796
   - *Fax. (work)*: +962 2 727 4725
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5. Dr. Yaser Al-Haj, associate professor of physical chemistry at Yarmouk University,
   - *Address*: Chemistry Department, Yarmouk University Irbid, 21163 JORDAN
   - *Tel. (work)*: +962 2 721 1111 ext.: 2621
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