

CURRICULUM VITAE

Pr. Abdelkader CHOUAIIH

الأستاذ: عبد القادر شوايح

Faculté des Sciences et de la Technologie — Université Abdelhamid Ibn Badis de Mostaganem — 2026

1. État civil

Nom & Prénom	CHOUAIIH Abdelkader
Date et lieu de naissance	25/08/1974 – Oued Rhiou (48300), Algérie
Laboratoire de recherche	Laboratoire de Technologie et Propriétés du Solide (LTPS), Université Abdelhamid Ibn Badis de Mostaganem
Adresse professionnelle	BP 227, Faculté des Sciences et de la Technologie, Université Abdelhamid Ibn Badis de Mostaganem, 27000 Mostaganem, Algérie
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Langues maîtrisées	Arabe, Français, Anglais

2. Situation professionnelle

Grade actuel	Professeur (CUN N°31 du 26 décembre 2013)
Depuis 2002	Enseignant-Chercheur à l'Université de Mostaganem
2016 – 2022	Directeur du Laboratoire de Technologie et Propriétés du Solide (LTPS)
2018 – 2022	Chargé de mission au vice-rectorat de la Formation Supérieure de troisième cycle, Habilitation Universitaire et Recherche Scientifique, et de la Formation Supérieure de Post-Graduation
Depuis 2014	Responsable du parcours Master « Génie des procédés des matériaux »
2013 – 2015	Vice-doyen chargé de la post-graduation, de la recherche scientifique et des relations extérieures, Faculté des Sciences et de la Technologie
2012 – 2013	Chargé de mission auprès du vice-recteur chargé de la post-graduation et de la recherche scientifique
2008 – 2009	Adjoint chef de département de Chimie

3. Études et diplômes

Diplôme obtenu (graduation, post-graduation)	Année	Établissement
Habilitation Universitaire – Sciences des Matériaux	2008	Université de Mostaganem
Doctorat en Sciences – Sciences des Matériaux	2006	Université de Mostaganem
Magister – Sciences des Matériaux	2002	Université de Mostaganem
Ingénieur d'État en Chimie Industrielle	1998	Université de Mostaganem
Baccalauréat Mathématiques	1993	Lycée H. Boumediene – Oued Rhiou

4. Domaines de compétences

Recherche scientifique (spécialités)

- Structure des matériaux (poudres et monocristaux)
- Modélisation moléculaire
- Cristallographie
- Matériaux de construction

Pédagogie (modules assurés)

- Technique de diffraction des rayons X (Cours, TD, TP)
- Théorie des groupes et symétrie des cristaux
- Cinétique chimique et catalyse
- Chimie analytique et méthodes d'analyse
- Thermodynamique chimique
- Classe et structure des matériaux
- Technologie des fours industriels
- Matériaux polymériques et composites
- Cristallographie
- Matériaux de construction : les liants

5. Expérience dans les projets et programmes de recherche

Responsable de projets

1. Synthèse, structure et réactivité de certains dérivés des thiazolidinones (2019) — Ministère de l'Enseignement Supérieur et de la Recherche Scientifique
2. Étude structurale par diffraction des rayons X et modélisation moléculaire des molécules biologiquement actives (2015) — Ministère de l'Enseignement Supérieur et de la Recherche Scientifique
3. Nouveaux composés organiques photovoltaïques pour l'énergie solaire : synthèse et structure (2013) — Ministère de l'Enseignement Supérieur et de la Recherche Scientifique

Membre de projets

1. Composés hétérocycliques d'intérêt pharmaceutique : synthèse, structure et applications (2023) — Ministère de l'Enseignement Supérieur et de la Recherche Scientifique
2. Structure des matériaux à propriétés optiques non linéaires (2007) — Ministère de l'Enseignement Supérieur et de la Recherche Scientifique

6. Production scientifique

131 publications internationales dans des revues de renommée internationale.

1. A. R. Guerroudj, E. U. Mughal, N. Naeem, H. A. Alrafai, A. Y. Abdullah Alzahrani, M. Fathalla, M. Damou, **A. Chouaih**, Structural and electronic insights into vanillin sulfonates: a spectroscopic and DFT study, *Structural Chemistry*, 1-20, (2026). <https://doi.org/10.1007/s11224-026-02837-y>
2. A. Zerhouni, M. Termoul, Z. D. Benyahlou, A. Çoruh, **A. Chouaih**, B. Bestani, N. Benderdouche, N. Kheddami, J. Kajima Mulengi, Integrated experimental and computational study of a thiazolidinone hydrazone: Insights into reactivity, drug-likeness, and molecular docking behavior, *Functional materials*, 33 (2), 282-297 (2026). <http://dx.doi.org/10.15407/fm33.02.282>
3. A. Benkanoun, M. H. M. Belhachemi, S. Djehni, F. Balegroune, **A. Chouaih**, N. E. H. Belkafouf, Synthesis, structural investigation, thermal behavior, Hirshfeld analysis, DFT computation and molecular docking of a new magnesium diphenate coordination polymer, *Journal of Coordination Chemistry*, 79(11), 1305-1325 (2026). <https://doi.org/10.1080/00958972.2026.2689684>
4. S. Sambandam, A. Ramalingam, A. R. Guerroudj, M. Ramasamy, M. Thiyagarajan, B. Arumugam, A. Arumugam, M. Saidj, **A. Chouaih**, A. Y. Abdullah Alzahrani, Synthesis, Spectroscopic Characterization, DFT Analysis, and Molecular Docking Studies of a Nitrosopiperidin-4-one Derivative toward Antiviral Applications,

5. N. Benhalima, N. Boukabcha, S. Chetoui, **A. Chouaih**, Molecular structure, theoretical and experimental vibrational spectroscopy, NBO investigation, RDG, IRI, AIM analyses, and NLO study of 1-[(E)-2-(5-chloro-2-hydroxyphenyl) hydrazine-1-ylidene] naphthalen-2(1H)-one, **ChemistrySelect** 11(20):e73530 (2026). <https://doi.org/10.1002/slct.73530>
6. Z. D. Benyahlou, F. Triki Baara, S. Yahiaoui, M. Saidj, K. Dermeche, M. Harir, Y. Megrouss, A. Djafri, **A. Chouaih**, H. Bendif, W. Elfalleh, T. H. Taha, A. A. Chaudhary, S. Garzoli, Atom-in-Molecule Analysis, Density Function Theory Research, Spectroscopy, Charge Transfer, and (Static, Dynamic) Nonlinear Optical Effects of (Z)-4,4'-Bis[3-N-Ethyl-2-N'-(Phenylimino) Thiazolidin-4-One] Methane, **ChemistryOpen**, 15(6), e70205, (2026). <https://doi.org/10.1002/open.702057>
7. Z. D. Benyahlou, M. H. M. Belhachemi, A. Oueslati, Ö. Tamer, S. Yahiaoui, M. Azayez, Y. Megrouss, S. A. Kaas, **A. Chouaih**, Y. Atalay, Electronic Structure, Nonlinear Optical Response, and Non-Covalent Interactions in Bi-(2-Amino-5-Methylpyridinium) Hexachlorostannate: Experimental and DFT Investigation, **Physics of the Solid State**, 68, 449–463, (2026). <https://doi.org/10.1134/S1063783425604291>
8. N. E. H. Belkafouf, S. Chetoui, R. Rahmani, O. Al-Dossary, M. Saidj, N. Boubegra, L. G. Bousiakou, **A. Chouaih**, N. Issaoui, Experimental and theoretical investigation of photoinduced electronic transitions and charge-transfer properties in a novel azo compound: (E)-1-((3-Methoxyphenyl)diazonyl)naphthalen-2-ol, **Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy**, 360, 128062 (2026). <https://doi.org/10.1016/j.saa.2026.128062>
9. M. Medjekane, Y. Nait Bachir, Z. D. Benyahlou, F. Nemar, H. Medjahed, S. Ali Haimoud, M. Sadoud, H. Naas, A. Nehari, M. Mansouri, C. Mimouni, **A. Chouaih**, R. Foligni, Juniperus phoenicea L. Essential Oil from Ain El Orak (Algeria): Chemical Analysis by GC/MS, In-Vitro Antioxidant and In-Vivo/In-Silico Gastroprotective and Hepatoprotective Effects, **Foods**, 15, 1667, (2026). <https://doi.org/10.3390/foods15101667>
10. M. Benzekri Benallou, N. Douara, Z. Mekibes, S. Yaslam Saleh Gamal, B. Bestani, N. Benderdouche, **A. Chouaih**, Preparation and Characterization of activated carbon prepared from pomegranate peel for efficient removal of Rhodamine B and Acid Red 114 dyes, **Iranian Journal of Chemistry and Chemical Engineering**, (2026). <https://doi.org/10.30492/ijcce.2026.2083568.7450>
11. H. Messiad, T. Yousfi, S. Hayaham, Z. D. Benyahlou, A. Bouhadiba, K. Belguidoum, H. Belbah, F. Z. Hmammadia, L. Nouar, F. Madi, **A. Chouaih**, H. Amira-Guebailia, Cyclodextrin-Mediated Protection and Delivery of Esculetin: A Combined DFT, TD-DFT, and Docking Investigation, **Journal of Molecular Liquids**, 454, 129552 (2026). <https://doi.org/10.1016/j.molliq.2026.129552>
12. A. R. Guerroudj, S. Chetoui, M. Saidj, R. Rahmani, N. E. H. Belkafouf, N. Boubegra, M. Damou, **A. Chouaih**, Effect of fluorine position on the structural, electronic, and docking properties of conjugated hydrazone and diazenium naphthalenone derivatives: experimental and computational insights, **Spectroscopy letters**, (2026). <https://doi.org/10.1080/00387010.2026.2650370>
13. T. Ouis, N. Boubegra, M. Saidj, N. E. H. Belkafouf, **A. Chouaih**, S. Saidi-Besbes, K. Khezami, M. Durmuş, DFT investigation of electronic structure, optical and photovoltaic properties of 1, 2, 3-triazole functionalized phthalocyanine derivatives, **Polyhedron**, 292, 118097, (2026). <https://doi.org/10.1016/j.poly.2026.118097>
14. S. K. Gandhi, R. P. Gangadharan, A. R. Guerroudj, N. Boukabcha, **A. Chouaih**, Crystal growth, structural scrutiny, optical properties, Hirshfeld surface examination and DFT calculations of an organic NLO material -2,4,6-trinitrophenyl benzoate, **Next Materials**, 11, 101820, (2026). <https://doi.org/10.1016/j.nxmte.2026.101820>
15. S. Arabi, K. Dermeche, R. Rahmani, Y. Makhlof, S. Gheraibia, **A. Chouaih**, Ethnobotanical documentation and pharmacological potential of medicinal plants in Relizane, Algeria, **Bangladesh Journal of Botany** 55 (1), 77–84 (2026). <https://doi.org/10.3329/bjb.v55i1.88601>
16. K. Hammou, M. Azayez, M. C. Terkhi, N. Boukabcha, Y. Megrouss, **A. Chouaih**, Z. D. Benyahlou, M. H. M. Belhachemi, Computational and Crystallographic Insights into 4,4'-Dibromo-2,5-dimethoxy-[1,1'-biphenyl]-2,5'-dione: DFT, Hirshfeld Surface, and Molecular Docking Studies, **Doklady Chemistry (Dokl Chem)**, 520, 210–221 (2026). <https://doi.org/10.1134/S0012500825600464>
17. S. Chetoui, M. Azayez, O. Brihi, D. Hadji, Z. D. Benyahlou, Y. Megrouss, **A. Chouaih**, M. Drissi, J.-P. Djukic, S. Yahiaoui, Design, synthesis, X-ray structure, Hirshfeld surface, and NLO behavior of 3-bromo-2-[(2E)-2-(2-oxonaphthalen-1(2H)-ylidene)hydrazinyl]benzoic acid, **Acta Chim. Slov.**, 73(1), 140–153 (2026). <https://doi.org/10.17344/acsi.2025.9398>
18. M. Benabdallah, S. Djabbour, N. Boukabcha, N. Choukhou-Braham, **A. Chouaih**, Synthesis, Crystal Structure, Electronic Properties, and Molecular Docking Study of bis [5-Imino-7-phenyl-5H-thiazolo [3, 2-a] pyrimidine-6-carbonitrile], **Journal of Molecular Structure**, 1353 (2), 144721, (2026). <https://doi.org/10.1016/j.molstruc.2025.144721>

19. M. Karadag-Alpaslan, A. Benmohammed, E. Berrin Poyraz, **A. Chouaih**, N. Dege, R. Rahmani, Y. Megrouss, A. Djafri, Crystallographic, Hirshfeld Surface, and DFT Analyses of a Fluorine–Bromine Schiff Base: Insights into Structural Features and MAO-A Binding Potential, *Journal of Molecular Structure*, 1351 (1), 144218, (2026). <https://doi.org/10.1016/j.molstruc.2025.144218>
20. F. Baghdad Benabed, S. Attouti, M. Termoul, N. Douara, M. İmamoğlu, A. Çoruh, B. Bestani, N. Benderdouche, **A. Chouaih**, Removal of paraChlorophenoxyacetic acid and Linuron herbicides using pine cone-based activated carbon, *Journal of Dispersion Science and Technology*, 47(2), 191-203 (2026)
21. K. Dermeche, K. Errouane, Z. D. Benyahlou, S. Gheraibia, **A. Chouaih**, In Vitro Evaluation of Antioxidant and Anti-inflammatory Activities of Aristolochia clematitis L roots supported by Computational Investigation, *Journal of Molecular Structure*, 1349 (3), 143892, (2026). <https://doi.org/10.1016/j.molstruc.2025.143892>
22. A. Lahouali Dit Yahyaoui, M. H. M. Belhachemi, A. Ould Rabah, K. Hammou, L. Bensassi, **A. Chouaih**, M. Saidj, Ö. Tamer, D. Avcı, Y. Atalay, DFT-based investigation of structural, optoelectronic and molecular docking analysis of thiosemicarbazone derivatives, *Next Materials*, 10, 101391, (2026). <https://doi.org/10.1016/j.nxmte.2025.101391>
23. M. Azayez, Y. Megrouss, S. Yahiaoui, R. Rahmani, S. A. Kaas, Z. D. Benyahlou, N. Boukabcha, Y. Bouhadda, **A. Chouaih**, Spectroscopic analysis, chemical reactivity, and nonlinear optical properties of (Z)-3-N-(methyl)-2-N'-(4-methoxyphenylimino) Thiazolidin-4-one: DFT/TD-DFT approach, *Turkish Computational and Theoretical Chemistry*, 10 (2), 40-53 (2026). <https://doi.org/10.33435/tcandtc.1055649>
24. S. Attouti, M. Termoul, Z. Bahnes, F. Baghdad-Benabed, N. Boukabcha, B. Bestani, N. Benderdouche, **A. Chouaih**, J. Srénscek-Nazzal, B. Michalkiewicz, Reduction of 2,4-dichlorophenoxy acetic acid herbicide toxicity from aqueous media by adsorption: Experimental and theoretical study using DFT method, *Journal of Dispersion Science and Technology*, 47(2), 179-190, (2026). <https://doi.org/10.1080/01932691.2024.2414276>
25. M. Azayez, N. Khelloul, S. A. Kaas, S. Yahiaoui, M. Drissi, N. Benhalima, Y. Megrouss, **A. Chouaih**, S. Chetoui, Quantum chemical investigation, reactivity, NBO, docking-based exploration and in silico pharmacological properties of 3-bromo-2-[(2Z)-2-(2-oxonaphthalen-1(2H)-ylidene)hydrazinyl]benzoic acid, *Doklady Chemistry*, (2025).
26. H. Belbah, K. Belguidoum, Z. Ourdjini, F. Z. Hamamdia, F. Madi, L. Nouar, M. Nacef, M. H. M. Belhachemi, H. Amira-Guebailia, **A. Chouaih**, Enhancing the antioxidant potential of a coumarin derivative via nickel complexation: synthesis, spectral insights, DFT analysis, and molecular docking, *RSC Advances*, 15(37), 30102-30122 (2025). <https://doi.org/10.1039/D5RA03168K>
27. K. Hammou, A. Djafri, M. C. Terkhi, R. Rahmani, M. Goudjil, N. Boukabcha, E. Lunedei, N. Dege, **A. Chouaih**, A. Djafri, F. Abdelmalek, Design, Integrated Structural, and Theoretical Investigation of a Novel 4-Fluoro-thiazolidin-4-one Derivative Targeting Sirtuin-1, *ChemistrySelect* 10 (26), e01210 (2025). <https://doi.org/10.1002/slct.202501210>
28. S. K. Gandhi, N. Boukabcha, M.H.M. Belhachemi, Z.D. Benyahlou, **A. Chouaih**, Mixed solvent crystal development, structural, spectral, theoretical insights, linear, and non-linear optical qualities of N, N'-diphenylguanidinium phthalate, *Journal of Materials Science: Materials in Electronics* 36 (17), 1040 (2025). <https://doi.org/10.1007/s10854-025-15130-1>
29. N. E. H. Belkafouf, M. Saidj, R. Rahmani, N. Boubegra, A. R. Guerroudj, **A. Chouaih**, Structural and physicochemical properties of azo based materials for organic solar cell application: A DFT approach, *Journal of Photochemistry & Photobiology, A: Chemistry*, 468, 116526 (2025). <https://doi.org/10.1016/j.jphotochem.2025.116526>
30. S. Chetoui, N. Khelloul, N. Boukabcha, N. Benhalima, S. Smati, K. Drim, A. Chouaih, Synthesis, crystal structure, Hirshfeld surface analysis and experimental and theoretical study of new azo compound methyl 2-{2-[(E)-2-oxo-1,2-dihydronaphthalen-1-ylidene]hydrazin-1-yl}-benzoate, *Acta Cryst. C* 81 (2025). <https://doi.org/10.1107/S2053229625003523>
31. F. Allouche, N. Benyza, E. Lanez, A. Chouaih, T. Lanez, Electrochemical and UV-Visible Spectroscopic Investigation of Anthranilic Acid Interaction with DNA, *Journal of Electrochemical Science and Engineering*, 2738 (2025). <https://doi.org/10.5599/jese.2738>
32. A. Ould Rabah, A. Benmohammed, A. Chouaih, M. Goudjil, R. Rahmani, N. E. H. Belkafouf, M. H. M. Belhachemi, F. Z. Boudjenane, A. Djafri, N. Boukabcha, Synthesis, characterization, DFT investigation and in silico anti-eczema evaluation of a novel thiazolidinone derivative, *Acta Chim. Slov.*, 72, 247–260 (2025). <https://acsi-journal.eu/index.php/ACSi/article/view/9111>
33. M. A. Benaouda, A. Djafri, M. Azayez, Y. Megrouss, N. Boukabcha, K. Drim, A. Chouaih, N. Dege, Synthesis, Characterization, Hirshfeld Surface Analysis and DFT Calculation of (2Z,5Z)-3-(2-Methoxyphenyl)-2-[(2-methoxyphenyl)imino]-5-(3-nitrobenzylidene)-1,3-thiazolidin-4-one, *Russian Journal of Physical Chemistry A*, 99(4) 773–785 (2025). <https://doi.org/10.1134/S0036024425700384>

34. M. Azayez, C. Tabti, Y. Megrouss, F. Z. Boudjenane, S. A. Kaas, K. Drim, M. A. Benaouda, A. Chouaih, Reactivity Study, NCI-RDG Analysis, Molecular Docking and ADMET Investigation of N-(4-Acetyl-5-(4-(nitro)phenyl)-4,5-dihydro-1,3,4-thiadiazol-2-yl)-N-phenyl Acetamide, **Doklady Physical Chemistry (Dokl Phys Chem)** 515, 25–35 (2025). <https://doi.org/10.1134/S001250162460027X>
35. S. Djabbour, O. Besseboua, A. Benmohammed, N. Boukabcha, M. Goudjil, Y. Megrouss, M. Shahidul Islam, A. Chouaih, Theoretical Investigation, Spectroscopic Characterization, Global Chemical Reactivity, Nonlinear optical properties, and Antioxidant Activity of 2-(2, 4-Dimethoxybenzylidene)-hydrazono-1, 2-diphenylethanone, **Journal of Molecular Structure**, 1334, 141792, (2025). <https://doi.org/10.1016/j.molstruc.2025.141792>
36. S. Goumri-Said, R. Rahmani, A. Chouaih, M. Benali Kanoun, Probing DCV5T-Me for Organic Photovoltaics: A Comprehensive DFT and NEGF Study, **Chemical Physics Impact**, 10, 100842, (2025). <https://doi.org/10.1016/j.chphi.2025.100842>
37. M. Kadiri, A. Benmohammed, A. Cherif, F. Z. Boudjenane, N. Rekiba, O. Khoumeri, T. Terme, P. Vanelle, A. Djafri, A. Chouaih, Experimental and theoretical investigation of indole analogs as potential antibacterial agents: Design, synthesis, characterization, in-vitro bioevaluation, molecular docking and ADMET studies, **Journal of Molecular Structure**, 1330, 141514, (2025). <https://doi.org/10.1016/j.molstruc.2025.141514>
38. A. Boughoual, F. Monti, A. Guerraoui, N. Boukabcha, A. Chouaih, O. Naili, M. Goudjil, Comprehensive in-vitro antibacterial and in-silico anti-viral evaluations of selected fluorinated-quinolone ligands and their Ag/Zn-based coordination polymers, **Journal of Molecular Structure**, 141280, (2025). <https://doi.org/10.1016/j.molstruc.2024.141280>
39. L. Bensassi, F. Triki-Baara, Y. Megrouss, K. Drim, A. Chouaih, M. Saidj, N. E. H. Belkafouf, A. Benmohammed, A. Djafri, A. Hatzidimitriou, Synthesis, characterization, NCI-RDG, Hirshfield surface analysis, chemical reactivity and quantum chemical calculations of Z-3-N-ethyl-2-N-[(2-methoxyphenyl) imino] thiazolidin-4-one, **Journal of Molecular Structure**, 141301, (2025). <https://doi.org/10.1016/j.molstruc.2024.141301>
40. N. Benharkat, F. Triki-Baara, A. Chouaih, Ş. Atalay, M. Aygün, N. E. H. Belkafouf, N. Dege, M. H. M. Belhachemi, A. Djafri, N. Boukabcha, Synthesis, structure, DFT investigation, and in silico anticancer activity of N-(4-methoxyphenyl)-N'-methyl thiourea, **ChemistrySelect**, 10(1), e202404732 (2025). <https://doi.org/10.1002/slct.202404732>
41. K. Drim, H. Khaldi, Y. Megrouss, M. Azayez, N. Boukabcha, S. A. Kaas, M. A. Benaouda, M. Drissi, A. Chouaih, A. Djafri, Investigation of a New Benzo Imidazothiazole Derivative and Their Inhibition Activity Against Myeloid Leukemia 1 (Mcl-1): Synthesis, Single-Crystal X-Ray Structure, In Silico Study, and Intermolecular Interaction Assessments Using the DFT Method, **Journal of Molecular Structure**, 141206, (2025). <https://doi.org/10.1016/j.molstruc.2024.141206>
42. Y. Megrouss, S. Chetioui, F. C. Kaouche, S. Yahiaoui, K. Drim, Z. D. Benyahlou, M. Azayez, S. A. Kaas, M. Drissi, A. Chouaih, Theoretical investigations, Molecular Docking, ADMET analysis, Molecular Dynamic Simulation, and Drug-Likeness Scoring of (E)-1-[2-(3,4-Dimethylphenyl) Diazen-2-yl]-1-Naphthalen-2-Olate as a Corticosteroid Side-Chain-Isomerase Inhibitor, **Turkish Comp Theo Chem (TC&TC)**, 9(3), 57-78 (2025). <https://doi.org/10.33435/tcandtc.1530717>
43. S. Djabbour, A. Benmohammed, O. Besseboua, N. Boukabcha, M. Goudjil, Y. Megrouss, M. Azayez, N. Dege, A. Chouaih, Y. Atalay, A. Djafri, Synthesis, Crystal Structure, Hirshfeld Surface Analysis, NCI-RDG, Molecular Docking, Molecular Dynamic Simulations, and the activity biologic of 2-((2, 4-dimethoxybenzylidene) hydrazono)-1, 2-diphenylethanone, **Journal of Molecular Structure** (2025), <https://doi.org/10.1016/j.molstruc.2024.140756>
44. R. Rahmani, A. Djafri, H. Khaldi, Y. Megrouss, A. R. Guerroudj, N. Dege, A. Djafri, A. Chouaih, Synthesis, structure, spectra, NLO behavior, and in-silico study on anti-tumor and anti-tuberculosis efficacy of (Z)-3-((Z)-3-phenylallylidene)benzo[4,5]imidazo[1,2-c]thiazole-1(3H)-thione, **Journal of Molecular Structure**, 139661 (2025).
45. F. Z. Boudjenane, R. Rahmani, Y. Megrouss, A. Chouaih, N. Benhalima, DFT theoretical calculations on (Z)-2-hydroxy-N'-(4-oxo-1,3-thiazolidin-2-ylidene) benzohydrazide as a methylene tetrahydrofolatereductase inhibitor: An in silico study, molecular docking, and molecular dynamics simulations, **Turkish Comp Theo Chem (TC&TC)**, 9(1), 90-114 (2025). <https://doi.org/10.33435/tcandtc.1493008>
46. S. Belhachemi, K. Argoub, R. Rahmani, M. Boulakoud, A. Djafri, N. Kheddami, C. Tabti, K. Toubal, A. Chouaih, Synthesis, crystal structure, intermolecular interactions, HOMO-LUMO, MEP, NLO properties, and DFT/TD-DFT investigation of (Z)-5-(4-nitrobenzylidene)-3-N(3-chlorophenyl)-2-thioxothiazolidin-4-one, **Polycyclic Aromatic Compounds** (2025).
47. M. Mostefai, A. Benmohammed, N. Benhalima, N. Dege, R. Rahmani, O. Kourat, A. R. Guerroudj, A. Chouaih, A. Djafri, Synthesis, structural analysis, and molecular docking of a novel 1,3,4-thiadiazole derivative: An experimental and molecular modeling studies, **Journal of Molecular Structure**, 139308 (2025).

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109. K. Toubal, N. Boukabcha, Ö. Tamer, N. Benhalima, S. Altürk, D. Avci, A. Chouaih, Y. Atalay, A. Djafri, F. Hamzaoui, Spectroscopic (FT-IR, 1H and 13C NMR) characterization and density functional theory calculations for (Z)-5-(4-nitrobenzyliden)-3-N(2-ethoxyphenyl)-2-thioxo-thiazolidin-4-one (ARNO), *Journal of Molecular Structure*, 1147, 569-581 (2017).
110. R. Rahmani, A. Djafri, A. Chouaih, A. Djafri, F. Hamzaoui, R. Rizzi, A. Altomare, Synthesis, molecular and solid state structure of 5-(5-nitro furan-2-ylmethylene), 3-N-(2-methoxy phenyl), 2-N'-(2-methoxyphenyl) imino thiazolidin-4-one: X-ray powder diffraction and DFT studies, *Journal of Molecular Structure*, 1143, 259-264 (2017).
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112. S. Altürk, N. Boukabcha, N. Benhalima, Ömer Tamer, A. Chouaih, Davut Avci, Yusuf Atalay, Fodil Hamzaoui, Conformational, spectroscopic and nonlinear optical investigations on 1-(4-chlorophenyl)-3-(4-chlorophenyl)-2-propen-1-one: a DFT study, *Indian Journal of Physics*, 1, 1-11, (2017).
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115. N. Khelloul, K. Toubal, N. Benhalima, R. Rahmani, A. Chouaih, A. Djafri, F. Hamzaoui, Crystal Structure, Hirshfeld Surface Analysis and Computational Studies of Thiazolidin-4-one derivative: (Z)-5-(4-Chlorobenzylidene)-3-(2-ethoxyphenyl)-2-thioxothiazolidin-4-one, *Acta Chim. Slov.*, 63(3), 619-626 (2016).
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127. N. Benhalima, K. Toubal, A. Chouaih, G. Chita, S. Maggi, A. Djafri, F. Hamzaoui, Synthesis and Molecular Structure Investigation by DFT and X-Ray Diffraction of ARNO, *Journal of Chemical Crystallography*, 41(11):1729-1736, (2011). DOI:10.1007/s10870-011-0165-9
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130. Fodil Hamzaoui, Charef Tabti, Abdelkader Chouaih, Gérard Vergoten, Evolution structurale en fonction de la température du composé LiNbO₃, *European Journal of Control*, 31(4):431-438, (2006). DOI:10.3166/acsm.31.431-438
131. Abdelkader Chouaih, Fodil Hamzaoui, Gérard Vergoten, Capability of X-ray diffraction to the determination of the macroscopic linear susceptibility in a crystalline environment: The case of 3-Methyl 4-Nitropyridine N-oxide (POM), *Journal of Molecular Structure*, 738(1):33-38, (2005). DOI:10.1016/j.molstruc.2004.10.067

Liste des communications nationales et internationales

1. A. Chouaih, Unveiling the therapeutic potential of Berbamine from *Berberis vulgaris*: An in silico exploration of nicotinic receptor activation, 1er Séminaire International Scientifique Tuniso-Algérien - Valorisation des Ressources Naturelles et Bio-surveillance SISTA1-VRNB, 20-22 décembre 2023, Monastir, Tunisie.
2. A. Chouaih, Détermination des structures des matériaux par diffraction des rayons X, International Workshop on Applied Chemistry, 12-14 décembre 2018, Chlef, Algérie.
3. N. Boukabcha, Y. Megrouss, M. Drissi, S. Yahiaoui, A. Chouaih, F. Hamzaoui, X-ray diffraction and ab initio investigations of the electrostatic potential and NLO properties of new organic compounds, International Workshop on Applied Chemistry, 12-14 décembre 2018, Chlef, Algérie.
4. Y. Megrouss, N. Boukabcha, S. Yahiaoui, A. Djafri, A. Nekrouf, A. Chouaih, M. Drissi, Synthesis and characterization of a thiazole derivative compound, International Workshop on Applied Chemistry, 12-14 décembre 2018, Chlef, Algérie.
5. N. Belkafouf, K. Toubal, N. Boukabcha, Y. Megrouss, A. Chouaih, F. Hamzaoui, Propriétés structurales, optiques et électroniques d'un nouveau matériau organique, International Workshop on Applied Chemistry, 12-14 décembre 2018, Chlef, Algérie.
6. A. Djafri, N. Khelloul, N. Boukabcha, O. Talhi, N. Taibi, A. Djafri, A. Chouaih, Synthèse, analyse vibrationnelle et propriétés structurales d'un nouveau composé organique, International Workshop on Applied Chemistry, 12-14 décembre 2018, Chlef, Algérie.
7. A. Djafri, N. Khelloul, N. Boukabcha, Y. Megrouss, A. Djafri, A. Chouaih, Synthèse, étude structurale et propriétés physico-chimiques associées du composé 5-Arylidène Imino Thiazolidinones, 4ème journées internationales de chimie organique JICOA-18, 1-3 décembre 2018, Annaba, Algérie.
8. N. Khelloul, A. Djafri, A. Chouaih, F. Hamzaoui, Crystal structure, Hirshfeld surface analysis and DFT calculations of organic compound, 4ème journées internationales de chimie organique JICOA-18, 1-3 décembre 2018, Annaba, Algérie.
9. N. Khelloul, N. Benhalima, A. Chouaih, F. Hamzaoui, Spectroscopic studies, HOMO-LUMO and NBO calculations, Premier colloque maghrébin sur la chimie des hétérocycles CMCH 1-2017, 16-17 mai 2017, Tunis, Tunisie.

10. N. Belkafouf, A. Chouaih, F. Hamzaoui, Détermination de propriétés structurales d'un composé organique : étude DFT, 12ème journées de chimie théorique et computationnelle UMMTO, 28-30 mars 2017, Tizi Ouzou, Algérie.
11. N. Boukabcha, S. Yahiaoui, Y. Megrouss, A. Chouaih, F. Hamzaoui, Theoretical investigations and electron density study of Aniline compound, International conference on progress in applied science ICPAS'17, 4-6 janvier 2017, Turquie.
12. S. Yahiaoui, N. Boukabcha, Y. Megrouss, A. Chouaih, F. Hamzaoui, X-ray diffraction and Theoretical investigations of new merocyanines dyes, International conference on progress in applied science ICPAS'17, 4-6 janvier 2017, Turquie.
13. A. Djafri, N. Boukabcha, N. Benhalima, A. Djafri, A. Chouaih, Synthèse, Caractérisation et Etude Structurale de 5-Arylidine-2-Imino-4-Thiazolidines, Premières Journées Internationales de Chimie Hétérocyclique et ses Applications JICHA 1-2016, 1-2 juin 2016, Tunis, Tunisie.
14. R. Bahoussi, H. Benaissi, A. Chouaih, N. Benhalima, Analyse structurale et calcul théorique des propriétés photovoltaïques d'un composé organique, Premières Journées Internationales de Chimie Hétérocyclique et ses Applications JICHA 1-2016, 1-2 juin 2016, Tunis, Tunisie.
15. R. Rahmani, A. Djafri, A. Chouaih, A. Djafri, F. Hamzaoui, Étude structurale et spectroscopique d'un composé hétérocyclique : approche théorique et expérimentale, Premières Journées Internationales de Chimie Hétérocyclique et ses Applications JICHA 1-2016, 1-2 juin 2016, Tunis, Tunisie.
16. H. Benaissi, S. Yahiaoui, R. Bahoussi, A. Chouaih, F. Hamzaoui, Étude théorique et expérimentale du transfert de charge intramoléculaire d'un composé organique C₂₁H₁₃N₃O₂, Premières Journées Internationales de Chimie Hétérocyclique et ses Applications JICHA 1-2016, 1-2 juin 2016, Tunis, Tunisie.
17. M. Boulakoud, A. Chouaih, F. Hamzaoui, Conformation and Molecular Interaction Studies of New Organic Compound, Congress of Theoretical Chemists of Latin Expression (CHITEL Meeting 2015), 26-31 juillet 2015, Turin, Italie.
18. A. Chouaih, N. Benhalima, R. Rahmani, N. Boukabcha, F. Hamzaoui, Electrostatic potential and Nonlinear Optical Properties of Zwitterionic compound: 6-methyl-2-oxo-3-(1-(ureidoiminio)ethyl)-2H-puran-4-monohydrate, 23rd Annual meeting of the German Crystallographic Society, 16-19 mars 2015, Göttingen, Allemagne.
19. R. Rahmani, A. Djafri, A. Chouaih, N. Benhalima, F. Hamzaoui, Molecular and solid-state structure of 5-(5-nitro furan-2-ylmethylene), 3-N-(2-methoxy phenyl), 2-N'-(2-methoxyphenyl) imino thiazolidin-4-one, 23rd Annual meeting of the German Crystallographic Society, 16-19 mars 2015, Göttingen, Allemagne.
20. Séminaire Matériaux 2014, novembre 2014, Montpellier, France.
21. Congrès de l'Union internationale de Cristallographie - IUCr2014, août 2014, Montréal, Canada.
22. International Conference on Environmental, Biological and Ecological Sciences, and Engineering (ICEBESE 2013), 27-28 février 2013, Barcelone, Espagne.
23. The 13th European Powder Diffraction Conference EPDIC 13, 28-31 octobre 2012, Grenoble, France.
24. Twenty-Second Congress and General Assembly of the International Union of Crystallography, 22-30 août 2011, Madrid, Espagne.
25. North African Conference on Computational Physics and Chemistry, 12-14 décembre 2010, Sidi Bel Abbès, Algérie.
26. Deuxièmes Journées Nationales du Génie des Procédés (2ème JNGP), 3-4 novembre 2010, Tlemcen, Algérie.
27. European Crystallographic Meeting (ECM26), 29 août - 2 septembre 2010, Darmstadt, Allemagne.
28. Première journée du Génie des procédés, 5 avril 2010, Mostaganem, Algérie.
29. 7ème Congrès de la SAC, 16-18 mai 2006, Oran, Algérie.
30. 7ème Journées de Chimie quantique, novembre 2005, Université Es-Senia, Oran, Algérie.
31. IXèmes Journées Maghrébines des Sciences des Matériaux, mai 2004, Université d'Oran, Algérie.
32. International Congress of Photovoltaic and Wind Energy, décembre 2003, Université de Tlemcen, Algérie.
33. Colloque de l'Association Française de Cristallographie, juillet 2003, Université de Caen, France.
34. 6ème journées d'études de chimie quantique, mai 2003, Université Mentouri Constantine, Algérie.
35. Congrès algérien de cristallographie 1, novembre 2002, USTHB, Alger, Algérie.

7. Encadrement et co-encadrement

Thèses de doctorat soutenues — Encadrement

- 1) **Benhalima Nadia** — *Modélisation de la structure cristalline d'un nouveau composé à propriétés optiques non linéaires* (Soutenance : 09/04/2013)
- 2) **Yahiaoui Salem** — *Analyse structurale et thermique du composé C₁₂H₁₈ONFBr₂* (Soutenance : 07/05/2014)
- 3) **Boubegra Naima** — *Étude de la distribution de charge dans un composé organique à propriétés optiques non linéaires, le Diméthyl amino cyano Biphenyl (DMACB)* (Soutenance : 29/05/2014)
- 4) **Boulakoud Manel** — *Étude structurale des composés organiques à transfert de charges : approche expérimentale et modélisation moléculaire* (Soutenance : 05/06/2016)
- 5) **Bahoussi Rawia Imane** — *Étude structurale, vibrationnelle et thermique d'un nouveau composé organique, le C₁₈H₂₀O₃N₄S* (Soutenance : 10/06/2017)
- 6) **Khelloul Nawel** — *Étude structurale et vibrationnelle du composé thiazolique C₁₈H₁₄O₂S₂NCI* (Soutenance : 02/07/2017)
- 7) **Boukabcha Nourdine** — *Étude des propriétés structurales des composés organiques poly-substitués* (Soutenance : 21/12/2017)
- 8) **Megrouss Youcef** — *Détermination des grandeurs physiques de composés moléculaires à propriétés optiques non linéaires* (Soutenance : 21/12/2017)
- 9) **Djafri Ahmed** — *Synthèse, étude structurale et propriétés physico-chimiques associées de quelques composés hétérocycliques* (Soutenance : 22/10/2018). Co-encadrant : Pr. Ayada Djafri.
- 10) **Benaissi Hafida** — *Analyse de la densité électronique précise d'un composé organique à propriétés optiques non linéaires* (Soutenance : 02/05/2019). Co-encadrant : M. Drissi.
- 11) **Belkafouf Nour El Houda** — *Analyse structurale et spectroscopique de nouveaux matériaux fonctionnels* (Soutenance : 18/07/2019). Co-encadrant : Pr. Fodil Hamzaoui.
- 12) **Kourat Oumria** — *Analyses structurale et conformationnelle de matériaux organiques conjugués* (Soutenance : 07/01/2021). Co-encadrant : Dr. Nadia Benhalima.
- 13) **Benelhadj Djelloul Yamina** — *Structure moléculaire de substances organiques et relation avec leur activité biologique* (Soutenance : 18/06/2021). Co-encadrant : Dr. Nourdine Boukabcha.
- 14) **Nekrouf Asma** — *Étude combinée par diffraction X et calcul théorique de la distribution de la densité électronique des matériaux moléculaires* (Soutenance : 09/03/2023). Co-encadrant : Dr. Y. Megrouss.
- 15) **Boudjenane Fatima Zohra** — *Contribution au développement de nouveaux matériaux organiques pour l'optoélectronique : caractérisation, structure et propriétés associées* (Soutenance : 25/04/2024). Co-encadrant : Dr. Nourdine Boukabcha.
- 16) **Kheddam Narimane** — *Synthèse, structure et activité biologique du composé C₂₄H₁₅O₃N₃F₂S* (Soutenance : 08/04/2025). Co-encadrant : Dr. Ahmed Djafri.
- 17) **Ould Rabah Amine** — *Analyse structurale et vibrationnelle et activité biologique de certains dérivés de thiazolidinones d'intérêt pharmaceutique* (Soutenance : 09/07/2025). Co-encadrant : N. Boukabcha.
- 18) **Bensassi Latifa** — *Étude structurale et activité biologique du composé C₁₂H₁₄O₂N₂S* (Soutenance : 13/04/2026). Co-encadrant : M. Saidj — inscription 2021.
- 19) **Belhachemi Soumia** — *Analyses spectroscopique et structurale, et propriétés physico-chimiques de nouvelles molécules de la famille des thiazolidinones* (Soutenance : 14/04/2026). Co-encadrant : C. Tabti — inscription 2021.
- 20) **Benharkat Noureddine** — *Design, structure et propriétés des composés hétéro-atomiques d'intérêt pharmaceutique* (Soutenance : 07/07/2026). Co-encadreur : N. Boukabcha — Université de Chlef, inscription 2023.

Thèses de doctorat soutenues — Co-encadrement

- 1) **Guerroudj Ahlem Roufieda** — *Analyse spectroscopique et structurale de nouveaux composés organiques à transfert de charge* (Soutenance : 18/02/2023). Encadrant : N. Boukabcha.

- 2) **Belhachemi Mohamed Hadj Mortada** — *Étude vibrationnelle et structurale de nouvelles molécules pour l'optoélectronique* (Soutenance : 02/05/2024). Encadrant : N. Boukabcha.
- 3) **Benyahlou Zohra Douaa** — *Analyse spectroscopique et structurale de dérivés de thiazolidinones à propriétés optiques non linéaires* (Soutenance : 04/05/2024). Encadrant : S. Yahiaoui.
- 4) **Kaas Sid Ahmed** — *Détermination de la structure, étude des propriétés et réactivités moléculaires du composé $C_{11}H_{12}N_2O_2S$, $2H_2O$ par diffraction X et calcul théorique* (Soutenance : 08/07/2025). Encadrant : Y. Megrouss.
- 5) **Chebli Amar** — *Analyse cristallographique et spectroscopique d'un nouveau composé à propriétés optiques non linéaires de la famille des quinoléines* (Soutenance : 22/01/2026). Encadrant : M. Drissi.

Thèses de doctorat en cours

- 1) **Mostefai Mohammed** — *Structure, caractérisation et électrochimie d'un nouveau composé hétérocyclique des dérivés de thiadiazoles : étude expérimentale et modélisation moléculaire* (Soutenance : Inscription 2020). Co-encadrant : N. Benhalima.
- 2) **Lahouali dit Yahyaoui Amina** — *Étude structurale et électrochimie d'un nouveau composé hétérocyclique à transfert de charge* (Soutenance : Inscription 2022). Co-encadrant : M. Saidj.

Mémoires de Magister soutenus

- 1) **Bensenouci Said** — *Application de la méthode de Rietveld à l'analyse quantitative du Clinker Portland* (Soutenance : Décembre 2008)
- 2) **Benelhadj Djelloul Yamina** — *Analyse structurale d'un nouveau composé organique de la famille des thiazolidinones* (Soutenance : 02/07/2010)
- 3) **Benkadari Abdelkarim** — *Résolution et affinement de la structure d'un nouveau pyréthroïde* (Soutenance : 14/07/2010)
- 4) **Boukabcha Noureddine** — *Effet de la substitution sur le moment dipolaire d'un composé à propriétés optiques non linéaires : modélisation moléculaire* (Soutenance : 16/06/2012)
- 5) **Zahraoui Mehdi** — *Étude comparative par diffraction X et modélisation moléculaire de la structure d'un intermédiaire réactionnel d'un insecticide* (Soutenance : 16/06/2012)
- 6) **Sahraoui Badreddine** — *Analyse de la densité de charge de composés organiques photovoltaïques, cas du tri (8-hydroxy quinolinate) Aluminium* (Soutenance : 25/05/2013)

Mémoires de Master soutenus

Plus d'une vingtaine (20) de mémoires de Master soutenus.

8. Ouvrage scientifique

1. F. Hamzaoui, A. Chouaih, *Electron Charge Density in Organic Compounds: Non-Linear Optical Properties*, Lap Lambert Academic Publishing, ISBN : 9783659710339 (2015).
2. M. Zahraoui, K. Dahmani, A. Chouaih, *Étude Comparative par Diffraction de RX et Modélisation Moléculaire : DRX et Modélisation Moléculaire de la Structure d'un intermédiaire réactionnel d'un insecticide RU 67273*, Editions Universitaires Européennes (2019).

9. Animation scientifique

- Expert ATRST de bilans scientifiques des laboratoires de recherche
- Expert ATRST PNR 2023 et 2025
- Membre expert de la sous-commission de l'habilitation universitaire en génie des procédés et environnement (depuis novembre 2021)
- Président de CSD de Génie des Procédés (2022 – 2025)
- Membre du comité scientifique du 1er séminaire national en génie des procédés, 18-19 octobre 2021, Ouargla
- Membre du comité scientifique de la 1ère conférence nationale de synthèse et catalyse, 26 octobre 2021, Tiaret

- Membre du comité scientifique de la journée de génie des procédés, 02 juin 2021, Mostaganem
- Responsable de la formation doctorale : Technologie, structure et propriétés des solides
- Chef d'équipe de cristallographie – Laboratoire de Technologie et Propriétés du Solide (LTPS)
- Membre de la sous-commission d'élaboration des programmes du CPND, spécialité Génie des procédés des matériaux
- Membre du conseil scientifique de la Faculté des Sciences et de la Technologie
- Membre du comité scientifique du département de Génie des Procédés
- Président de CPC – Master en Génie des Procédés des Matériaux
- Reviewer, revue Journal of Molecular Structure – Elsevier/ScienceDirect
- Reviewer, revue Polycyclic Aromatic Compounds Journal
- Reviewer, revue Acta Chimica Slovenica
- Reviewer, revue Chemical Physics Impact – Elsevier/ScienceDirect
- Reviewer, revue Crystal Research & Technology
- Reviewer, revue Journal of Molecular Liquids
- Reviewer, revue Organometallic Applied Chemistry
- Reviewer, revue Arabian Journal of Chemistry
- Reviewer, revue Journal of Photochemistry and Photobiology A: Chemistry – Elsevier/ScienceDirect
- Reviewer, revue Phosphorus, Sulfur, and Silicon and The Related Elements
- Membre de jury de plus de 40 soutenances de doctorat, en tant que président ou examinateur

10. Compétences

- Sens du contact
- Communication
- Capacité d'adaptation
- Polyvalence
- Logique
- Rigueur
- Autonomie

11. Centres d'intérêt

- Recherche scientifique
- Lecture
- Bénévolat
- Voyage