

Dr. Zainab Husain Abdulaziz Alsunaidi

Assistant Professor in Physical Chemistry
Vice Dean of Scientific Research and Innovation

Personal Data

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Department | Chemistry

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Language Proficiency

Language	Read	Write	Speak
Arabic	√	√	√
English	√	√	√

Academic Qualifications (Beginning with the most recent)

Date	Academic Degree	Place of Issue	Address
2017	PhD in Chemistry	Michigan State University	East Lansing, MI, USA
2009	MS in Chemistry	Imam Abdulrahman Bin Faisal University (Formerly known as King Faisal University)	Dammam, Saudi Arabia
2003	BS in Chemistry	Imam Abdulrahman Bin Faisal University (Formerly known as College of Science in Dammam)	Dammam, Saudi Arabia

PhD, Master or Fellowship Research Title: (Academic Honors or Distinctions)

PhD	Prediction of Structural and Thermochemical Properties: Computational Strategies for Small Molecules to Periodic Systems. Advisor: Prof. Angela K. Wilson
Master	Computational Study of Structural Stability, Rotational Barriers and Analysis of Vibrational Spectra of Some Amides. Advisor: Prof. Hassan M. Badawi

Professional Record: (Beginning with the most recent)

Job Rank	Place and Address of Work			Date
Assistant Professor	Chemistry Department	College of Science, Imam Abdulrahman bin Faisal University	Dammam, Saudi Arabia	2018-present
Research Assistant	Chemistry Department	Michigan State University	East Lansing, Michigan, USA	Jun 2016-May 2017
Research Assistant	Chemistry Department	University of North Texas	Denton, Texas, USA	May 2014-May 2016
Lecturer	Chemistry Department	Imam Abdulrahman bin Faisal University	Dammam, Saudi Arabia	2009-2018
Teaching Assistant	Chemistry Department	Imam Abdulrahman bin Faisal University	Dammam, Saudi Arabia	2008-2009

Administrative Position Held: (Beginning with the most recent)

Administrative Position	Office	Date
Vice Dean of Scientific Research and Innovation	College of Science	March 2021-present
General Supervisor of the postgraduate programs of the College of Science	College of Science	March 2021-present
Coordinator of Graduate Studies	Chemistry Department	Jan 2020-Jan 2021
Vice Dean of Training Affairs	College of Science	Dec 2018-Jan 2019

Administrative Responsibilities, Committee and Community Service (Beginning with the most recent)

Committee Membership

#	From	To	Position	Organization
1	Oct 2023	present	Vice- Head	Committee for developing professional multidiscipline master programs in the College of Science
2	Oct 2023	present	Member	The Higher Committee for Quality and Academic Accreditation at the College of Science
3	March 2022	present	member	Committee of Scientific and Health postgraduate programs, Deanship of Graduate Studies, IAU
4	Nov 2021	present	member	Committee of the second strategic plan of the College of Science
5	March 2021	present	member	Standing Committee of contracting with Saudi faculty members and others, and extending their services
6	March 2021	present	member	College of Science Council
7	March 2021	present	member	Scientific research committee in the chemistry department
8	Jan 2020	Jan 2021	Head	Graduate studies and scientific research committee in the chemistry department
9	Jan 2019	May 2019	Head	Midterm exams committee in the chemistry department
10	Jan 2018	present	member	Chemistry department Council
11	Jan 2018	Dec 2018	Head	Tables committee in the chemistry department

12	Dec 2017	Jan 2018	member	Final exams committee in the chemistry department
13	Aug 2017	May 2018	member	The development of PhD program committee in the Chemistry department
14	Aug 2017	Dec 2019	member	Graduate studies committee in the Chemistry department
15	Aug 2017	Jan 2018	Activities coordinator	Saudi Chemical Society branch committee in the Eastern Province
16	Aug 2017	Dec 2017	Head	Midterm exams committee in the chemistry department
17	2008	2009	Member	Monitoring exams committee in the Mathematics department
18	2008	2010	Member	Academic advising committee in the Chemistry department

Scientific Achievements

Published Refereed Scientific Researches

(In Chronological Order Beginning with the Most Recent)

#	Name of Investigator(s)	Research Title	Publisher and Date of Publication
1	Md. Shamim Hossain, Sanaa S. Al Abbad, <u>Zainab H. A. Alsunaidi</u> , Shofiur Rahman, Abdullah N. Alodhayb, Md. Mainul Hossain, Raymond A. Poirier, Kabir M. Uddin	Evaluation of novel pyridoxal isonicotinoyl hydrazone (PIH) derivatives as potential anti-tuberculosis agents: An in silico investigation	International Journal of Quantum Chemistry. 2024, 142, 9, e27381. Q2
2	Syeda Tasnim Quayum, Nusrat Jahan Ikbal Esha, Siam Siraji, Sanaa S Al Abbad, <u>Zainab H A Alsunaidi</u> , Mansour H Almatarneh, Shofiur Rahman, Abdullah N Alodhayb, Khuloud A Alibrahim, Sarkar M A Kawsar, Kabir M Uddin	Exploring the effectiveness of flavone derivatives for treating liver diseases: Utilizing DFT, molecular docking, and molecular dynamics techniques	MethodsX. 2024, 12, 102537. Q2
3	Muhammad Usman Khan, Faiza Shafiq, Sanaa S. Al Abbad, Junaid Yaqoob, Riaz Hussain, <u>Zainab H. A. Alsunaidi</u> , Ghulam Mustafa, Shabbir Hussain	Designing Electron-Deficient Diketone Unit Based Non-Fused Ring Acceptors with Amplified Optoelectronic Features for Highly Efficient Organic Solar Cells: A DFT Study	Molecules. 2023, 28, 8, 3625. Q1
4	Mansour H. Almatarneh, Ghada G. Kayed, Sanaa S. AlAbbad, <u>Zainab H. A. Alsunaidi</u> , Mohammed S. Al-Sheraideh, Yuming Zhao	Mechanistic Study on DNA Mutation of the Cytosine Methylation Reaction at C5 Position	Arabian Journal of Chemistry. 2022, 15, 8, 103956. Q1
5	Al Omari, Rima; Almatarneh, Mansour; Alnajajrah, Asmaa; Al-Sheraideh, Mohammed; Al Abbad, Sanaa; <u>Alsunaidi, Zainab</u>	Thermal Degradation and Bimolecular Decomposition of 2-Ethoxyethanol in Binary Ethanol and Isobutanol Solvent Mixtures: Computational Mechanistic Study	ACS Omega. 2021, 6, 20, 13365–13374. Q2

6	E. Mliki, T. K. Srinivasa, A. Messaâdi, N. O. Alzamel, <u>Z. H. A. Alsunaidi</u> , N. Ouerfelli	Hyperbolic Correlation between the Viscosity Arrhenius Parameters at Liquid Phase of Some Pure Newtonian Fluids and Their Normal Boiling Temperature	Russian Journal of Physical Chemistry A. 2020, 94 (01), 30-40. Q4
7	<u>Alsunaidi, Z. H. A.</u> ; Cundari, T. R.; Wilson. A. K.	Towards a Better Rational Design of a Catalytic Surface for the Direct Synthesis of Aniline: A DFT Study.	ACS Omega. 2017, 2(7), 3214-3227. Q2
8	<u>Alsunaidi, Z. H. A.</u> ; Wilson. A. K.	DFT and Composite Methods: Investigation of Oxygen Fluoride Species.	Computational and Theoretical Chemistry. 2016, 1095, 71-82. Q2
9	Badawi, H. M.; Al-Saadi, A.A.; Al-Khalidi, M. A. A.; Al-Abbad, S. S. A.; <u>Al-Sunaidi, Z. H. A.</u>	Potential Energy Scans and Vibrational Assignments of Cyclopropanecarboxylic acid and Cyclopropanecarboxamide.	Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy. 2008, 71, 1540. Q2
10	Badawi, H. M.; Al-Khalidi, M. A. A.; <u>Al-Sunaidi, Z. H. A.</u> ; Al-Abbad, S. S. A.	Conformational Properties and Vibrational Analyses of Monomeric Pentafluoropropionic Acid CF_3CF_2COOH and Pentafluoropropionamide $CF_3CF_2CONH_2$.	Canadian Journal of Analytical Sciences and Spectroscopy. 2007, 52, 5. Q3
11	Badawi, H. M.; Al-Khalidi, M. A. A.; Al-Abbad, S. S. A.; <u>Al-Sunaidi, Z. H. A.</u>	Rotational Barriers in Monomeric $CH_2=CX-COOH$ and $CH_2=CX-CONH_2$ (X is H or CH_3) and Vibrational Analysis of Methacrylic Acid and Methacrylamide.	Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy. 2007, 68, 43. Q2

Current Research Projects

#	Name of Investigator(s) (Supported by)	Research Title	Grant number
2	Ahmed Maarouf, Fatimah Alahmari, Sarah Aldulaijan, Dana Almohazey, Nouf Al-Saleem, Zainab Alsunaidi	Design of biosensor and chemical sensor based on mixed-phase transition metal dichalcogenide materials	2019-092-IRMC, end

Research Interests

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1	Catalyst design: Conducting research on heterogeneous catalyst activity using first principles plane wave density functional theory; Studying the direct amination of benzene on surfaces; Examining adsorption energies and structures, possible reaction pathways, catalyst activity, and electronic density of states.
2	Atmospheric Thermochemistry: Investigating structures and accurate thermochemical properties of species involved in atmospheric reactions using <i>ab initio</i> composite methods and density functional theory; Examining

	the effect of basis sets size, spin contaminations, and electron lone pairs; Determining reliable methods for these species.
3	Physical Organic chemistry: organoselenium thermochemistry; Calculating thermochemical energetics of organoselenium compounds using hypohomodesmotic reaction schemes via <i>ab initio</i> composite methods; Investigating different mechanisms of some important chemical reactions involving Organoselenium compounds
4	Computational methods for lanthanides and actinides thermochemistry
5	Green Chemistry: converting biomass to chemicals

Contribution to Scientific Conferences and Symposia

#	Conference Title	Place and Date of the Conference	Extent of Contribution
1	The 2 nd Annual Scientific Forum of College of Science	12 May 2024, College of Science, IAU	إلقاء محاضرة بعنوان: (الأولويات البحثية لكلية العلوم ودورها في تعزيز البحوث البيئية)
2	The 2 nd Annual Scientific Forum of College of Science	9-13 May 2024, College of Science, IAU	Vice Chairwomen of the forum
3	Human Capability Initiative Conference (Preparing for the Future)	29-28 Feb 2024, Human Capacity Development Program, Riyadh	Attendance
4	Chemical Research Forum	12-13 Dec 2023, Chemistry Department, College of Science, IAU	Attendance
5	The 1 st Annual Scientific Forum of College of Science	4 June 2023, College of Science, IAU	إلقاء محاضرة بعنوان: (تحديد الأولويات البحثية بكلية العلوم)
6	The 1 st Annual Scientific Forum of College of Science	31 May - 5 June 2023, College of Science, IAU	Vice Chairwomen of the forum
7	International Conference and Exhibition for Science	6-8 Feb 2023, College of Science, King Saud University	Attendance
8	مؤتمر الشركات المستدامة (البحث و الابتكار لبناء مستقبل مزهر)	23-24 Nov 2022, Ministry of Education, Riyadh	Attendance
9	The Gulf Chemists Union (GCU) & The Saudi Arabian International Chemical Sciences Chapter (SAICSC)	13-17 Nov 2022, Manama, Kingdom of Bahrain	Attendance
10	Symposium 7th Annual National Academic Talent Development Program (NATDP)	24 March 2022, KAUST, Thoul, Saudi Arabia	Attendance
11	Student Scientific Poster Day, SSDE 2022	17 Feb 2022, College of Science, IAU	Head of Organizing the event
12	Webinar INTERNATIONAL WEBINAR, SUSTAINABLE DEVELOPMENT AND	14-17 Feb 2022, College of Science, IAU (virtual)	Attendance and Organizing Committee

	ECOSYSTEMS IN SAUDI Arabia (SSDE'22)		
13	The International Webinar on Science, Sustainable, Development and Ecosystems in Saudi Arabia (SSDE'21)	College of science at Imam Abdulrahman bin Faisal University, Dammam, Saudi Arabia 6-7 April, 2021	Attendance and Organizing Committee
14	سلسلة محاضرات الفريق STEAMomentos التطوعي	STEAMomentos, volunteer team 14 Nov, 2020	إلقاء محاضرة "الكيمياء الحاسوبية وأهم تطبيقاتها"
15	Saudi Arabian Section of the Combustion Institute 10th SASCI Annual Meeting	SASCI , 14-15 October 2020	Attendance
16	ACS Fall 2020 Virtual Meeting & Expo	ACS, Aug 2020	Attendance
17	Teaching and Learning Exhibition	Deanship of Academic Development, IAU, Dammam, SA 17-20/2/2020	"Promoting confidence and performance in solving thermodynamic problems through Jigsaw Technique" Zainab H. A. Alsunaidi, poster
18	Scientific Research committee in the chemistry department	College of science at Imam Abdulrahman bin Faisal University, Dammam, Saudi Arabia (13/1/2019)	"Theoretical investigation of the direct amination of benzene on the Ni(111) surface" Zainab H. A. Alsunaidi, oral presentation
19	الندوة التثقيفية الأولى (الكيمياء الحاسوبية وأهم تطبيقاتها الحديثة)	فرع الجمعية الكيميائية السعودية بالمنطقة الشرقية/ كلية العلوم 19/3/2019	إلقاء محاضرة – منسقة
20	ملتقى الطاقة الشمسية و طاقة الرياح 2 nd solar & wind symposium and exhibition(يومان)	College of Engineering, IAU 12-13/3/2019	Attendance
21	ملتقى الكيميائيين الخليجيين الثاني – دور الكيميائيين في مواجهة التحديات في الصناعات النفطية	اتحاد الكيميائيين الخليجي/ البحرين 24/4/2019	Attendance
22	"Chemistry in our life" Symposium and exhibition sponsored by Saudi Chemical Society and the Chemistry club	College of science at Imam Abdulrahman bin Faisal University, Dammam, Saudi Arabia (Jan 2018)	Attendance and organization
23	Talent Enrichment Program	College of science at Imam Abdulrahman bin Faisal University, Dammam, Saudi Arabia (Jan 2018)	"computational modelling in chemistry" Zainab H. A. Alsunaidi, oral presentation
24	Scientific Research committee in the chemistry department	College of science at Imam Abdulrahman bin Faisal University, Dammam, Saudi Arabia (March 2018)	"Application of several computational strategies to small molecules and periodic systems" Zainab H. A. Alsunaidi, oral presentation
25	"Chemistry of petroleum industry and	Al Khobar Le Meridien Hotel, Al Khobar, Saudi Arabia (April 2018)	Attendance

	environment” First Gulf Chemists Symposium		
26	The 49th Annual Midwest Theoretical Chemistry Conference	East Lansing, Michigan (June 2017).	"Enthalpies of Formation for Organoselenium Compounds via Several Thermochemical Schemes." Zainab H. A. Alsunaidi and Angela K. Wilson; Poster presentation
27	Physical seminar series	Chemistry department, Michigan State University, East Lansing, Michigan. (Jan 2017).	"Towards a Better Design of a Catalytic Surface For the Direct Synthesis of Aniline: A DFT Study" Zainab H. A. Alsunaidi. Oral presentation
28	the 49 th American Chemical Society DFW Meeting-in-Miniature	Texas Woman's University, Denton, Texas (April 2016).	"Application of Thermochemical Schemes for the Prediction of Enthalpies of Formation of Organoselenium Compounds." Zainab H. A. Alsunaidi and Angela K. Wilson; Oral presentation
29	The 26 th Austin Symposium on Molecular Structure	Dallas, Texas (March 2016).	"DFT and Ab Initio Composite Method Investigations of Oxygen Fluorides and Related Hydrides." Zainab H. A. Alsunaidi and Angela K. Wilson; Poster presentation
30	the 251 st ACS National Meeting	San Diego, California (March 2016).	"Catalytic activity of the Ni-surface on the "green" synthesis of Aniline" Zainab H. A. Alsunaidi, Thomas R. Cundari, and Angela K. Wilson; Oral presentation
31	The 249 th ACS National Meeting, Denver, Colorado (March 2015).	Denver, Colorado (March 2015).	"DFT and Ab Initio Composite Method Investigations of Oxygen Fluorides and Related Hydrides" Zainab H. A. Alsunaidi and Angela K. Wilson; Poster presentation
32	A Celebration of Graduate Student Research	University of North Texas, Denton, Texas (May 2014).	"Computational Investigations of the Amination of Benzene on the Ni(111) Surface" Zainab H. A. Alsunaidi; Oral presentation
33	The 47 th American Chemical Society DFW Meeting-in-Miniature	Texas Wesleyan University, Fort Worth, Texas (April 2014).	"Computational Investigations of the Amination of Benzene on the Ni (111) Surface." Zainab H. A. Alsunaidi, Thomas R. Cundari, and Angela K. Wilson; Oral presentation
34	The 25 th Austin Symposium on Molecular Structure	Dallas, Texas (March 2014).	"Theoretical study of direct amination of benzene on a Ni(111) surface." Zainab H. A. Alsunaidi, Thomas R. Cundari, and Angela K. Wilson; Poster presentation
35	The 247 th ACS National Meeting, Dallas, Texas (March 2014).	Dallas, Texas (March 2014).	"Theoretical study of direct amination of benzene on a Ni(111) surface." Zainab H. A. Alsunaidi, Thomas R.

			Cundari, and Angela K. Wilson; Poster presentation
36	Monthly CASCaM Post-Doc and Graduate Student Research Presentations	University of North Texas, Denton, Texas (November 2013).	"Theoretical Investigations of Fluorine Oxides Using <i>Ab Initio</i> Composite Methods, M06, and M06-2X." Zainab H. A. Alsunaidi. Oral presentation
37	Departmental seminar	University of North Texas, Denton, Texas. (April 2013)	Theoretical Investigations of FO _x and FO _x H, x=1-3, using <i>Ab Initio</i> Composite Methods, M06, and M06-2X." Zainab H. A. Alsunaidi. Oral presentation

Membership of Scientific and Professional Societies and Organizations

- American Chemical Society 2014-present
- Saudi Chemical Society 2017-present

Teaching Activities

Undergraduate

#	Course/Rotation Title	No./Code	Extent of Contribution (no. of lectures/Tutorials. Or labs, Clinics)
1	General Chemistry I	CHEM 203	5 semesters (15Lecture/semester) + 2 semester (15 lab/ semester)
2	Research project	CHEM 474N, CHEM 508	3 semesters, 14 students supervision
3	Thermodynamic Chemistry	CHEM 306	3 semesters (15Lecture + Lab/semester)
4	Surface Chemistry and Catalysis	CHEM 507	3 semesters (15Lecture + Lab/semester)
5	Physical Chemistry 1	CHEM 201	1 semester

Course Coordination

#	Course Title and Code	Coordination	Co-coordination	Undergrad.	Postgrad.	From	to
1	General Chemistry (CHEM 203)	√		√		18/9/2017	30/10/2017
2	General Chemistry (CHEM 203)	√		√		Jan 2019	May 2019
3	Surface Chemistry and Catalysis (CHEM 507)	√		√		Aug 2020	Dec 2020
4	Surface Chemistry and Catalysis (CHEM 507)	√		√		Jan 2022	May 2022

Student Academic Supervision and Mentoring

#	Level	Number of Students	From	to
1	Graduate student (research mentoring)	2	Aug 2016	May 2017
2	Graduate student (software training)	3	March 2016	May 2016
3	Undergraduate students (research mentoring)	6	Jan 2018	May 2018
4	Undergraduate students (research mentoring)	1	Aug 2018	Dec 2018
5	Undergraduate students (research mentoring)	7	Jan 2020	May 2020

Supervision/Examination of Master and/or PhD Thesis

#	Degree Type	Title	Institution	Date
1	MSc/as Examiner	Computational Study and Modelling of Some Catalyst Reactions by Graphene	Chemistry Department, College of Science, IAU	31 March 2022
2	MSc/as co-Supervisor	Microwave Synthesis of Metal-Free Doped Hexagonal Boron Nitride for Photocatalytic Hydrogen Production	Chemistry Department, College of Science, IAU	Sep 2020 - 2022

Scientific research centers that have been utilized:

#	
1	The center for advanced scientific computing and modeling (CASCaM) at UNT (May 2014-May2017)
2	Institute for Cyber-Enabled Research (iCER) at MSU (June 2016-June2017)
3	Basic and Applied Scientific Research Center at IAU (Sep 2020 – present)

Scientific contribution to scientific Journals:

#	
1	Working as a scientific reviewer for the Computational and Theoretical chemistry (CTC), 2017

Scientific presentation:

#	
1	Van der Waals Density Functionals (vdW-DFs) Applied to Water Adsorption on Metals, literature talk series, UNT, Denton, TX, May 22 nd , 2013.
2	Computational Considerations of Noncovalent Interactions. Zainab H. A. Alsunaidi, literature talk series, UNT, Denton, TX, July 16 th , 2013.
3	Introduction to VASP. Zainab H. A. Alsunaidi, summer workshop, UNT, Denton, TX, Aug 22 nd , 2013.
4	Plane-wave basis sets. Zainab H. A. Alsunaidi, summer workshop, UNT, Denton, TX, Aug 7 th , 2014
5	Solid-state calculations. Zainab H. A. Alsunaidi, summer workshop, UNT, Denton, TX, July 9 th , 2015.
6	Surface Modeling. Zainab H. A. Alsunaidi, summer workshop, MSU, East Lansing, MI, Aug 2 nd , 2016.

Volunteer Work

#	From	To	Type of Volunteer	Organization
2	4/2/2024	11/2/2024	برنامج الباحث العلمي الناجح – النسخة الثانية- تم تقديمه عن بعد للمجتمع	المشرف العام على تنفيذ البرنامج، كلية العلوم، جامعة الإمام عبد الرحمن بن فيصل
1	1/1/2022	present	تنسيق الكثير من الورش و المحاضرات عن بعد في مجال البحث العلمي و الابتكار	كلية العلوم – جامعة الإمام عبد الرحمن بن فيصل
2	11/12/2022	8/1/2023	برنامج الباحث العلمي الناجح – تم تقديمه عن بعد للمجتمع	المشرف العام على تنفيذ البرنامج، كلية العلوم، جامعة الإمام عبد الرحمن بن فيصل
3	31/1/2021	31/3/2021	برنامج التلمذة البحثية (إشراف أكاديمي على الطالبات الموهوبات من المرحلة الثانوية بتعليم الخبر)	كلية العلوم – جامعة الإمام عبد الرحمن بن فيصل
4	Aug 2020	Dec 2020	البرنامج التدريبي للخريجات (تدريب خريجات)	مكتب الخريجين و التنمية المهنية - كلية العلوم – جامعة الإمام عبد الرحمن بن فيصل
5	Aug 2016	May 2017	Chemistry tutoring	Muslim Students Association, MSU, East Lansing, MI
6	Aug2013	May 2016	Helping and guiding many Saudi students with academic issues (admission, conducting research, academic writing, choosing major/courses, choosing advisor, and	Saudi Club in Denton, Texas

			tutoring), in social life, and in personal development	
7	2009	2009	Organizing graduation party for chemistry students	Chemistry Department, King Faisal University, Dammam

Personal Key Competencies and Skills: (Computer, Information technology, technical, etc.)

1	Extensive experience with software code Gaussian, VASP, Vista, Mercury, and OVITO, and proficient with MOLPRO, NWCHEM, MATLAB, MOLPAC, quantum espresso, and ADF
2	Extensive experience using UNIX/Linus based systems
3	Experience in using Chemdraw, chemcraft, and Gaussian view
4	Professional in academic use of Microsoft Office and proficient use of Adobe Photoshop

Personal Key Competencies and Skills:

1	Professional in academic writing, scientific reviewing, writing proposal, white papers, and critiques
2	Professional in scientific presentation and poster
3	Professional communication skills and networking
4	Leading and coordinating many group teams and meetings
5	Professional in research publishing process
6	Advance Leadership skills
7	Very committed, responsible and dedicated to work

Last Update

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