CURRICULUM VITAE

PERSONAL DATA

Name	Sahar Shamseldden Mohammed Abdalla
Nationality	Sudanese
Position	Associate Professor
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EDUCATION

Year	Academic Degree	Institution
2001	B.Sc	University of Khartoum
2007	M.SC	University of Khartoum
2012	Ph.D	University of Saarland

WORK EXPERIENCE

Period	Position	Address
2001-2007	Teashing assistant	Depatment of Chemistry-Faculy of Science-Universiy of Khartoum-Khartoum-Sudan
2007-2012	Lecturer	Depatment of Chemistry-Faculy of Science-Universiy of Khartoum-Khartoum-Sudan
2012-2013	Assistant researcher	University of tuebingen-Tuebingen-Germany
2012-2017	Assistant professor	Depatment of Chemistry-Faculy of Science-Universiy of Khartoum-Khartoum-Sudan
2017-up to now	Associate professor	Depatment of Chemistry-Faculy of Science-Universiy of Khartoum-Kharoum-Sudan
2022-up to now	Associate professor	Department of Chemistry- Faculty pf Science-Iman Mohammed Ibn Saud University-Riyadh-KSA

RESEARCH INTERESTS

***** Theoretical studies of the effect of substitutions and media on the molecular structures of organic molecules.

***** Improvement of Semiconductor materials that uses in the solar cells, Organic light emitting diodes (OLED), and organic light effect transistors (OLFT) applications.

***** Analysis of the interaction energies using quantum mechanical methods (an approach toward improving the force field methods).

* Isolated and deposited metal clusters.

* Drug design and Molecular docking

PUBLICATIONS

1. **S. Abdalla** and M. Springborg,"Theoretical study of the effect of solvation, substitution, and structure on the properties of imidazoline, oxazolines, and thiazoline". *J. Phys. Chem. A 114 (**2010**) 5823-5829.* DOI: 10.1021/jp9102096.

2. **S. Abdalla** and M. Springborg,"Theoretical Study of tautomerization and isomerization of methylaminoand phenylamino substituted cyclic azaphospholine, oxaphospholine, and thiaphospholines in gas phase and aqueous phase". *J. Mol. Struct. THEOCHEM 962 (**2010**) 101-107.* DOI:10.1016/j.theochem.2010.09.024.

3. **S. Abdalla** and M. Springborg, "A DFT Study of the Properties of Substituted Pyrrolidines and Phospholanes in Gas and in aqueous phase". *Compu. Theor. Chem.978 (**2011**) 143-151*. DOI:10.1016/j.comptc.2011.10.007.

4. **S. Abdalla**, M. Springborg and Y. Dong, "Isolated and deposited

potassium clusters". *Surface Science 608 (**2013**) 255-264.* DOI: 10.1016/j.susc.2012.10.016.

5. **S. Abdalla**, R. R. Fink, "Analyzing Interaction Energy of Polycyclic Aromatic Hydrocarbons (PAHs) Dimers", *Chapter in a book, Springer,* DOI: 10.1007/978-3-319-31759-5_8 *Chapter In book: Crystallizing Ideas – The Role of Chemistry,113-126.*

6. Y. Umar and **S. Abdalla**, "Experimental FTIR and Theoretical Investigation of the Molecular Structure and Vibrational Spectra of Terephthaloyl Chloride by Density Functional Theory", *IOSR Journal of Applied Chemistry (IOSR-JAC, Vol 8, Issue 9 (**2015**) 26-34.*DOI: 10.9790/5736-08912634

7. **S. Abdalla**, Y. Umar, and I. Mokhtar, "Conformational and Vibrational Analysis of 2-, 3- and 4 Pyridinecarbonyl Chloride Using DFT", *z. phys. chem.*, 230 (5-7) (***2016***) 867-882 DOI: 10.1515/zpch-2015-0700

8. Y. Umar, J. Tijani and **S. Abdalla**, "Density functional theory studies of conformational barrier of 2-and 3-Thiophenecarboxaldehydes", *Journal of Structural Chemistry, 57(8), (**2016**) 1642-1650.*DOI: 10.1134/S0022476616080084

9. Y. Umar and **S. Abdalla**," DFT Study of the Molecular Structure, Conformational Preference, HOMO, LUMO, and Vibrational Analysis of 2-, and 3-Furoyl Chloride", *Journal of Solution Chemistry, 46(4), (**2017**) 741-758.* DOI: 10.1007/s10953-017-0601-3

10. R. Oshi, **S. Abdalla** and M. Springborg, "Study of the Influence of Functionalization on the Reorganization Energy of Naphthalene using DFT"**,** *Computational and Theoretical Chemistry, 1099, (**2017**) 209–215.*DOI:10.1016/j.comptc.2016.12.002

11. R. Oshi, **S. Abdalla**, and M. Springborg, "Theoretical study on functionalized anthracene and tetracene as starting species to produce

promising semiconductor materials", *Computational and Theoretical Chemistry 1128, (**2018**) 60-69*.DOI: 10.1016/j.comptc.2018.01.016.

12. R. A. Alnajjar and **S. Abdalla**, Y. Umar, "A DFT study of the effect of halogenation on the conformation of 1,4-dithiin and its S-oxide derivatives", *Revue Roumaine de Chimie*, *63(4), (**2018**) 293-298.*

13. Y. Umar, J. Tijani, and **S. Abdalla**, "Conformational Stabilities, Rotational Barriers, and Vibrational Spectra of 2-Pyrrolecarboxaldehyde and 3-Pyrrole carboxaldehyde using Density Functional Theory", *Journal of Structural Chemistry 60(2) (**2019**) 199-210.*DOI: 10.1134/S0022476619020033.

14. N. Edres, S. Abdalla and Y. Umar, "Theoretical Study of Mono-Terminal Functionalized Oligo-acetylene [$C_nH_{n+2}X$] (*n*=3-5, X= - COOH, and - PO_3H_2) in Gas and Aqueous Phases", *Current Physical Chemistry, 8(2), (**2018**), 95-108.*DOI: 10.2174/1877946808666180703121522.

15. R. Oshi, **S. Abdalla**, and M. Springborg, "The impact of functionalization of organic Semiconductors by electron donating groups on the reorganization energy", *Eur. Phys. J. D 73, (**2019**), 124-132 .*DOI: 10.1140/epjd/e2019-100020-1.

16. Y. Umar, **S. Abdalla**, S. K M. Haque, G. S. Moran, W.C. Villada, J. Dagnino-Leone, M. Bunster, "Theoretical investigation of the molecular structure, vibrational spectra and molecular docking of tramadol using density functional theory", *J Chin Chem Soc. (**2019**);1–10.* DOI: 10.1002/jccs.201900051.

17. W. Fathalrahman, **S. Abdalla**, N. Seriani, "Quasiparticle and Optical Properties of Hydrogen Titanate and Its Defective Systems: An Investigation by Density Functional Theory with Hubbard Correction, Many-Body Perturbation Theory, and Bethe–Salpeter Equation", *Phys. Status Solidi B (**2020**) , 257, 1900054-1900062.* DOI: 10.1002/pssb.201900054.

18. S. Ahmed, **S. Abdalla**, A. Ishaq, Y. Umar," DFT Study of the Structure,

Conformational Profile and Vibrational Analysis of 2-furancarbothialdehyde, and 3-furancarbothialdehyde", *Journal of Structural Chemistry, 62(10), (**2021**) 1485-1497.* DOI: 10.1134/S0022476621100012.

19. A. El-Naeem, S. Abdalla, I. Ahmed, G. Alhassan," Phytochemicals and in Silico Investigations of Sudanese Roselle", *South African Journal of Science (sajs), 118 No.1/2 (**2022**)*. DOI: https://doi.org/10.17159/sajs.2022/10383.

20. Z. Ali, **S. Abdalla***, E. A. Hassan, Y. Umar, and M. M. Al-Mogren," A DFT and TD-DFT Study on Emodin and Purpurin and their Functionalized Molecules to Produce Promising Organic Semiconductor Materials, *Journal* of King Saud University-Science 34 (**2022**) 102117-102125. DOI: https://doi.org/10.1016/j.jksus.2022.102117

21. S. Ahmed, **S. Abdalla**, A. Ishaq, Y. Umar, "Molecular Structure, Conformational Preference and Vibrational Spectral Analysis of 2-, and 3-Furancarboselenaldehyde Using DFT" Accepted for Publication in the *Egyptian Journal of Chemistry* 65 (12) (**2022).** DOI: 10.21608/EJCHEM.2022.120948.5431

22. Z. Ali, **S. Abdalla***, E. A. Hassan, and M. M. Al-Mogren, "Theoretical Study of Electronic and Optical Properties of Functionalized Indigo and Alizarin as Potential Organic Semi-Conductors for Solar Cells Applications" (2022) *Materials Today Communications* 32 104048-104055. https://doi.org/10.1016/j.mtcomm.2022.104048.

23. F. Fadl, **S. Abdalla**, A. Ishaq and Y.Umar," DFT Study of the Molecular Structure, Conformational Preference, Spectroscopic and Vibrational Analysis of Cinnamic acid and Cinnamaldehyde" (2022) J. Mex. Chem. Soc. 2022, 66(4). 543-559. DOI: http://dx.doi.org/10.29356/jmcs.v66i4.1757.

24. S. Shantier; N. S. Mohamed; **S. Abdalla**; R. Elhag; R. Mothana; W. Osman; Y. Umar" Prediction of ADMET, Molecular Docking, DFT and QSPR of Potential

Xanthine Oxidase Inhibitors from *Ambrosia martima* L" Submitted to the *Molecular Structure* 2023.

25. S.Babikir, S. Abdalla, W. Mohamed, Y.Umar, "The impact of Substitution of diphenyl dialumene on the Molecular Structure and Energetic Properties" , submitted to JCCS 2023

26. L. Yagoub, T. A. Awad, **S. Abdalla**, A. Ali, F. Fadul Alla," Docking and in vitro Analysis of Coumarins and Flavonoids Acting as Potential Anti-Alzheimer and Antioxidant Agents". *Submitted to Monatshefte für Chemie - Chemical Monthly 2023.*

27. A. El-Naeem, **S. Abdalla**, I. Ahmed "New Identified Anthocyanins from Sudanese Roselle: Potential Candidates for Inhibition of Xanthine Oxidase", *in preparation*.

28. G. M. Taha, **S. Abdalla**, Y. Abdelmalik, M. Dawood, and A. Khalid," The Structural Properties of Acetylcholinesterase in the presence of Organic Cosolvents", *in preparation.*