

CURRICULUM VITAE

Personal Data

Name. Muneerah Mogren Abdulaziz Al-Mogren

Nationality: Saudi ,Languages: Arabic and English

Contact Information

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Saudi Arabia Email mmogren@ksu.edu.sa

Work Experience

2003- 2007: lecture,

2008- Assistant Professor of Quantum Chemistry Chemistry Science

Department, College of Sciences, King Saud University. Riyadh, Saudi

Arabia

2015- Associate Professor of Quantum Chemistry Chemistry Science

Department, College of Sciences, King Saud University. Riyadh, Saudi

Arabia

Academic Qualifications

Assistant Professor of Quantum Chemistry

In Chemistry Science, Quantum chemistry King Saud University, KSA.

Title of Ph.D. Dissertation: " Structural and Stability of Some Carbon and

Silicon Clusters: an ab initio study 2008

1998 M.Sc. Chemistry Science, Quantum chemistry King Saud University, KSA. Title of M.Sc. Thesis: "Calculations of Molecular Properties of Some Pyrimidine and Purine Derivatives Using X-ray Results and MO Methods ".

1990 B.Sc. Chemistry Science, College of Sciences,

SKILLS

In quantum Computer programs

Foreign Languages:

English (Toefl)

TRAININGS/ SEMINARS

Workshop on Nanotechnologies and Applications

In KACST and KSU and E-learning and distance learning

Publications

<u>Title</u>	<u>Cited by</u>	<u>Year</u>
<u>Theoretical spectroscopic investigations of HNS_q and HSN_q (q= 0,+ 1,- 1) in the gas phase</u> SB Yaghlane, NE Jaidane, CE Cotton, JS Francisco, MM Al Mogren, ... The Journal of chemical physics 140 (24), 244309	<u>11</u>	2014
<u>Synthesis, spectroscopic, molecular orbital calculation, cytotoxic, molecular docking of DNA binding and DNA cleavage studies of transition metal complexes with N-benzylidene-N'-salicylidene-1, 1-diaminopropane</u> MM Al-Mogren, ANMA Alaghaz, EA Ebrahim Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy 114, 695-707	<u>9</u>	2013
<u>On the use of explicitly correlated treatment methods for the generation of accurate polyatomic-He/H₂ interaction potential energy surfaces: The case of C₃-He complex and generalization</u>	<u>8</u>	2014

<u>Title</u>	<u>Cited by</u>	<u>Year</u>
MM Al Mogren, O Denis-Alpizar, DB Abdallah, T Stoecklin, P Halvick, ... The Journal of chemical physics 141 (4), 044308		
<u>Accurate spectroscopic characterization of ethyl mercaptan and dimethyl sulfide isotopologues: A route toward their astrophysical detection</u> C Puzzarini, ML Senent, R Domínguez-Gómez, M Carvajal, M Hochlaf, ... The Astrophysical Journal 796 (1), 50	<u>7</u>	2014
<u>A G3 Study of the Structure of Carbon– Nitrogen Nanoclusters</u> MMA Mogren, AA El-Azhary, WZ Alkiali, M Hochlaf The Journal of Physical Chemistry A 114 (46), 12258-12268	<u>6</u>	2010
<u>Characterization and reactivity of the weakly bound complexes of the [H, N, S]– anionic system with astrophysical and biological implications</u> T Trabelsi, Y Ajili, SB Yaghlane, NE Jaidane, MM Al-Mogren, ... The Journal of chemical physics 143 (3), 034303	<u>5</u>	2015
<u>Vibrationally Resolved Photoelectron Spectroscopy of Electronic Excited States of DNA Bases: Application to the \tilde{A} State of Thymine Cation</u> M Hochlaf, Y Pan, KC Lau, Y Majdi, L Poisson, GA Garcia, L Nahon, ... The Journal of Physical Chemistry A 119 (7), 1146-1153	<u>5</u>	2015
<u>Characterization of Zn q+–imidazole (q= 0, 1, 2) organometallic complexes: DFT methods vs. standard and explicitly correlated post-Hartree–Fock methods</u> K Boussouf, R Boulmene, M Prakash, N Komiha, M Taleb, MM Al-Mogren, ... Physical Chemistry Chemical Physics 17 (22), 14417-14426	<u>5</u>	2015
<u>Theoretical and experimental photoelectron spectroscopy characterization of the ground state of thymine cation</u> Y Majdi, M Hochlaf, Y Pan, KC Lau, L Poisson, GA Garcia, L Nahon, ... The Journal of Physical Chemistry A 119 (23), 5951-5958	<u>4</u>	2015
<u>Theoretical studies of 2-quinolinol: Geometries, vibrational frequencies, isomerization, tautomerism, and excited states</u> Y Pan, KC Lau, MM Al-Mogren, A Mahjoub, M Hochlaf Chemical Physics Letters 613, 29-33	<u>4</u>	2014

<u>Title</u>	<u>Cited by</u>	<u>Year</u>
<u>Synthesis, Spectral and Quantum Chemical Calculations of Mononuclear Nickel (II), Copper (II) and Cadmium (II) Complexes of New Schiff–Base Ligand</u> MM Al-Mogren, ANMA Alaghaz Int. J. Electrochem. Sci 8, 8669-8685	<u>4</u>	2013
<u>On the role of HNS and HSN as light-sensitive NO-donors for delivery in biological media</u> T Trabelsi, R Linguerr, SB Yaghlane, NE Jaidane, MM Al-Mogren, ... The Journal of chemical physics 143 (13), 134301	<u>3</u>	2015
<u>Experimental and quantum chemical studies of the electronic absorption spectra of pyrimidine derivatives</u> M Mogren, K Al-Farhan, AA Hasanein Journal of Saudi Chemical Society 17 (1), 87-95	<u>3</u>	2013
<u>pH-Metric Studies of Acid-Base Equilibria on the mixed Cu (II) Complexes with Pyrazine-2, 3-Dicarboxylic Acid and Amino Acids</u> RA Ammar, A Nafady, MF Amin, MM Al-Mogren, EM Shoukry Int. J. Electrochem. Sci 8, 1501-1510	<u>3</u>	2013
<u>VUV photoionization and dissociative photoionization spectroscopy of the interstellar molecule aminoacetonitrile: Theory and experiment</u> A Bellili, M Schwell, Y Bénilan, N Fray, MC Gazeau, MM Al-Mogren, ... Journal of Molecular Spectroscopy 315, 196-205	<u>2</u>	2015
<u>VUV photoionization and dissociative photoionization of the prebiotic molecule acetyl cyanide: Theory and experiment</u> A Bellili, M Schwell, Y Bénilan, N Fray, MC Gazeau, MM Al-Mogren, ... The Journal of chemical physics 141 (13), 134311	<u>2</u>	2014
<u>Theoretical investigations of the IO, q+ (q= 2, 3, 4) multi-charged ions: Metastability, characterization and spectroscopy</u> H Hammami, O Yazidi, MBEH Rhouma, MM Al Mogren, M Hochlaf The Journal of chemical physics 141 (1), 014302	<u>2</u>	2014
<u>Theoretical characterization of C7, C7–, and C7+</u> MM Al-Mogren, ML Senent, M Hochlaf The Journal of chemical physics 139 (6), 064301	<u>2</u>	2013

<u>Title</u>	<u>Cited by</u>	<u>Year</u>
<u>SPECTROSCOPIC CONSTANTS OF THE X1Σ⁺ AND 13Π STATES OF AIO⁺</u> O Sghaier, R Linguerri, MM Al Mogren, JS Francisco, M Hochlaf The Astrophysical Journal 826 (2), 163	1	2016
<u>Electronic, structural and vibrational induced effects upon ionization of 2-quinolinone</u> A Bellili, Y Pan, MM Al Mogren, KC Lau, M Hochlaf Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy 164, 1-7	1	2016
<u>Toward the laboratory identification of [O, N, S, S] isomers: Implications for biological NO chemistry</u> T Ayari, NE Jaidane, MM Al Mogren, JS Francisco, M Hochlaf The Journal of Chemical Physics 144 (23), 234316	1	2016
<u>Rotational (de-) excitation of HNS by He: three-dimensional potential energy surface and collision rate coefficients</u> Y Ajili, DB Abdallah, MM Al-Mogren, JS Francisco, M Hochlaf Monthly Notices of the Royal Astronomical Society 458 (2), 1581-1589	1	2016
<u>Structure, Reactivity, and Fragmentation of Small Multi-Charged Methane Clusters</u> AS Zaag, O Yazidi, NE Jaidane, MW Ross, AW Castleman Jr, ... The Journal of Physical Chemistry A 120 (10), 1669-1676	1	2016
<u>Theoretical characterization of vanadyl and VO 3⁺ cations in gas phase</u> S Almenia, MM Al Mogren, DB Abdallah, R Linguerri, M Hochlaf Chemical Physics Letters 646, 142-147	1	2016
<u>Role of size and shape selectivity in interaction between gold nanoclusters and imidazole: a theoretical study</u> M Prakash, G Chambaud, MM Al-Mogren, M Hochlaf Journal of molecular modeling 20 (12), 1-14	1	2014
<u>Spectral and quantum chemical studies on 1, 3-bis (N 1-4-amino-6-methoxypyrimidinebenzenesulfonamide-2, 2, 4, 4-ethane-1, 2-dithiol)-2, 4-dichlorocyclodiphosph (V) azane and its erbium complex</u> MM Al-Mogren, ANMA Alaghaz, TM El-Gogary Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy 118, 481-487	1	2014

<u>Title</u>	<u>Cited by</u>	<u>Year</u>
<u>Synthesis, spectroscopic, thermal and quantum chemical studies on trivalent erbium NO chelating sulfamonomethoxine–cyclophosph (V) azane complex</u> MM Al-Mogren, ANMA Alaghaz, TM El-Gogary, SAH Albohy Journal of Molecular Structure 1048, 202-209	1	2013
<u>Theoretical investigation of the long-lived metastable AlO 2+ dication in gas phase</u> O Sghaier, HH Abdallah, HY Abdullah, NE Jaidane, MM Al Mogren, ... Chemical Physics 477, 32-38	-	2016
<u>HNS+ and HSN+ cations: Electronic states, spin-rovibronic spectroscopy with planetary and biological implications</u> T Trabelsi, SB Yaghlane, MM Al Mogren, JS Francisco, M Hochlaf The Journal of Chemical Physics 145 (8), 084307	-	2016
<u>Explicitly correlated three-dimensional potential-energy surface of the thiazyl-hydride–helium weakly bound system and implications for HSN detection</u> Y Ajili, DB Abdallah, MM Al-Mogren, F Lique, JS Francisco, M Hochlaf Physical Review A 94 (1), 012512	-	2016
<u>First principle investigations of organobismuth palladium-catalyzed C–C coupling reaction: mechanism, chemoselectivity and solvent effects</u> P Kutudila, R Linguerri, MM Al-Mogren, C Pichon, S Condon, M Hochlaf Theoretical Chemistry Accounts 135 (7), 1-10	-	2016
<u>Vibrational memory in quantum localized states</u> Y Ajili, T Trabelsi, O Denis-Alpizar, T Stoecklin, AG Császár, ... Physical Review A 93 (5), 052514	-	2016
<u>Ab Initio and DFT Studies on CO2 Interacting with Znq+–Imidazole (q= 0, 1, 2) Complexes: Prediction of Charge Transfer through σ-or π-Type Models</u> R Boulmene, K Boussouf, M Prakash, N Komiha, MM Al-Mogren, ... ChemPhysChem	-	2016
<u>Collisional excitation of MgO by He</u> MM Al Mogren, Y Ajili, S Almania, DB Abdallah, M Hochlaf Monthly Notices of the Royal Astronomical Society 452 (2), 1561-1566	-	2015

<u>Title</u>	<u>Cited by</u>	<u>Year</u>
<u>Structure, stability, energy barrier and ionization energies of chemically modified DNA-bases: Quantum chemical calculations on 37 favored and rare tautomeric forms of tetraphosphoadenine</u> MM Al-Mogren, TM El-Gogary Computational and Theoretical Chemistry 1052, 35-41	-	2015
<u>Ab initio treatment of gas phase GeO 2+ doubly charged ion</u> MM Al Mogren, DB Abdallah, M Hochlaf Chemical Physics 446, 13-17	-	2015
<u>Understanding of matrix embedding: a theoretical spectroscopic study of CO interacting with Ar clusters, surfaces and matrices</u> K Mahjoubi, DM Benoit, NE Jaidane, MM Al-Mogren, M Hochlaf Physical Chemistry Chemical Physics 17 (26), 17159-17168	-	2015
<u>State-to-state vacuum ultraviolet photodissociation study of CO 2 on the formation of state-correlated CO (X 1 Σ^+; v) with O (1 D) and O (1 S) photoproducts at 11.95–12.22 eV</u> Z Lu, YC Chang, Y Benitez, Z Luo, AB Houria, T Ayari, MM Al Mogren, ... Physical Chemistry Chemical Physics 17 (17), 11752-11762	-	2015
<u>Substituent effects on vibrational and electronic excitation spectra of pyridone tautomers and ions: The case of the cyano group</u> MB Messaouda, A Mahjoub, MM Al-Mogren, M Abderrabba, M Hochlaf Journal of Molecular Structure 1074, 422-428	-	2014
<u>Characterization of gas phase WC 2+: a thermodynamically stable carbide dication</u> S Sabor, AT Benjelloun, MM Al Mogren, M Hochlaf Physical Chemistry Chemical Physics 16 (39), 21356-21362	-	2014
<u>Synthesis, Spectral and Quantum Chemical Calculations of Mononuclear Nickel (II), Copper (II) and Cadmium (II) Complexes of New Schiff-Base Ligand</u> MM Al-Mogren, AN Alaghaz INTERNATIONAL JOURNAL OF ELECTROCHEMICAL SCIENCE 8 (6), 8669-8685	-	2013
<u>Electronic structure and properties of neutral, anionic and cationic silicon–nitrogen nanoclusters</u> MM Al Mogren, AA El-Azhary, WZ Alkiali, M Hochlaf Journal of molecular modeling 19 (6), 2657-2668	-	2013

<u>Title</u>	<u>Cited by</u>	<u>Year</u>
<u>Synthesis, Spectral Characterization and Quantum Chemical Calculations on Pyridine Cyclodiphospho- (V) Azane Derivative and Its Cu (II) Complex</u>	-	2013
MM Al-Mogren, ANMAA Alaghaz		
Int. J. Electrochem. Sci 8, 6951-6971		

Scientific Conferences

“XXI edition of the European Conference on the Dynamics of Molecular Systems” (MOLEC 2016), that Celebrated between the 11th to 16th September 2016.

“Anharmonicity in medium-sized molecules and clusters” (AMOC 2015), that Celebrated between the 26-30 of April of 2015.

The poster is

“Structure, properties and energetics of carbon-nitrogen and silicon-nitrogen nanoclusters: a comparative study”

M. M. Al-Mogren, A. A. El-Azhary and W. Z. Alkiali, Majdi Hochlaf “A G3 study of the structure of Carbon-Nitrogen C_mN_n ($m = 1-4$, $n = 1-4$, $m + n = 5$) Nanoclusters”, J. Phys. Chem. A, 12258, 114, 2010.

M. M. Al-Mogren, A. A. El-Azhary, Majdi Hochlaf A. A. AlWarthan and K. A. M. Al-Farhan, A G3 study of the Carbon-Silicon Si_nC_m ($n = 0-4$, $m = 0-4$, $n + m = 4$) Nanoclusters, CHEM. 4, Cairo University, Giza, Egypt, 3-6 Mar., 2008.

Muneerah M. Al-Mogren, Adel A. El-Azhary, Wad Kealie , Majdi Hochlaf, Khalid A. M. Al-Farhan, A G3 study of the Carbon-Nitrogen C_nN_m ($n = 1-4$, $m = 1-4$, $n + m = 5$) Nanoclusters, The International Conference on Nanotechnology (ICON008), Jeddah, Saudi Arabia, 17 – 19 June, 2008.

Muneerah M. Al-Mogren, Adel El-Azhary and Wad Kealie, Majdi Hochlaf, A G3 study of the structure of carbon-nitrogen ($n = 1-4$, $m = 1-4$, $n + m = 5$) anion nanoclusters, Taibah International Chemistry Conference, 2009, 23-25 March, 2009.

Muneerah M. Al Mogren, Adel A. El-Azhary, Wad. Z. Alkiali, and Majdi Hochlaf, A G3 study of the structure of Carbon-Nitrogen Nanoclusters, The Third International Syrian Chemical Conference in Chemsitry, Aleppo, Syria, 2010, 27-29 Oct., 2010.