بسم الله الرحمن الرحيم

أ.د. فخر محمد أبو عواد
بروفيسور الكيمياء البيوفيزيائية النظرية
الجامعة الإسلامية – غزة

Prof. Fakhr M. Abu-Awwad
Biophysical & Computational Chemistry
Islamic University - Gaza

Chemistry Department
P. O. Box 108 – Gaza - Palestine
www.dr-fakhr.ps / site.iugaza.edu.ps/fakhr/
dr-fakhr@live.com / fakhr@iugaza.edu.ps
Office: +970 8 2863554 (ext. 2638)
Home: +970 8 2874876 / +970 599 932932

Curriculum Vitae

EDUCATION:

Graduate:

- Emporia State University, Emporia, KS, USA, 1996

Degree: **Master of Physical Computational Chemistry**

Thesis Title: ***A quantum Mechanical Study of Nitration of Simple Aromatic Systems***.

- University of New Orleans, New Orleans, LA, USA, 1999

Degree: **Ph.D. of Physical/Computational Chemistry**

Dissertation Title: ***The Physical Significance of Kohn-Sham Orbitals.***

FIELDS OF INTEREST:

- **Electronic Calculations:**

1. Electrostatic Potential
2. Hydrogen Energy
3. Hydrogen Bonded Clusters
4. Chemical Reactivity

- **QSAR:**

1. Biophysical Systems
2. Toxicology
3. Drugs Potency

AWARDS AND SCHOLARSHIPS:

- The Islamic University Grant of Research (2011)
- Visiting Professor: Uppsala University – Sweden (2010/2011) www.pac.uu.se/ViewPage.action?siteNodeId=32903&languageId=1&contentId=-1
- Arab Fund Fellowship, Kuwait, (2009 – 2010)
- The Islamic University Grant of Research (2006)
- The Islamic University Grant of Research (2005)
- The Islamic University Grant of Research (2003)
- Research Assistantship 1996-1999, USA
- Fulbright scholarship 1994-1996, USA

LANGUAGES

- Arabic (Native)
- English (Excellent Skills)
- Hebrew (good)

EDITOR OF:

- Research & Reviews: J. Chemistry: (www.rroij.com/jc/index.php/jc)
- Der Pharma Chemica: (//derpharmachemica.com)
- Pelagia Res. Library: http://pelagiaresearchlibrary.com/editorial-board.html

PAPERS/POSTERS PRESENTED AT MEETINGS OF PROFESSIONAL SOCIETIES

1- **"A Quantum mechanical Study of Nitration of Simple Aromatic Systems"** Greenlief, C.; Abu-Awwad, F. presented at the regional meeting of the American Chemical Society, S. Dakota U.S.A., 1996.

2- **"The Physical Significance of Kohn-Sham Orbitals"** Politzer, P.; Abu-Awwad, F.; Murray, J. presented at the Conference of Theoretical Chemistry. New Orleans, Louisiana, U.S.A., 1997. (Poster).

3- **"Systematic Study of Average Local Ionization Energy"** Politzer, P.; Abu-Awwad, F.; Murray, J. presented at the Conference of recent trends in Computational Chemistry. Jackson, Mississippi, U.S.A., 1998. (Poster).

4- **"A lecture on Computational Chemistry"** Abu-Awwad, F. presented at The Day of Chemistry Symposium. Islamic University, Gaza, 2000.

5- **"An Overview of Average Local Ionization Energy"** Abu-Awwad, F. presented at the day of Chemistry Symposium. Islamic University, Gaza, 2000. (Poster session).

PUBLICATIONS

1. **Synthesis, antibacterial and QSAR evaluation of 5-oxo and 5-thio derivatives of 1,4-disubstituted tetrazoles,** Morjan, R.Y., El-Attar, N.H., Abu-Teim, O.S., Ulrich, M., Awadallah, A.M., Mkadmh, A.M., Elmanamae, A.A., Raftery, J., Abu-Awwad, F.M., Yaseen, Z.J., Elqidrea, A.F., Gardiner, J.M., Bioorganic & Medicinal Chemistry Letters(in Press, Accepted Manuscript)
2. **Stability and Antimicrobial Activity of Transition Metal (II) Complexes with SNO and ONO Functionalized Ligand: A Computational Study,** *Abu*-Awwad, F.M., El Halabi, N.M., American Chemical Science Journal, 4(6): 759-773, (2014).
3. **Synthesis, structural characterization, and computational study of novel (E)-N^0-(1-p-tolylethylidene)furan-2-carbohydrazide.** Morjan, R.Y., Mkadmh, A.M., Abu-Awwad, F.M., Helliwell, M., Awadallah, A. M., Gardiner. J. M., J. Mol. Struct, 1051;5 (2013).
4. **Minimum Local Ionization Potential as a Measure of Inorganic and Organic Corrosion Inhibition: A Computational Study,** El Halabi, N. M., Abu-Awwad, F.M., Morjan, R.Y., Research and Reviews: J of Chem., Vol. 2, No 4 (2013).
5. **QSAR Study of the Biologically Active Organosulfurs in Natural Products**, Abu Awwad, F.M., E J Chem., Vol.7(S1), (2010).
6. **The Role of Various Theoretical Descriptors in QSAR Investigations of Toxicity of Benzodiazepine Drugs,** Abu Awwad, F.M., Der Pharma Chemica, Vol. 2, No. 1, (2010).
7. **A QSAR Study of the Activity of Some Fluorinated Anesthetics,** Abu Awwad, F.M., Der Pharma Chemica, Vol. 2, No. 1, (2010).
8. **A Computational Study of Toxicity of Nitrobenzenes Using QSPR and DFT-Based Molecular Surface Electrostatic Potential**, Abu Awwad, F.M., Islamic Univ J. (Series Nat. St. Eng) Vol.18, No.1, (2010).
9. **A Density Functional Based Molecular Surface Electrostatic Potentials of Histamine H_1-Agonists,** Abu-Awwad, F. M., Mkadmh A. M., Int. J. ChemTech Res., Vol. 1, No. 3, (2009).

10. **A Computational Study of Histamine H_1- Receptor Agonist Activity Using QSPR and DFT-Based Molecular Surface Electrostatic Potential**, Abu Awwad, F.M., Int. J. ChemTech Res., Vol. 1, No. 3, (2009)

11. **Synthesis and Computational Verification of New Nickel(II) Complexes,** Halabi, N. M., Awadalla, A. M., Abu-Awwad, F.M., Safi, Z. S., Int. J. PharmTech Res., Vol. 1, No. 2, (2009).

12. **Atom additive model based on dipole field tensor to compute static average molecular dipole polarizabilities.** Mkadmh, A.M., Hinchliffe, A., Abu-Awwad, F.M., J. Molec. St. (THEOCHEM), Vol. 901, No. 1-3, 9-17, (2009).

13. **Tautomerism of 5-methyl imidazolidine Thio derivatives in the Gas Phase: A Density Functional Study.** Abu Awwad, F.M., Safi, Z., E J Chem, Vol. 5, No. 4, (2008)..

14. **Density functional studies on trialkyl phosphorus selenide dibromide complexes R_3PSeBr_2 (R=H, Me, Et, $N(CH_3)_2$, $N(C_2H5)_2$, Ph, and C_6H_{11}),** Mkadmh, A.M., Hinchliffe, A., Abu Awwad, F.M. J. Molec. St. (THEOCHEM), Vol. 848, No. 1-3, 87-93, (2008).

15. **Enhancement of molecular polarizabilities by the push-pull mechanism; a Density Functional study of substituted benzene, furan, thiophene and related molecules**. Hinchliffe, A., Mkadmh, A., Nikolaidi , B., Soscún, H.J., Abu-Awwad, F.M., CEJC 4(4) 743–759 (2006).

16. **Density Functional and CIS(D) Studies on the Ground and Excited Electronic State Properties of Nitrogen Dioxide,** Hinchliffe, A., Soscun, H.J., Mkadmh, A., Abu-Awwad, F.M., J. of Comp Methods in Science and Engineering, 6, 165 (2006).

17. **Ab Initio studies of the excited state polarizabilities of Ozone and Thiozone,** Hinchliffe, A., Soscun, H.J., Mkadmh, A., Abu-Awwad, F.M., Int. J. Applied Chem., Vol. 1, No. 1, 71-83, (2005).

18. **On the Electronic Excited States of Sulfur Dioxide**, Hinchliffe, A., Soscun Machado, H.J., Mkadmh, A., Abu-Awwad, F.M., J. Molec. St. (THEOCHEM), Vol. 717, No. 1-3, 231-234, (2005).

19. **A Comparative Study of Structure and Electrostatic Potential of Hydrogen-Bonded Clusters of Neutral Ammonia, $(NH3)_n$ (n=2-6),** Abu-Awwad, F.M., J. Molec. St. (THEOCHEM) Vol. 683, No.1-3 (2004).

20. **The Gas-Phase Heats of Formation of n-Alkanes as A Function of The Electrostatic Potential Extrema on their Molecular Surfaces.** Abu-Awwad, F. M., E J Chem, Vol. 01, No. 02, 81, (2004).

21. **Ab-initio Study of Molecular Surface Electrostatic Potential of Hydrogen Fluoride Clusters $(HF)_n$, (n=2-15),** Abu-Awwad, F.M., Chem. Phys. Lett. 360, 3-4 (2002).

22. **The Reaction of Methyl Thioacetate with Nitrilimines: An Experimental Local Ionization Energy and Electrostatic Potential Investigation**, Abu Thaher, B., and Abu-Awwad, F.M., Asian J. Chem.,14-3 (2002)

23. **Variation of Parameters in Hybrid Density Functional Theory**, Politzer, P.; Lane, P.; Thomas, E. J.; Abu-Awwad, F.M.; O'Connor, C. J, Recent Res. Devel. Quantum Chem., 2, 41. (2001)

24. **Computational Study of Chemical Reactivity of Vinylpyrrole Derivatives,** Hania, M. M.; Abu-Awwad, F.M., Asian J. Chem, (2000).

25. **Prediction of Solvation Free Energies from Computed Properties of Solute Molecular Surfaces,** Politzer, P.; Murray, J. S.; Abu-Awwad, F.M., Int. J. Quant. Chem., VOL 76; PART 5; 643. (2000).

26. **Characterization of Aromatic Hydrocarbons by Means of Average Local Ionization Energies on Their Molecular Surfaces,** Murray, J. S.; Abu-Awwad, F.; Politzer, P. J. Molec. Struct., VOL 501/502; No; 241-250, (2000).

27. **Variation of Parameters in Becke-3 Hybrid Exchange-Correlation Functional,** Abu-Awwad, F.M.; Politzer, P., J. Comp. Chem., VOL 21; PART 3; 227-238, (2000)

28. **Molecular Dynamics Simulations of Liquid Nitromethane,** Alper, H. E.; Abu-Awwad, F.M.; Politzer, P. J. Phys. Chem. B, 1999 VOL 103; No 4; 1089-5647.
29. **Prediction of Aqueous Solvation Free Energies from Properties of Solute Molecular Surface Electrostatic Potentials,** Murray, J. S.; Abu-Awwad, F.M.; Politzer, P. J. Phys. Chem. A, 1999, VOL 103; No 12; 1853-1856.
30. **Molecular Surface Electrostatic Potentials of Anticonvulsant Drugs,** Murray, J. S.; Abu-Awwad, F.M.; Politzer, P.; Wilson, L. C.; Troupin, A. S.; Wall, R. E, Int. J Quant Chem 1998, VOL 70; No 6; 1137-1144.
31. **Some approximate Kohn-Sham molecular energy formulas, Politzer, P.;** Abu-Awwad, F.M., Molec. Phys., 1998, VOL 95; No 4; 681-688.
32. **A comparative analysis of Hartree-Fock and Kohn-Sham orbital energies,** Politzer, P.; Abu-Awwad, F.M., Theoretical Chem. Accounts, 1998, VOL 99; NUMB 2; 83-84.
33. **Comparison of Density Functional and Hartree-Fock Average Local Ionization Energies on Molecular Surfaces.** Politzer, P.; Abu-Awwad, F.M.; Murray, J. S. Int. J. Quant Chem. 1998, VOL 69; No 4; 607-614.

TEACHING and SUPERVISION

- 2010 – Yet: Professor, Islamic University of Gaza
- 2003 – 2007: Co-Supervisor a PhD Student, Manchester University, England.
- 2005 – 2010: Associate Prof., Islamic University of Gaza.
- 2001 – 2003: Part time Professor, Al-Aqsa University, and The Open Quds University.
- 1999 – 2005: Assistant Prof., Islamic University of Gaza
- 1996 – 1999: Teaching Assistant, University of New Orleans, La, USA

Courses

- ✓ General Chemistry I
- ✓ General Chemistry II
- ✓ Physical Chemistry II – Kinetics, Catalysis
- ✓ Introductory Quantum Chemistry
- ✓ Chemistry Literature
- ✓ Thermodynamics (graduate level)
- ✓ Quantum and Computational Chemistry (graduate level)
- ✓ Chemical Literature and Computers
- ✓ Research Projects and Seminar
- ✓ Advanced Physical Chemistry (graduate level)

PROFESSIONAL / ADMINISTRATIVE POSITIONS and COMMUNITY SERVICES:

- Visiting Professor: Uppsala University – Sweden (2010/2011)
- Professor, Islamic University of Gaza, Palestine (2010- yet).
- Editor, Der Pharma Chemica, E-J. Chemistry, and Pelagia Res. Library.
- Associate Professor, Islamic University of Gaza, Palestine (2005- 2010).
- Active participant of political and cultural events including workshops, debates, and conferences.
- Founder and director general of The Academy for Security and Strategic Studies (SSSA), Gaza (2007 -)
- Strategic Policy Counselor, Technical Team of Reform, Palestinian Authority, (2006 – 2007)
- Strategic planning committee, Islamic University of Gaza (2005-2006)
- Associate Professor, Islamic University of Gaza, Palestine (2005 - 2010)
- Vice dean of Scientific Research, Islamic University of Gaza (2003 – 2005)
- Cofounder and deputy of director general, Al Mostaqbal Research center, Gaza (2003 -2005)
- Steering committee, Al Nour Center for Research and Studies, Gaza (2002 – 2005)
- Assistant Professor, Islamic University of Gaza, Palestine (1999- 2004).
- Research Assistant, University of New Orleans, LA, USA, 1997-1999.
- Teaching Assistant, Emporia State University, KS, USA, 1995 -1996.
- Teacher of Chemistry , Lab Technician, Al Abiyar, Benghazi, Libya

COMPUTER SKILLS

- Fluent use of personal computers and Networking
- Excellent knowledge of Physics and Chemistry software packages, such that Gaussian, Spartan, Hyperchem, CODESSA, and Chemoffice.
- Excellent knowledge with software of many different applications in both the general and academic fields including different operating systems (DOS, Windows, UNIX), Word processing, Spreadsheets, and Statistics.
- Very good background in FORTRAN.

REFEREES

1. Prof. Francesco Aquilante francesco.aquilante@gmail.com
2. Prof. Adel M. Awadallah awada@iugaza.edu.ps