

Liste des productions scientifiques (publications, communications,...)

Année 2024

Etablissement Universitaire: Université 8 Mai 1945 de Guelma

Faculté: Mathématique, Informatique et Sciences de la Matière

Laboratoire de chimie computationnelle et nanostructures "LCCN"

|                              | Productions Scientifiques 2024                                                                                                                                |                                                                                                                                                 |                                           |       |                                                                            |        |               |                                                                                           |
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|                              | Publications                                                                                                                                                  |                                                                                                                                                 |                                           |       |                                                                            |        |               |                                                                                           |
|                              | Titre                                                                                                                                                         | Auteurs                                                                                                                                         | Revue                                     | Année | Catégorie de la revue: A+ , A , B-<br>Scopus, B-non Scopus, C, non classée | Volume | Page          | URL                                                                                       |
| Publications internationales | Intermolecular interactions of Guanosine/ $\beta$ -Cyclodextrine and Guanosine-hydroxypropyl/ $\beta$ -Cyclodextrin inclusion complexes using DFT calculation | Sakina Hayahem<br>Hanane Messiad<br>Tarek Yousfi<br>Leila Nouar<br>Fatiha Madi<br>Mohamed Rahim<br>Abdelaziz Bouhadiba                          | Studies in Engineering and Exact Sciences | 2024  | B                                                                          | Vol. 5 | e11649-e11649 | <a href="https://doi.org/10.54021/seesv5n2-649">https://doi.org/10.54021/seesv5n2-649</a> |
|                              | Computational study of the encapsulation of an organic pollutant with beta-CD, in vacuum and in water                                                         | Mohamed Rahim<br>Abdelaziz Bouhadiba<br>Ahlem Benmerabet<br>Hassina Chekroud<br>Fatiha Madi<br>Leila Nouar<br>Imane Djellala<br>Sulaiman Mogali | Studies in Engineering and Exact Sciences | 2024  | B                                                                          | Vol. 5 | e9518-e9518   | <a href="https://doi.org/10.54021/seesv5n2-376">https://doi.org/10.54021/seesv5n2-376</a> |

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| Publications internationales | Synthesis of ultramicroporous zeolitic imidazolate framework ZIF-8 via solid state method using a minimum amount of deionized water for high greenhouse gas adsorption: A computational modeling | C.H. Belgacem<br>N. Missaoui<br>M.A.H. Khalafalla<br>G. Bouzid<br>H. Kahri<br>A.H. Bashal<br>A. Dhahri<br>L. Nouar<br>F.J. Melendez<br>M.E. Castro<br>H. Ghalla<br>Y. Zhou | Journal of Environmental Chemical Engineering | 2024 | A | Vol 12 | 112086    | <a href="https://doi.org/10.1016/j.jece.2024.112086">https://doi.org/10.1016/j.jece.2024.112086</a>       |
|                              | Host-Guest Inclusion Systems of Vanillic Acid into $\alpha$ -Cyclodextrin: Structures, Electronic Properties, QTAIM, NCI and IGM Analyses with Dispersion Corrected Calculations                 | Fatiha Madi<br>Leila Nouar<br>Nora Merabet<br>Imane Djellala<br>Abdelkrim Guendouzi<br>Abdelaziz Bouhadiba                                                                 | Polycyclic Aromatic Compounds                 | 2024 | A | Vol 44 | 1682-1696 | <a href="https://doi.org/10.1080/10406638.2023.2202866">https://doi.org/10.1080/10406638.2023.2202866</a> |
|                              | Theoretical Study of the Elastic, Electronic, and Thermodynamic Properties of the Cs <sub>2</sub> MF <sub>6</sub> (M = Cr and Mo) Perovskites                                                    | Nedjoua Cheghib<br>Rafik Maizi<br>Abdelghani Boudjahem<br>Rabah Ksouri<br>Meryem Dardare                                                                                   | Russian Journal of Inorganic Chemistry        | 2024 | A |        | 1-7       | <a href="https://doi.org/10.1134/S0036023624601983">https://doi.org/10.1134/S0036023624601983</a>         |

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| Publications internationales | DFT Study of Structural, Elastic, Electronic, and Thermodynamic Properties of Compounds Cs <sub>2</sub> TiCl <sub>6</sub> and Cs <sub>2</sub> TiBr <sub>6</sub>                                                                 | A-G Boudjahem<br>R Ksouri<br>R Maizi<br>N Cheghib<br>I Djaghout<br>M Derdare                                                                                         | Russian Journal of Inorganic Chemistry  | 2024 | A |      | 1-6  | <a href="https://doi.org/10.1134/S0036023624601223">https://doi.org/10.1134/S0036023624601223</a>   |
|                              | Electronic, Structural, Elastic, and Thermodynamic Properties of X <sub>2</sub> TiBr <sub>6</sub> (X = Li and Na) under Pressure: A DFT Investigation                                                                           | R Maizi<br>R Ksouri<br>AG Boudjahem<br>M Derdare<br>N Cheghib<br>I Djaghout                                                                                          | Russian Journal of Inorganic Chemistry  | 2024 | A |      | 1-11 | <a href="https://doi.org/10.1134/S0036023624600722">https://doi.org/10.1134/S0036023624600722</a>   |
|                              | Plasma-flash sintering: Metastable phase stabilization and evidence of ionized species                                                                                                                                          | Ahmed Taibi<br>Antonio Perejón<br>Eva Gil-González,<br>L. A. Pérez-Maqueda<br>P. E. Sánchez-Jiménez                                                                  | Journal of the American Ceramic Society | 2024 | A | V108 |      | <a href="https://doi.org/10.1111/jace.20105">https://doi.org/10.1111/jace.20105</a>                 |
|                              | Synthesis, structural characterization, computational studies, and in silico and in vitro biological activities of cyclodextrin inclusion complex with sulfonamide derived from L-valine as antimicrobial and anti-HIV-1 agents | Zineb Attou<br>Yamina Abdi<br>Yassamina Arbia<br>Belgacem Bezzina<br>Hadjer Merazka<br>Messaouda Mohamdi<br>Dhaouiya Siziani<br>Meziane Brahimi<br>Nadjia Bensouilah | Structural Chemistry                    | 2024 | A |      | 1-24 | <a href="https://doi.org/10.1007/s11224-024-02393-3">https://doi.org/10.1007/s11224-024-02393-3</a> |

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| Publications internationales | Effect of morphology on the electrochemical performance of NiO thin films                  | A Houssou<br>S Amirat<br>W Bouchelaghem<br>A Sayah<br>H Ferkous<br>R Rehamnia                                                                                                                                                                                                        | Bulletin of Materials Science | 2024 | A | 47  | 126    | <a href="https://doi.org/10.1007/s12034-024-03190-8">https://doi.org/10.1007/s12034-024-03190-8</a>     |
|                              | Experimental and computational investigations on mechanically alloyed Fe55Co30Ni15 powders | Abdelkrim Houssou<br>Samia Amirat<br>Hana Ferkous<br>Safia Alleg<br>Karima Dadda<br>Yacine Benguerba<br>Rahima Boulechfar<br>Lakhdar Abadlia<br>Wahiba Bouchelaghem<br>Javed Khan Bhutto<br>Krishna Kumar Yadav<br>Alessandro Erto<br>Noureddine Elboughdiri<br>Maha Awjan Alreshidi | Powder Technology             | 2024 | A | 433 | 119203 | <a href="https://doi.org/10.1016/j.powtec.2023.119203">https://doi.org/10.1016/j.powtec.2023.119203</a> |

|                           | Productions Scientifiques 2024                                                                       |                                                                                                                                                      |                                                             |       |                                                             |        |      |                                                                                                                                                                     |
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|                           | Communications                                                                                       |                                                                                                                                                      |                                                             |       |                                                             |        |      |                                                                                                                                                                     |
|                           | Titre                                                                                                | Auteurs                                                                                                                                              | Intitulé de manifestation                                   | Année | Proceeding de la conférence indexé dans Scopus ( oui /non ) | Volume | Page | URL                                                                                                                                                                 |
| Communications nationales | Investigation of cytosine-guanine interactions with free radicals OH*: a computational investigation | Samia AMIRAT,<br>Oualid Alioui<br>Abir Boublia<br>Amel Boudechicha<br>Fatiha Madi<br>Nouar Leila<br>Abdelhak Gheid<br>Barbara Ernst<br>Manawwer Alam | 3ème Séminaire National sur la Chimie Appliquée (3ème NSAC) | 2024  |                                                             |        |      | <a href="https://www.univ-guelma.dz/sites/default/files/2024-09/sem14-11-2024CA.pdf">https://www.univ-guelma.dz/sites/default/files/2024-09/sem14-11-2024CA.pdf</a> |
|                           | Computational investigation of simazine by $\beta$ -cyclodextrin                                     | Ahlem Benmerabet<br>Bouhadiba Abdelaziz<br>Rahim Mohamed<br>Nouar Leila<br>Madi Fatiha                                                               | 3ème Séminaire National sur la Chimie Appliquée (3ème NSAC) | 2024  |                                                             |        |      | <a href="https://www.univ-guelma.dz/sites/default/files/2024-09/sem14-11-2024CA.pdf">https://www.univ-guelma.dz/sites/default/files/2024-09/sem14-11-2024CA.pdf</a> |
|                           | In silico investigation to predict pharmacokinetic and drug-likeness features of bioactive molecule  | Samah HADJAR<br><br>Harkati Brahim                                                                                                                   | 3ème Séminaire National sur la Chimie Appliquée (3ème NSAC) | 2024  |                                                             |        |      | <a href="https://www.univ-guelma.dz/sites/default/files/2024-09/sem14-11-2024CA.pdf">https://www.univ-guelma.dz/sites/default/files/2024-09/sem14-11-2024CA.pdf</a> |
|                           | Theoretical study of host-guest interactions in complexes of cucurbit[7]uril                         | Sakina HAYAHM<br><br>Leila Nouar                                                                                                                     | 3ème Séminaire National sur la Chimie Appliquée (3ème NSAC) | 2024  |                                                             |        |      | <a href="https://www.univ-guelma.dz/sites/default/files/2024-09/sem14-11-2024CA.pdf">https://www.univ-guelma.dz/sites/default/files/2024-09/sem14-11-2024CA.pdf</a> |

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| Communications nationales | Inclusion complex formation of $\beta$ -cyclodextrin with the dimethoate computational study                                                              | Abdelaziz Bouhadiba<br>Rahim Mohamed<br>Bouneb Wahiba<br>Nouar Leila<br>Madi Fatiha           | 5ème Séminaire National sur la Chimie Appliquée (3ème NSAC) | 2024 |  |  |  | <a href="https://www.univ-quelma.dz/sites/default/files/2024-09/sem14-11-2024CA.pdf">https://www.univ-quelma.dz/sites/default/files/2024-09/sem14-11-2024CA.pdf</a> |
|                           | Etude in silico de l'inhibition des cyclooxygénases-2 par le cyclocoumarol et ses dérivés                                                                 | Nadia LACHI                                                                                   | 6ème Séminaire National sur la Chimie Appliquée (3ème NSAC) | 2024 |  |  |  | <a href="https://www.univ-quelma.dz/sites/default/files/2024-09/sem14-11-2024CA.pdf">https://www.univ-quelma.dz/sites/default/files/2024-09/sem14-11-2024CA.pdf</a> |
|                           | Etude par modélisation moléculaire du système emodine @ $\beta$ -CD                                                                                       | Nora MERABET<br>Lafifi Ismahane<br>Nouar Leila<br>Madi Fatiha                                 | 7ème Séminaire National sur la Chimie Appliquée (3ème NSAC) | 2024 |  |  |  | <a href="https://www.univ-quelma.dz/sites/default/files/2024-09/sem14-11-2024CA.pdf">https://www.univ-quelma.dz/sites/default/files/2024-09/sem14-11-2024CA.pdf</a> |
|                           | Revêtement et étude morphologique et structurale des composés d'alliages binaires Ni-Fe électro déposées dans le milieu liquide ionique [BuMePyr][Tf2N]   | Rafik MAIZI<br>Nedjoua Cheghib<br>Rousse Céline<br>Fricoteaux Patrick<br>Abdelghani Boudjahem | 8ème Séminaire National sur la Chimie Appliquée (3ème NSAC) | 2024 |  |  |  | <a href="https://www.univ-quelma.dz/sites/default/files/2024-09/sem14-11-2024CA.pdf">https://www.univ-quelma.dz/sites/default/files/2024-09/sem14-11-2024CA.pdf</a> |
|                           | Exploring the properties of hydroxytriazenes and triazenes and fragmentation molecules for quantum chemical torsion scans using density functional theory | Leila LARGATE<br>Ali Athmani<br>Rachid Merdes<br>Abdelghani Boudjahem                         | 3ème Séminaire National sur la Chimie Appliquée (3ème NSAC) | 2024 |  |  |  | <a href="https://www.univ-quelma.dz/sites/default/files/2024-09/sem14-11-2024CA.pdf">https://www.univ-quelma.dz/sites/default/files/2024-09/sem14-11-2024CA.pdf</a> |

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| Communications nationales | Computational study of DNA methylation in cytosine base                                                                                                              | Ismahan LAFIFI<br>Leila Nouar<br>Noura Merabet<br>Imane Djilani                                             | 3ème Séminaire National sur la Chimie Appliquée (3ème NSAC) | 2024 |  |  |  | <a href="https://www.univ-guelma.dz/sites/default/files/2024-09/sem14-11-2024CA.pdf">https://www.univ-guelma.dz/sites/default/files/2024-09/sem14-11-2024CA.pdf</a> |
|                           | Etude par la méthode TD-DFT des spectres de fluorescence de p-aminobenzoate de méthyle et leurs complexes d'inclusion par les $\alpha$ - et $\gamma$ -cyclodextrines | Sonia BADI<br><br>Leila Nouar<br><br>Fatiha Madi                                                            | 3ème Séminaire National sur la Chimie Appliquée (3ème NSAC) | 2024 |  |  |  | <a href="https://www.univ-guelma.dz/sites/default/files/2024-09/sem14-11-2024CA.pdf">https://www.univ-guelma.dz/sites/default/files/2024-09/sem14-11-2024CA.pdf</a> |
|                           | Deleterious effects of classically activated macrophages (M1) modulated by selenium supplementation in human type 1 diabetes onset                                   | LAFIFI Ismahan<br><br>Mouna NOUAR<br><br>Leila Nouar<br><br>Fatiha Madi                                     | 3ème Séminaire National sur la Chimie Appliquée (3ème NSAC) | 2024 |  |  |  | <a href="https://www.univ-guelma.dz/sites/default/files/2024-09/sem14-11-2024CA.pdf">https://www.univ-guelma.dz/sites/default/files/2024-09/sem14-11-2024CA.pdf</a> |
|                           | A theoretical study of the elastic, electronic and thermodynamic properties of NaNbO <sub>3</sub> and NaTaO <sub>3</sub> perovskites                                 | Rabah KSOURI<br>Ilhem Djaghout<br>Rafik Maizi<br>Nadjoua Cheghib<br>Meryem Derdare<br>Abdel Ghani Boudjahem | 3ème Séminaire National sur la Chimie Appliquée (3ème NSAC) | 2024 |  |  |  | <a href="https://www.univ-guelma.dz/sites/default/files/2024-09/sem14-11-2024CA.pdf">https://www.univ-guelma.dz/sites/default/files/2024-09/sem14-11-2024CA.pdf</a> |
|                           | Étude théorique du complexe zinc pyrithione : un antimicrobien doté de qualité pharmaceutique                                                                        | LAFIFI Ismahane<br>MERABET Nora<br>DJILANI Imane<br>NOUAR Mouna                                             | Le 2ème colloque national de chimie (CNC2@2024)             | 2024 |  |  |  | <a href="http://virtuelcampus.univ-msila.dz/facscience/?p=8514">http://virtuelcampus.univ-msila.dz/facscience/?p=8514</a>                                           |

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| Communications internationales | "QSAR and molecular docking studies of H2 receptor antagonists"                               | LAFIFI Ismahan<br>Fayçal Nouar<br>Mouna Nouar                  | 14th International Days of Theoretical and Computational Chemistry JCTC14, Tlemcen, March 2-3 |      |  |  |  | The 14th International Days of Theoretical and Computational Chemistry   University of Tlemcen                            |
|                                | Étude théorique du complexe zinc pyrithione : un antimicrobien doté de qualité pharmaceutique | LAFIFI Ismahan<br>MERABET Nora<br>DJILANI Imane<br>NOUAR Mouna | 2ème colloque national de chimie (CNC2@2024) 6 - 7 mai 2024                                   | 2024 |  |  |  | <a href="http://virtuelcampus.univ-msila.dz/facscience/?p=8514">http://virtuelcampus.univ-msila.dz/facscience/?p=8514</a> |