ESEF-Berrechid

EST-Safi

Faculté Polydisciplinaire de Safi

Livret

1ère édition du colloque national eau, matériaux et modélisation moléculaire (E3M-2025)

sous le thème:

Intelligence artificielle : Enjeux pour une recherche doctorale de qualité, applications à la détection de la pollution de l'eau et à la modélisation moléculaire avancée

Organisé par:

Faculté Polydiscilpnaire de Safi-Université Cadi Ayyad
&
Laboratoire Education, Sciences et Techniques, Ecole Supérieure de l'Education et de la Formation de Berrechid-Université Hassan 1er

Mercredi 25 juin à 9h00
Salle de conférences
Faculté Polydisciplainaire de Safi

Coordonnateurs: – Pr. Zouhair LAKBAIBI Enseignant–Chercheur FP–Safi
– Pr. Adil JAAFAR Enseignant–Chercheur ESEF–Berrechid

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Mot de bienvenue

Mesdames, Messieurs, Cher(e)s participant(e)s,

Nous avons le grand plaisir de vous accueillir à la première édition du colloque national eau, matériaux et modélisation moléculaire (E3M-2025), sous le thème: Intelligence artificielle: enjeux pour une recherche doctorale de qualité, applications à la détection de la pollution dans l'eau et à la modélisation moléculaire avancée.

Ce colloque vise à réunir chercheurs, enseignants, doctorants et professionnels autour des thématiques actuelles en relation avec l'intelligence artificielle (IA), visant à se rencontrer, échanger et coopérer.

Nous vous souhaitons un excellent colloque et des échanges fructueux.

Le Comité d'organisation E3M-2025

Préambule

Cet événement explore l'impact de l'intelligence artificielle sur la qualité de la recherche académique, en particulier les thèses de doctorat, en abordant les enjeux et les opportunités qu'offre cette technologie pour améliorer les méthodes de recherche, l'analyse des données et proposer des solutions innovantes. Il met également en lumière les applications récentes de l'IA dans la modélisation moléculaire et la détection de la pollution des eaux souterraines, en mettant l'accent sur la conception de médicaments et l'ouverture de nouvelles perspectives dans la médecine moderne. Ce rassemblement réunira des chercheurs, des universitaires et des professionnels de divers domaines pour échanger des connaissances et des idées sur le rôle de l'IA dans l'avancement de la science.

Argumentaire

À l'heure où l'intelligence artificielle transforme en profondeur l'ensemble des disciplines scientifiques, la recherche doctorale se doit d'intégrer ces avancées technologiques pour renforcer la qualité, la rigueur méthodologique de ses productions. Ce colloque national entend explorer les enjeux, défis et opportunités qu'offre l'IA à la recherche doctorale, en se focalisant sur deux champs d'application stratégiques : la détection des polluants dans l'eau et la modélisation moléculaire.

Face aux défis environnementaux majeurs, notamment la contamination des ressources hydriques, l'IA s'impose comme un outil précieux pour automatiser la détection de polluants, améliorer la précision des diagnostics, et optimiser les réponses en matière de gestion et de traitement de l'eau. Par des approches d'apprentissage automatique (machine Learning), l'IA permet une surveillance intelligente, continue et prédictive de la qualité de l'eau.

Parallèlement, en modélisation moléculaire, domaine-clé pour les sciences chimiques, biologiques et pharmaceutiques, l'IA révolutionne la conception et la simulation des interactions moléculaires. Grâce aux algorithmes d'apprentissage profond, il devient possible de prédire des structures moléculaires, d'accélérer la découverte de nouveaux composés, et de réduire le temps et les coûts de recherche expérimentale.

Objectifs du colloque

1. Explorer les enjeux méthodologiques de l'intégration de l'intelligence artificielle dans la recherche doctorale, notamment en termes de qualité scientifique, de reproductibilité, et d'éthique.

2. Présenter et valoriser des travaux de recherche appliquant l'IA à la détection des polluants dans l'eau, en mettant en lumière les outils, les algorithmes et les résultats obtenus par des doctorants et des chercheurs.

3. Mettre en évidence les contributions de l'IA à la modélisation moléculaire, en particulier pour la prédiction de structures, la simulation d'interactions et l'accélération des découvertes scientifiques dans les disciplines de chimie et de biologie.

4. Favoriser les échanges interdisciplinaires entre doctorants, encadrants, chercheurs, ingénieurs et professionnels, afin de stimuler les synergies entre les sciences de l'environnement, les sciences moléculaires, et les sciences informatiques.

5. Identifier les défis techniques, éthiques et réglementaires liés à l'usage de l'IA dans la recherche, et proposer des pistes d'action pour assurer une utilisation responsable et durable de ces technologies.

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ENS de Meknès

REFLEXIONS SUR L'IA ET L'ENJEU DE LA QUALITE DE LA THESE DE DOCTORAT POUR LES ETUDIANTS CHERCHEURS

Pr. Moulay Brahim SEDRA

Directeur ENS de Meknès et ancien doyen de la FST d'Errachidia (Maroc).

Biographie du Professeur Moulay Brahim SEDRA

Le Professeur Moulay Brahim Sedra est une figure éminente de l'enseignement supérieur et de la recherche scientifique au Maroc. Physicien théoricien de formation, il occupe actuellement le poste de Directeur de l'Ecole Normale Supérieure de Meknès, relevant de **l'Université Moulay-Ismaïl.**

Tout au long de son parcours, le Professeur Sedra s'est illustré par une excellence académique soutenue, tant sur le plan de la recherche que de l'encadrement. Auteur de nombreuses publications scientifiques de renommée internationale en physique théorique, il a dirigé un grand nombre de thèses de doctorat, déjà soutenues ou en cours, et participe activement à la formation de chercheurs de haut niveau. Ses contributions lui ont valu plusieurs distinctions et prix internationaux. Il est également membre de l'Académie de Réflexion Stratégique de la région Drâa-Tafilalet.

Entre 1997 et 2014, il a fondé et dirigé l'un des laboratoires de recherche les plus prolifiques de la Faculté des Sciences de Kénitra, contribuant à y instaurer une dynamique de recherche interdisciplinaire, propice à l'innovation scientifique. En tant qu'expert reconnu, il est régulièrement sollicité comme évaluateur par de nombreuses revues scientifiques internationales.

Son parcours institutionnel est marqué par des responsabilités académiques majeures : il a exercé les fonctions de directeur adjoint à l'ENSA d'Al Hoceima, puis de Doyen de la Faculté des Sciences et Techniques d'Errachidia, où il a mené d'importantes réformes pour le développement de la recherche et de l'enseignement.

Par ailleurs, le Professeur Sedra s'illustre par son engagement intellectuel dans les domaines de l'épistémologie, de l'histoire et de la philosophie des sciences. Conférencier de renom, il a animé de nombreux débats et rencontres scientifiques au niveau national et international, contribuant ainsi activement à la réflexion sur le rôle des sciences dans la société contemporaine. Son travail se caractérise par une volonté constante de concilier rigueur scientifique et profondeur philosophique.

Professeur Mohamed Taib MOHTADI

l'ESEF-Berrechid

IMPACT DE L'IA SUR L'INTEGRITE ACADEMIQUE: DEFIS ET SOLUTIONS POUR GARANTIR L'AUTHENTICITE DE LA RECHERCHE DOCTORALE A L'ERE DES GENERATEURS DE CONTENU AUTOMATISES

Pr. Mohamed TAIB MOHTADI

Professeur à l'ESEF-Berrechid, Université Hassan 1er, Settat (Maroc).

Biographie du Professeur Mohamed Taib MOHTADI

Mohammed Taib MOHTADI est un expert reconnu de l'enseignement technologique et de l'innovation pédagogique au Maroc. Spécialiste en technologie éducative et enseignant chercheur passionné, il occupe actuellement le poste d'enseignant chercheur à l'École Supérieure de l'Éducation et de la Formation (ESEF) de Berrechid, relevant du ministère de l'Enseignement supérieur, de la recherche scientifique et de l'innovation.

Tout au long de sa carrière qui a commencé en 1990, M. Mohamed Taib MOHTADI s'est distingué par son engagement envers l'amélioration de l'enseignement de la technologie, de l'informatique et l'intégration des nouvelles technologies dans les pratiques pédagogiques. Titulaire d'un Doctorat en Informatique et Technologies Éducatives, il possède une expertise pointue dans le développement informatique, la robotique, l'intelligence artificielle et les systèmes d'information.

Entre 2018 et aujourd'hui, il a contribué activement à l'ESEF de Berrechid, en tant qu'enseignant chercheur, coordonnateur de la filière "Informatique pédagogique" et responsable du FabLab. Il a développé des modules de formation innovants, encadré des étudiants et promu l'utilisation des technologies éducatives.

Son parcours institutionnel est marqué par des responsabilités importantes au sein du ministère de l'Éducation Nationale, où il a supervisé les enseignants d'informatique des cycles secondaires et conduit des projets d'intégration des TICE et de la robotique dans les établissements scolaires. Il a également participé à des projets internationaux, tels que le programme Erasmus+ et le projet HEP-M avec USAID, témoignant de son ouverture à l'innovation et à la collaboration internationale.

Par ailleurs, le professeur Mohtadi s'illustre également par son engagement envers la diffusion des connaissances et la promotion de la culture scientifique et technologique. Il est l'auteur et coauteur de plusieurs manuels scolaires et parascolaires en informatique, contribuant

ainsi à améliorer l'enseignement de cette discipline. Il est également membre actif de plusieurs associations professionnelles, telles que l'Association Marocaine des Enseignants de l'Informatique et l'association "Génération AI".

Mohammed Taib MOHTADI est un professionnel passionné et compétent, doté d'une solide expérience dans l'enseignement, la recherche et l'innovation pédagogique, ce qui fait de lui un acteur clé dans le domaine de la technologie éducative au Maroc.

Professeur Abdelhakim LAHJOUJ

FS - El Jadida

APPLICATION DE MACHINE LEARNING DANS L'EVALUATION DE LA VULNERABILITE DES EAUX SOUTERRAINES A LA POLLUTION

Pr. Abdelhakim LAHJOUJ

Professeur à la Faculté des Sciences d'El Jadida, Université Chouaib Doukkali, El Jadida (Maroc).

Biographie du Professeur Abdelhakim LAHJOUJ

Professeur Abdelhakim Lahjouj est titulaire d'un doctorat en hydrogéochimie et environnement de l'Université Moulay Ismail, Faculté des Sciences. Il occupe actuellement le poste de maître de conférences au département de Géologie, Faculté des Sciences, Université Chouaib Doukkali. Ses travaux de recherche portent sur l'application de l'intelligence artificielle à la gestion des ressources en eau et à l'optimisation des pratiques agricoles pour réduire la pression anthropique sur ces ressources.

Il s'intéresse particulièrement à la simulation du transfert des polluants dans les sols et à l'application de l'intelligence artificielle dans la surveillance de la qualité de l'eau, prévision de la pollution des eaux souterraines et l'évaluation de l'impact du changement climatique. Il a participé activement à plusieurs projets de recherche nationaux, en particulier la cartographie de la fertilité des sols cultivés au Maroc. Il a également exercé la fonction d'éditeur académique pour diverses revues spécialisées et indexées dans des bases bibliographiques internationales et continue aujourd'hui d'intervenir comme relecteur auprès de plusieurs revues scientifiques.

Le professeur Lahjouj il est auteur de plusieurs articles scientifiques publiés, il co-dirige actuellement plusieurs projets de recherche portant sur la vulnérabilité spécifique des ressources en eau face à la pollution anthropique.

Professeur Samir CHTITA

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L'IA AU SERVICE DE LA MODELISATION MOLECULAIRE: NOUVELLES PERSPECTIVES EN DRUG DESIGN

Pr. Samir CHTITA

Professeur à la Faculté des Sciences Ben M'Sick, Université Hassan II, Casablanca (Maroc).

Biographie du Professeur Samir CHTITA

Professeur Samir Chtita est enseignant-chercheur au Département de Chimie de la Faculté des Sciences Ben M'Sick, Université Hassan II de Casablanca. Titulaire d'un doctorat obtenu en 2017 à l'Université Moulay Ismaïl de Meknès, il s'est spécialisé dans la modélisation des molécules organiques hétérocycliques à l'aide des méthodes QSAR/QSPR appliquées au Drug design.

Ses travaux de recherche portent principalement sur la chimie computationnelle, la modélisation moléculaire, le criblage virtuel, les relations structure-activité/propriété (SAR/QSPR), la dynamique moléculaire, les calculs DFT, ainsi que l'application de l'intelligence artificielle à la découverte de nouveaux médicaments.

Le professeur Chtita il est auteur de plus de 200 publications scientifiques dans des revues internationales de renom et participe activement à plusieurs collaborations nationales et internationales. En 2024, il a été classé parmi les 2 % des meilleurs chercheurs au monde, selon le classement de l'Université de Stanford.

COMMUNICATIONS ORALES

Hydroxyapatite from Sardine Waste for Water Purification: A Critical Review of Extraction Techniques, Artificial Intelligence Applications, and Economic Feasibility

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Abstract:

Water pollution caused by heavy metals, dyes, and emerging contaminants continues to pose serious environmental and health threats, especially in regions with limited wastewater treatment infrastructure. Hydroxyapatite (Hap), a calcium phosphate bioceramic, has emerged as a sustainable and efficient adsorbent for water purification. This review explores the potential of valorizing Moroccan sardine waste as a rich source of Hap through thermal calcination. It highlights the physicochemical properties of fish-derived Hap, its pollutant removal performance, and key extraction protocols. In addition, recent advances in the integration of artificial intelligence (AI); notably artificial neural networks (ANN) and random forest (RF) models; are discussed as innovative tools for optimizing Hap synthesis and adsorption processes. A five-year economic feasibility analysis is presented, confirming the viability of large-scale Hap production in Morocco. This multidisciplinary review underscores the potential of sardine-based Hap as a circular economy solution for sustainable water treatment.

Keywords: hydroxyapatite, sardine waste, water treatment, adsorption, artificial intelligence, circular economy, Morocco.

Artificial Intelligence-Driven Optimization of Advanced Oxidation of Ponceau S in Saline Water

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Abstract:

Advanced Oxidation Processes (AOPs) are among the most effective technologies for treating wastewater containing persistent pollutants including synthetic dyes such as Ponceau S, commonly found in textile and food industry effluents. However, their efficiency is influenced by several interdependent parameters, including oxidant dosage, pH, reaction time, and light intensity. Recent advancements in Artificial Intelligence (AI) provide powerful tools to enhance the performance, efficiency, and sustainability of AOPs. This study explores the application of AI techniques such as artificial neural networks (ANNs), support vector machines (SVMs), fuzzy logic, and reinforcement learning for process modeling, optimization, real-time control, and fault detection in AOP-based water treatment systems.

Keywords: Advanced Oxidation Processes (AOPs), Azo dyes, Wastewater Treatment, Pollutants, Artificial Intelligence (AI), Process Optimization, Predictive Modeling.

Artificial Intelligence-Driven Modeling of Magnetic Properties in AB_2X_4 - Type Compounds: From First-Principles to Predictive Design

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Abstract

AB_2X_4-type compounds, encompassing spinels and thiospinels, exhibit a wide range of magnetic phenomena due to their rich cationic distribution and complex exchange interactions. These materials are of particular interest for spintronics, magnetic storage, and sensing applications. In this study, we combine density functional theory (DFT+U) calculations with machine learning (ML) models to investigate and predict the magnetic properties of selected AB_2X_4 compounds, including ferrites and chalcogenides. Magnetic moments, and density of states are extracted from ab initio calculations and used to train ML algorithms (Random Forest and Neural Networks). The trained models enable the prediction of magnetic ordering and magnetic properties across a broader compositional space. Our AI-assisted framework accelerates the identification of promising AB_2X_4 compounds with enhanced magnetic performance, paving the way for data-driven materials discovery in magnetism.

Keywords: AB_2X_4 compounds, spinels, magnetic materials, DFT+U, exchange interaction, machine learning, data-driven materials science.

Artificial Intelligence Enhanced Heavy Metal Removal Using Calcium Phosphate in Wastewater Treatment

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Abstract:

The removal of heavy metal ions from wastewater is critical for environmental protection and human health. Calcium phosphate (CaP) has emerged as a promising adsorbent due to its ability to precipitate heavy metals as insoluble metal phosphate complexes. This study explores the integration of artificial intelligence (AI) to optimize the process of heavy metal removal using CaP, enhancing efficiency and predictive accuracy. Machine learning (ML) models, including neural networks and genetic algorithms, were employed to analyze key parameters such as pH, CaP dosage, contact time, and initial metal concentration. AI-driven predictive modeling facilitated real-time adjustments, improving adsorption capacity and reducing experimental iterations. Additionally, AI-enhanced characterization techniques, such as X-ray Photoelectron Spectroscopy (XPS), Scanning Electron Microscopy (SEM) Coupled with X-ray Energy Dispersive Spectroscopy (EDS), Inductively Coupled Plasma (ICP), Fourier Transform Infrared Spectroscopy (FT-IR) and X-ray diffraction (XRD), provided deeper insights into the mechanistic interactions between CaP and metal ions. Results indicate CaP removes >90% of metal ions (Pb^{2+}, Cd^{2+}, Ni^{2+}, Co^{2+}, Cu^{2+} and Hg^{2+}) through concurrent precipitation of insoluble $M_x(PO_4)y$ phases. The results demonstrate that AI-optimized CaP systems achieve superior heavy metal removal efficiency compared to traditional methods. This approach not only enhances wastewater treatment scalability but also reduces operational costs, offering a sustainable solution for industrial effluent management.

Keywords: Calcium phosphate, heavy metal removal, artificial intelligence, machine learning, wastewater treatment, adsorption optimization.

Machine Learning Applications for Enhancing the Efficiency of Dye-Sensitized Solar Cells (DSSC)

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Abstract:

Dye-sensitized solar cells (DSSCs) represent a promising alternative to conventional photovoltaic technologies due to their cost-effectiveness, flexibility, and ability to function under diffuse light conditions. However, optimizing their performance remains a significant challenge due to the complexity of the parameters governing their design and fabrication.

This study explores the role of machine learning (ML) in enhancing DSSC performance. ML enables a paradigm shift by overcoming the limitations of traditional experimental methods, leveraging large datasets to efficiently identify optimal combinations of materials, structures, and synthesis conditions. Algorithms such as random forests and decision trees facilitate the prediction of conversion efficiency, guide dye selection, and optimize key device parameters.

By integrating artificial intelligence into photovoltaic research, this approach accelerates the development of high-performance DSSCs, paving the way for more efficient and durable solar cells tailored to the needs of the energy transition. Our contribution underscores the synergy between ML and DSSC innovation, proposing an advanced methodology to streamline solar cell design.

Keywords: DSSC, machine learning, materials, algorithms, conversion efficiency.

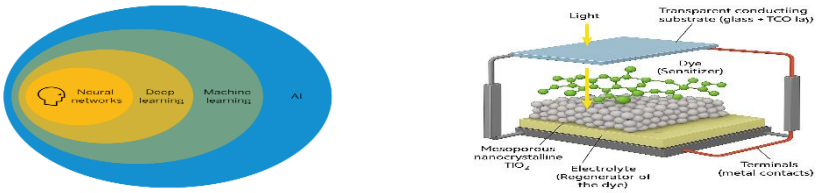

Fig. 1. (a) Basic concepts of artificial intelligence; (b) Components of the DSSC

Déchiffrer les Conformations Protéiques à l'Aide de l'Apprentissage Profond : Applications aux Protéines Kinases

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Résumé:

Le déchiffrage des conformations protéiques constitue un défi fondamental pour les protéines kinases, superfamille de plus de 500 famillles enzymes orchestrant tous les processus cellulaires. AlphaFold3, basé sur une architecture de diffusion et des transformers, représente l'état de l'art en apprentissage profond structural et un outil révolutionnaire pour décoder cette complexité conformationnelle du kinome grâce à sa capacité améliorée de modélisation des complexes multimoléculaires.

Nous avons assemblé 1024 structures cristallographiques haute résolution couvrant l'ensemble des kinases dans leurs états actif/inactif. Le dataset englobe toutes les familles du kinome (CMGC, AGC, CAMK, STE, tyrosine kinases, etc.) avec ligands physiologiques (ATP/ADP), cofacteurs (Mg^{2+}, Ca^{2+}), protéines régulatrices et modifications post-traductionnelles. L'évaluation utilise les métriques RMSD, précision des sites actifs et qualité des interfaces. AlphaFold3 démontre une capacité variable de déchiffrage conformationnel : excellente pour les domaines apo (RMSD 1,2 Å, 100% réussite), modérée pour les complexes ATP/ADP (75% du dataset, 67% précision), et limitée pour les assemblages multi-protéiques (29% du dataset, 57% réussite). La discrimination actif/inactif atteint 83% de précision, mais les états DFG-out restent problématiques (33% réussite). Cette analyse comprehensive révèle les capacités et limitations d'AlphaFold3 pour le déchiffrage du kinome. Le modèle excelle dans la prédiction des conformations canoniques mais montre des faiblesses pour les états rares et mécanismes allostériques complexes. Ces résultats établissent un benchmark robuste pour évaluer l'apprentissage profond structural et ouvrent de nouvelles perspectives pour la conception d'inhibiteurs ciblant des états conformationnels spécifiques à travers la diversité des kinases. L'approche établit un paradigme pour comprendre comment l'intelligence artificielle peut déchiffrer la complexité conformationnelle des grandes familles protéiques.

Mots-clés: Apprentissage profond; déchiffrage conformationnel; kinome; AlphaFold3; intelligence artificielle

Computational and Artificial Intelligence-Assisted Study of [3+2] Cycloaddition-Derived Compounds as Potential Antibacterial Agents: A Combined DFT, ADMET, Molecular Docking and Molecular Dynamics Approach

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Abstract:

In this study, we evaluated the antibacterial potential of compounds derived from [3+2] cycloaddition reactions using an integrated computational approach that combines physics-based methods, such as DFT, molecular docking and molecular dynamics, with artificial intelligence tools, notably the pkCSM server, which incorporates machine learning (ML) models to predict ADMET properties. The study begins with a classical analysis of reactivity using Molecular Electron Density Theory (MEDT) at the MPWB1K/6-311G(d) level. To explain the experimentally observed selectivity and solvent effects, the results reveal that the reaction follows a one-step mechanism with asynchronous bond formation. N-benzylfluoronitrone behaves as a zwitterionic species exhibiting a high activation barrier. Energy profiles show that the exo cycloadducts are favored both kinetically and thermodynamically, in agreement with the experimental findings.

The compounds derived from these reactions were studied *in silico* using molecular docking and molecular dynamics to evaluate their antimicrobial activity against the target protein from *Staphylococcus aureus* (PDB code 2X3F). The results show that all compounds exhibit stable antibacterial activity except for the product P2-2b. This stability was confirmed by analyzing the RMSD and RMSF trajectories using the molecular dynamics software GROMACS. In addition, the pharmacokinetic ADMET properties were predicted using artificial intelligence (AI) tools, notably the pkCSM server, which incorporates machine learning (ML) models. This approach enables rapid and accurate estimation of drug-like properties essential for drug development. All the studied compounds exhibit favorable pharmacokinetic and ADMET profiles, except for compound P1-2b, which shows hepatotoxicity.

From a future perspective, the integration of artificial intelligence-based approaches, such as QSAR models and deep learning algorithms applied to molecular docking, could significantly enhance the accuracy of predictions and accelerate the discovery of new bioactive molecules.

Keywords: AI-assisted Drug Discovery, Virtual Screening, Molecular Docking, Dynamics Molecular, pkCSM and Machine Learning.

A First-Principles Study of Surface Passivation Effects on the Stability, Electronic, and Optical Properties of Silicon Quantum Dots: Toward AI-Assisted Materials Design

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Abstract:

Silicon's transformation at the nanoscale reveals a departure from conventional bulk behavior, particularly through the relaxation of momentum conservation rules that enhance its optical activity. Here, we present a first-principles investigation of hydrogen-passivated zero-dimensional silicon nanostructures: $Si_{10}H_{16}$, $Si_{14}H_{20}$, $Si_{18}H_{24}$, and $Si_{22}H_{28}$ exploring how quantum confinement and surface passivation influence their thermal stability and optical response. Using time-dependent density functional theory (TD-DFT) and Car–Parrinello molecular dynamics via Quantum ESPRESSO on high-performance computing platforms, we assess their excited-state behavior and resilience to thermal fluctuations at 40 and 300 K.

Our results reveal systematic blue shifts in the absorption edge, as well as variations in dielectric properties such as permittivity, refractive index, and oscillator strength. While this study is grounded in ab-initio methods, the generated data and trends offer a valuable foundation for future integration with machine learning and deep learning models, particularly for accelerating the screening of nanostructures and predicting optoelectronic properties at scale. This work contributes to the evolving synergy between physics-based simulations and AI-driven materials discovery.

Keywords: Silicon Quantum Dots, Surface Passivation, Time-Dependent DFT, Optical Properties, AI-Assisted Materials Design

Reference

[1] A Holistic Understanding of Optical Properties in Amorphous H-Terminated Si-Nanostructures: Combining TD-DFT with AIMD - **Results in Optics** 16-100694 (2024) https://doi.org/10.1016/j.rio.2024.100694
F. Dnaya, D. Soubane, M. Bouhassoune, M. Bellioua, Y. Laaziz , A. Nafidi and T. Ozaki

Tuning Sunlight: First-Principles and Machine Learning Perspectives on TiO_2 for High-Performance Dye-Sensitized Solar Cells

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Abstract:

As a wide-bandgap semiconductor with strong UV absorption, chemical stability, and excellent charge transport at the nanoscale, titania (TiO_2) plays a central role in dye-sensitized solar cells (DSSCs). In this study, we employ density functional theory (DFT) and linear-response formalism to investigate the electronic band structure and optical response of bulk anatase and rutile TiO_2. Our results reveal distinct conduction band offsets, refractive behavior, and dielectric properties, with anatase emerging as the more favorable phase for efficient electron injection and light harvesting.

This work provides a theoretical foundation for optimizing dye selection, transparent conductive oxides (TCOs), and interfacial design. It is part of a broader multiscale project that integrates simulation and fabrication of TiO_2–TCO layers via magnetron sputtering. Looking forward, the integration of machine learning into this workflow is expected to accelerate the discovery of optimized TiO_2 modifications and support data-driven screening of nanostructures, bridging first-principles accuracy with scalable design strategies in photovoltaic research.

Keywords: Titanium Dioxide (TiO_2), Dye-Sensitized Solar Cells (DSSCs), Density Functional Theory, Optical Band Structure, Machine Learning Integration

AI for COD: resolving ambiguity between dissolved and undissolved matter in turbid matrices

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Abstract:

In the current context of environmental protection, the accuracy of water quality analyses is crucial, especially chemical oxygen demand (COD) analyses. COD is a key indicator of organic pollutants in water, and is often compromised by turbidity interference at UV wavelengths. Faced with this turbidity challenge, this innovative study proposes an integrated approach, using in situ UV sensors and advanced Chemometric techniques, exploiting the synergy between PLS (Partial Least Square) and ANN (Artificial Neural Network). The research is divided into three main sections: (i) assessment of turbidity interference, (ii) development of a turbidity prediction model and (iii) elaboration of the COD compensation and prediction model. Turbidity significantly alters the UV-Visible absorbance spectrum of COD. By analyzing mixed solutions of COD and turbidity, we quantified this interference and established a turbidity prediction model using spectral areas between 303.5 and 700 nm. Interval PLS identified the most informative spectral regions for COD concentration, highlighting the 200 to 250 nm interval. To address turbidity interference, we developed a hybrid model combining PLS and ANN regression, and turbidity measurements are incorporated as an explanatory term in the model. This hybrid approach relies on in situ UV sensors to directly capture UV absorbance data in the field and applies robust chemometric models to accurately distinguish the UV absorbance contributions of organic compounds and turbidity. The method not only compensates for the interfering effect of turbidity, but also allows turbidity information to be used to refine COD predictions. Model performance, evaluated using R^2, RMSE, and MAE, showed a significant increase in R^2 to 0.9972, and decreases in RMSE to 0.94 and MAE to 0.64, demonstrating the method's effectiveness in correcting turbidity-induced deviations and improving COD prediction accuracy. The results of the evaluation on real data show high performance metrics, with recovery percentages close to 100% and low RMSE and MAE values, indicating the model's robust ability to predict COD in the presence of suspended particles.

Keywords: Chemometric, COD (Chemical Oxygen Demand), Turbidity compensation, In-situ UV sensors, Partial Least Squares (PLS), Artificial Neural Networks (ANN).

Artificial Intelligence in Wastewater Treatment: A Bibliometric Analysis of Emerging Trends

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Abstract:

In a context marked by increasing water scarcity and the need to preserve aquatic ecosystems, wastewater treatment has become a strategic priority. Artificial Intelligence (AI) is emerging as an innovative tool to enhance process performance, predict pollutant behavior, and support decision-making.

This study, based on a bibliometric analysis, traces the evolution of research on the integration of AI in wastewater treatment. It identifies key trends, leading contributors, and dominant research directions.

The findings reveal that AI is primarily used to assess pollutant removal efficiency, optimize process models and operational parameters, and control membrane fouling. Future research should further explore the removal of organic compounds and emerging contaminants, as well as microbial dynamics and multi-objective optimization.

Promising avenues also include water quality prediction, synergies with other information technologies, and image analysis applied to wastewater treatment.

Keywords: Artificial intelligence, Bibliometric analysis, biblioshiny, Wastewater treatment.

Hybrid QSPR–DNN Framework for Photovoltaic Efficiency Prediction in Organic Semiconductors

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Abstract:

The increasing global demand for renewable energy has intensified research into alternative photovoltaic technologies. Organic solar cells (OSCs) have emerged as promising candidates due to their inherent advantages, including mechanical flexibility, lightweight construction, and potential for low-cost manufacturing. Recent progress in molecular design and synthesis has significantly improved power conversion efficiencies (PCEs), particularly in bulk heterojunction architectures that leverage optimized donor–acceptor interfaces for efficient exciton dissociation and charge transport. Despite these advancements, issues related to long-term stability and the slow pace of high-throughput materials discovery continue to impede large-scale commercialization. Conventional computational approaches such as density functional theory (DFT) and time-dependent DFT (TD-DFT) offer high accuracy but are computationally prohibitive for large molecular libraries. To address this limitation, we employed three machine learning models feedforward neural networks (FNN), one-dimensional convolutional neural networks (1D-CNN), and random forest (RF) as predictive tools for OSC performance. Molecular fingerprints of small-molecule donors were used as input descriptors to capture relevant structural features influencing PCE. This data-driven framework enables rapid and cost-effective screening of candidate materials, offering a scalable approach to accelerate the discovery and optimization of efficient organic photovoltaic systems.

Keywords: QSPR, Machine Learning, OSC, DFT, PCE.

Surveying Novel Pyrazine Acceptor Materials for Bulk Heterojunction Solar Cells: Computational Insights using AI and deep learning to study Photovoltaic Performance

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Abstract:

The design of organic electron acceptor materials is fundamental to advancing bulk heterojunction solar cells with outstanding photovoltaic performance. Among these, pyrazine-based π-conjugated electron acceptors have shown significant improvements over conventional acceptor materials, offering enhanced optoelectronic suitability, cost-effectiveness, and stability. In this comprehensive theoretical study, we investigate the potential of novel pyrazine derivatives (C1–C5) as acceptor materials in heterojunction solar cells. Time-dependent DFT (TD-DFT) were employed to analyze key electronic properties, including frontier molecular orbitals, density of states, reorganization energies, molecular electrostatic potential, and global reactivity descriptors.

To further enhance prediction accuracy and accelerate material screening, artificial intelligence (AI) and deep learning models were integrated into the analysis pipeline. These models enabled efficient pattern recognition and property prediction based on computed molecular descriptors. The study also explores how variations in acceptor terminal groups influence the electronic and photovoltaic performance of the designed compounds. Results indicate that C1–C5 derivatives exhibit excellent optical properties, low bandgaps, optimal open-circuit voltages, and energy level alignment with the PTB7-Th donor polymer. This AI-assisted approach demonstrates the power of combining quantum chemistry and machine learning in the rational design of next-generation solar cell materials.

Keywords: TD-DFT, Artificial Intelligence, deep learning, Acceptor materials, PTB7-Th.

Molecular Engineering of Organic Dyes for DSSCs: DFT/TD-DFT Insights and the Promising Role of Artificial Intelligence in Enhancing Photovoltaic Performance

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Abstract:

This research investigates the computational design and analysis of innovative organic electron-donor dyes for dye-sensitized solar cells (DSSCs), utilizing density functional theory DFT and TD-DFT time-dependent DFT with the B3LYP functional. In recent years, the increasing power of computational resources has driven the broader adoption of artificial intelligence (AI) in various sectors of photovoltaic PV systems, accelerating the pace of innovation and discovery.

In this work, we examined the structural, electronic, optical, and photovoltaic properties of newly synthesized dyes (MC28, MC20, MZ173, MZ175, MK162). Our analysis included key parameters such as reorganization energy, global reactivity descriptors, density of states, molecular electrostatic potential (MEP), charge mobility, and nonlinear optical (NLO) properties. Molecular modeling enabled us to identify promising dye candidates and optimize their interaction with other DSSC components, including semiconductors and electrolytes.

Machine learning approaches, as a growing branch of AI, were employed to enhance the selection of critical parameters and guide the cell design process. The results demonstrate that these designed molecules possess low band gaps, favorable optical properties, and strong photovoltaic potential, paving the way for the development of high-efficiency DSSCs while reducing the need for extensive laboratory experimentation. [1]

Keywords: TD-DFT, Artificial Intelligence, Non-linear Optical Properties (NLO), Dye-Sensitized Solar Cells.

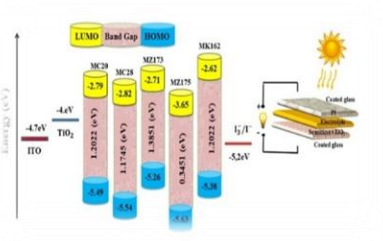

Fig.1. Energy level of the studied compounds

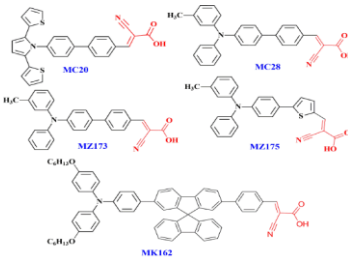

Fig.2. Molecular structure design (MC28, MC20, MZ173, MZ175 and MK162)

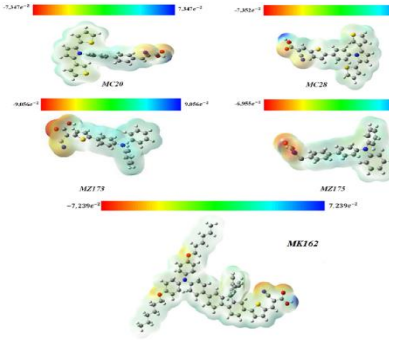

Fig.3. MEP surface of engineered compounds

Enhancing Organic Photovoltaic Cells: Quinoxaline-Based Small Molecule Acceptors andthe Role of AI and Deep Learning in Performance Optimization and Innovation

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Abstract:

In this investigation, we combine advanced quantum modeling methods, including time-dependent density functional theory (TD-DFT), with artificial intelligence (AI) and deep learning approaches to explore and optimize the structural, optical, electronic, and photovoltaic properties of eight thiophene-based π-conjugated organic molecules. This integrated approach aims to establish precise correlations between the chemical structure of these compounds and their optoelectronic performance. The results reveal that the studied molecules exhibit a low band gap, an appropriate open-circuit voltage (V_{OC}), and favorable energy level alignment with the donor material key features for their effective integration into organic bulk heterojunction photovoltaic cells. The use of artificial intelligence (AI) is increasing in various areas of photovoltaic (PV) systems, due to the increase in computing power, tools and data generation. This synergy between AI and quantum modeling significantly improves the reliability of the results, reduces experimental uncertainties, and opens new avenues for the streamlined design of innovative, high performance, and sustainable photovoltaic materials.

Keywords: TD-DFT, Artificial Intelligence, Acceptor materials, PTB7-Th.

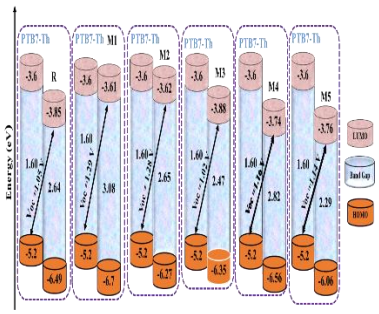

Fig.1. Voc variation of all engineered using PTB7-Th as a donor.

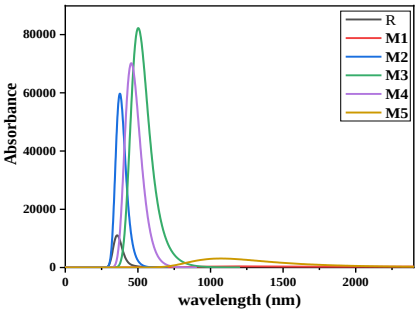

Fig.2. Computational UV-Visible spectra of developed compounds (R, M1-M5).

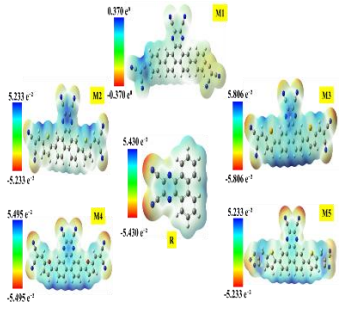

Fig.3. MEP surface of engineered compounds (R and M1-M5).

Comparative Study of Multiclass Brain Tumor Classification Using Efficientnet Architectures

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Abstract:

Brain tumors are one of the most serious health challenges worldwide and one of the leading causes of death. Early detection is crucial to improve survival rates. However, even with high-quality brain imaging techniques, obtaining reliable and accurate results remains a major challenge. The diagnosis of brain tumors is often a lengthy process that depends largely on the expertise and experience of radiologists. Artificial Intelligence (AI), particularly Deep Learning (DL), plays a growing role in medical diagnosis through medical imaging and to improve the efficiency of brain tumor diagnosis. This study focuses on the classification of the three most common types of brain tumors: meningiomas, gliomas, pituitary tumors, and benign tumors. We preprocessed the data, including resizing the images, standardizing pixels, and applying augmentation to the training data to increase diversity and limit overfitting. We then trained different types of EfficientNet architectures and compared their performance. EfficientNetB03 achieved an optimal performance of 98%, demonstrating its effectiveness in detecting and classifying brain tumors.

Keywords: Deep learning, EffiecientNet, Convolutional neural network, Image classification, Brain tumor.

Lewis Acid-Catalyzed Cycloaddition Reactions: DFT, Docking, and ADMET Study with future perspective on AI including Machine Learning, and Deep Learning.

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Abstract:

The [4+2] cycloaddition reaction between cyclopenta-1,3-diene and fluorescent enones was investigated using a theoretical framework based on Molecular Electron Density Theory (MEDT). Calculations were performed for both uncatalyzed and BF_3-catalyzed pathways to explore the influence of Lewis acid catalysis on reactivity and selectivity. The results indicate that product distribution is highly dependent on the reaction conditions: in the absence of BF_3, the formation of product P-2 is preferred, whereas the presence of the Lewis acid shifts selectivity toward product P-1. Topological analyses using the Electron Localization Function (ELF) and Bonding Evolution Theory (BET) revealed that both cycloaddition pathways proceed through a non-concerted and asynchronous mechanism.

To evaluate the pharmacological potential of the synthesized compounds, molecular docking simulations were carried out. The results showed that the introduction of a CF_3 group significantly increases the binding affinity of both P-1 and P-2 to viral proteins. Complementary ADMET analysis demonstrated favorable pharmacokinetic properties.

As a future perspective, the integration of artificial intelligence (AI), machine learning (ML), and deep learning (DL) techniques into DFT modeling, molecular docking, and ADMET prediction is anticipated to enhance accuracy, reduce computational cost, and accelerate the discovery of biologically active compounds.

Keywords: MEDT, Stereoselective, catalyst (BF_3), CF_3 group, ELF, BET

Computational Study of Triazole Derivatives Against Pseudomonas aeruginosa: Molecular Docking, DFT, and ADMET Analysis with Future Outlook on AI, Machine Learning, and Deep Learning Applications

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Abstract:

Pseudomonas aeruginosa is a notoriously resistant pathogen, largely due to its ability to form protective biofilms, making the search for new antibacterial compounds more urgent than ever. In this work, we investigated 21 triazole-based molecules using a computational approach combining molecular docking, pharmacokinetic (ADMET) analysis, and Density Functional Theory (DFT) calculations.

Molecular docking studies targeting the quorum-sensing regulator lasR identified compounds G, N, and U as having strong binding affinities. Among them, compound N emerged as the most promising, showing stable interactions with the active site. ADMET screening further supported its drug-like profile, with favorable absorption, low toxicity, and compliance with Lipinski's rule of five.

To better understand the compound's chemical behavior, we performed DFT calculations focusing on frontier molecular orbitals (HOMO and LUMO) and the energy gap, highlighting good electronic stability and potential biological activity.

Although classical computational methods were employed in this study, the future integration of artificial intelligence (AI), machine learning (ML), and deep learning (DL) techniques into molecular modeling, and virtual screening is expected to improve prediction accuracy and accelerate the discovery of novel antimicrobial agents.

This work lays a strong computational foundation for applying AI-assisted approaches in the rational design of bioactive molecules targeting *Pseudomonas aeruginosa*. It highlights the promising role of in silico methods in modern drug discovery and encourages further development of intelligent, data-driven strategies to fight bacterial resistance.

Keywords: AI, Antibiofilm, LasR, Molecular Docking, ADMET, DFT.

Entre Assistance et Autonomie : le Doctorant Face à l'IA

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Abstract:

À l'ère de l'intelligence artificielle, la posture traditionnelle du doctorant, fondée sur l'autonomie, la rigueur méthodologique et l'originalité intellectuelle, se trouve profondément transformée. Ce travail interroge comment l'IA redéfinit le rôle, les compétences et les responsabilités du chercheur doctorant, en remettant en question les frontières entre pensée humaine et traitement algorithmique.

L'étude vise à analyser les usages croissants de l'IA dans les différentes étapes du processus doctoral — de la formulation des problématiques à la rédaction — et à identifier les changements qu'ils induisent dans la manière de « faire de la recherche ». Elle explore également les tensions émergentes entre assistance technologique et autonomie scientifique, ainsi que les risques de dépendance, de dilution de l'effort intellectuel ou de perte de créativité.

Sur le plan méthodologique, une enquête qualitative auprès de doctorants et une analyse réflexive permettront d'examiner les postures adoptées face à ces outils. L'objectif est de proposer une typologie des rôles du chercheur à l'ère de l'IA (utilisateur, superviseur, co-créateur) et d'esquisser un cadre de formation éthique et méthodologique adapté aux nouvelles réalités académiques.

En définitive, ce travail propose une réflexion critique sur les mutations de la recherche doctorale et la nécessité de repenser la formation des jeunes chercheurs dans un contexte où l'intelligence humaine et artificielle coexistent et interagissent. Loin d'opposer technologie et pensée critique, il s'agit de réaffirmer la centralité du chercheur dans une recherche augmentée, mais responsable.

Mots-clés : Intelligence artificielle, Posture du chercheur, Autonomie scientifique, Éthique de la recherche, Humanités numériques, Repenser la formation doctorale.

Teaching Chemistry in the Era of Generative AI

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Abstract:

Chemistry occupies a central position in educational curricula, yet its instruction faces persistent pedagogical challenges stemming from the complexity of its multiple representational levels (macroscopic, sub-microscopic, and symbolic), the abstract nature of chemical phenomena, and the prevalence of alternative conceptions among learners. Addressing these challenges calls for innovative teaching approaches.

Science education, and chemistry in particular, is undergoing a profound transformation with the advent of generative artificial intelligence (Gen AI). This technology is opening up new prospects for teaching and learning through personalized content, adaptive conceptual explanations, and intelligent tutoring systems. Practical applications already include automated creation of tailored exercises, the generation of interactive molecular visualizations, and the development of personalized assessment tools.

Nevertheless, integrating such technologies raises important ethical concerns related to educational relevance, technological dependence, and equitable access to digital resources. The pedagogical effectiveness of these innovations remains under investigation through ongoing empirical studies, highlighting the need for regulatory frameworks and best-practice guidelines that optimize their use while safeguarding academic integrity and the quality of chemistry teaching and learning.

Keywords: Chemistry education, Teaching; Learning, Generative artificial intelligence, Educational technologies, Pedagogical effectiveness.

Optical and Electronic Characterization of TiO_2 to Dye Interfaces Using TD-DFT and Artificial Intelligence

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Abstract:

Dye-sensitized solar cells (DSSCs) represent a promising technology for clean energy production, combining efficiency, low cost and respect for the environment. They are based on an architecture with three functional layers: a working electrode composed of a mesoporous nanocrystalline semiconductor with a wide band gap - most often titanium dioxide (TiO_2) - sensitized by an absorbing dye in the visible range; a platinized counter-electrode ensuring electron recovery; and a redox electrolyte facilitating charge transfer between the two electrodes. TiO_2 is establishing itself as a reference material thanks to its excellent optoelectronic properties, particularly suited to photovoltaic conversion.

In this work, the optical and electronic properties of the dyes will be analyzed using quantum chemical methods, including DFT and TD-DFT, to model their behavior when adsorbed onto the TiO_2 surface. Different exchange-correlation functions will be evaluated to ensure reliable predictions. In addition, artificial intelligence techniques (IA) will be exploited to optimize interpretation of theoretical data, facilitate exploration of molecular structure space, and establish non-linear correlations between structural, electronic parameters and photovoltaic performance. This integrated approach is designed to enhance predictive accuracy and accelerate the design process for new high-performance dyes (Table 1).

Keywords: TD-DFT, Organic dyes, Photovoltaic, Artificial intelligence, DSCs.

Table 1. Charge transport rates and transfer of charge integrals and carrier mobility were calculated for all dye at B3LYP/6-31G(d,p).

Dye	$\lambda_{electonl}$(eV)	λ_{hol}(eV)	t_{hol}(eV)	$t_{electonl}$(eV)	k_{CT}^{elec} (s^{-1})	k_{CT}^{hol} (s^{-1})	$\mu_{electron}$ (cm^2/Vs)	μ_{hole} (cm^2/Vs)
C1	0.4578	0.1083	0.4040	0.3566	$3.243.10^{15}$	$8.636.10^{15}$	2.51×10^{-3}	6.69×10^{-3}
C2	0.3532	0.1981	0.2357	0.0409	$4.857.10^{13}$	$2.153.10^{15}$	3.76×10^{-5}	1.67×10^{-3}
C3	0.3187	0.2010	0.2621	0.2808	$2.410.10^{15}$	$2.644.10^{15}$	1.87×10^{-3}	2.05×10^{-3}
C4	0.3981	0.1811	0.8010	0.1623	$7.204.10^{14}$	$2.601.10^{16}$	5.58×10^{-4}	2.02×10^{-2}

Study of Lithium-Ion Intercalation and Deintercalation into $FePO_4$ Using Electrochemical Techniques

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Abstract:

Iron phosphate ($FePO_4$) is a promising, non-toxic, and earth-abundant material composed of naturally available elements such as iron and phosphate. Its simple structure and ease of synthesis make it attractive for various applications, especially in energy storage. $FePO_4$ is used directly as a cathode material and serves as a precursor for synthesizing $LiFePO_4$ and $NaFePO_4$, which are widely employed in lithium-ion and sodium-ion batteries due to their excellent stability and safety.

In this work, $FePO_4$ is investigated as a cathode material for lithium-ion batteries using simple yet effective electrochemical techniques, including cyclic voltammetry (CV), electrochemical impedance spectroscopy (EIS), and galvanostatic charge-discharge (GCD). These accessible methods provide valuable insights into the intercalation and deintercalation of lithium ions through reversible Fe^{3+}/Fe^{2+} redox reactions. They also enable the determination of key parameters, such as lithium-ion diffusion coefficients and charge-discharge capacity. Despite their simplicity, these techniques effectively characterize electrochemical behavior of the material, offering a deeper understanding of the underlying kinetics and transport mechanisms. The study confirms the potential of $FePO_4$ as an efficient cathode material for aqueous lithium-ion energy storage systems.

To further enhance the analysis, artificial intelligence (AI) was integrated into the data interpretation process. This integration accelerates the interpretation of complex electrochemical data, minimizes experimental time, and significantly improves the quality and reliability of the research outcomes.

Keywords: Iron phosphate, lithium-ion batteries, Electrochemical techniques, intercalation, Cathode material.

In Silico Design Of Pyridones Derivatives As Alpha-Glucosidase Inhibitors: A Qsar Study, Molecular Docking, Admet, And Molecular Dynamics Approach

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Abstract:

Alpha-glucosidase inhibitors are essential for managing type 2 diabetes by delaying carbohydrate absorption and controlling postprandial blood glucose levels. This study investigates 3-amino-2,4-diarylbenzo[4,5]imidazo[1,2-α]pyrimidine derivatives as potential alpha-glucosidase inhibitors using an in silico approach. The studied compounds with their values of IC50 against alpha glucosidase were retrieved from previous paper (Peytam et al. 2021). The objectives are to (1) develop a predictive QSAR model, (2) validate the model through statistical metrics, and (3) evaluate the binding affinity, pharmacokinetics, and stability of proposed compounds via molecular docking, ADMET analysis, and molecular dynamics simulations. By leveraging computational tools, the study aims to optimize these derivatives as promising therapeutic agents for type 2 diabetes. Approximately 400 molecular descriptors were computed using DataWarrior, PaDEL, and Gaussian. Principal Component Analysis was applied for dimensionality reduction, and a Multiple Linear Regression (MLR) model was developed to predict bioactivity. The model underwent rigorous validation, and five novel compounds were proposed for further investigation. Molecular docking studies revealed promising binding interactions with alpha-glucosidase, while ADMET analysis indicated favorable pharmacokinetic profiles. Molecular dynamics simulations confirmed the stability of the enzyme-inhibitor complexes. The MLR model demonstrated high predictive accuracy, with proposed compounds exhibiting pIC50 values higher than the most active molecule in the series. This study identifies five promising alpha-glucosidase inhibitors, offering a robust in silico framework for the design of therapeutic agents targeting alpha-glucosidase in type 2 diabetes.

Keywords: Alpha-glucosidase inhibitors, 3-amino-2,4-diarylbenzo[4,5]imidazo[1,2-α]pyrimidine, QSAR, Molecular Docking, ADMET, Molecular Dynamics.

Phytochemical-Based Modulation Of IL-4Rα For Developing Plant-Derived Therapeutics Against Eczema: Insights From In Silico Screening, ADMET Profiling And Molecular Dynamics

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Abstract :

Eczema, a chronic inflammatory skin disorder, affects a significant portion of the global population, leading to itching, redness, and skin damage. This study investigates the potential of 39 phytochemicals derived from Atractylis cancellata, Helianthemum sessiliflorum, and Euphorbia guyoniana as IL-4Rα modulators for the development of plant-derived therapeutics against eczema. Using advanced molecular docking and molecular dynamics simulations, we evaluated the binding affinity, stability, and potential efficacy of these compounds in targeting IL-4Rα. Our results demonstrate that 10 compounds show strong binding affinity, with values ranging from -12.421 kcal/mol to -8.157 kcal/mol. Among these, Isoolivil and Catechin stood out as particularly promising compounds. Both demonstrated favorable ADMET properties for topical administration, suggesting minimal irritation and optimal skin penetration. In terms of stability, both compounds exhibited RMSD fluctuations below 2 Å during 100 ns molecular dynamics simulations, indicating stable and effective binding to IL-4Rα. The study also highlights the anti-inflammatory and immunomodulatory properties of these compounds, suggesting their potential use in topical therapeutic formulations for eczema treatment. These findings provide a foundation for further experimental studies and the development of novel, plant-derived therapies for inflammatory skin diseases.

Keywords: Eczema, IL-4Rα, Molecular docking, Molecular dynamics, ADMET, Phytochemicals.

Modélisation Numérique 3D du Flambement de Poteaux en Acier Corrodés : Vers une Prédiction Assistée par Intelligence Artificielle

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Résumé :

Les poteaux en acier jouent un rôle fondamental dans la stabilité des structures métalliques. Cependant, une exposition prolongée à des environnements agressifs peut entraîner l'apparition de corrosion, en particulier dans les zones critiques. Cette dégradation altère significativement la capacité portante des poteaux, augmentant le risque d'instabilité structurelle. Dans ce contexte, la présente étude propose un modèle numérique tridimensionnel développé pour évaluer l'impact de la corrosion sur la résistance au flambement des poteaux en acier S235. L'approche adoptée se concentre sur les effets géométriques locaux, tels que les trous des platines, susceptibles d'amplifier les phénomènes de perte de stabilité. Afin de reproduire fidèlement les mécanismes de déformation sous charges critiques, un comportement élastoplastique du matériau a été intégré dans ce modèle.

Les simulations numériques effectuées ont permis de constater une réduction notable de la résistance au flambement en présence de corrosion, comparativement à des poteaux intacts. Cette perte de performance est principalement attribuée à l'augmentation des concentrations de contraintes et à l'apparition de déformations plastiques dans les zones endommagées. L'intégration de la corrosion et du comportement non linéaire du matériau s'avère donc indispensable pour des prédictions fiables de la sécurité des structures métalliques.

En perspective, cette étude ouvre la voie à l'intégration de l'intelligence artificielle, notamment des techniques d'apprentissage automatique en vue de faciliter l'identification des zones critiques, anticiper les évolutions de l'endommagement et optimiser les modèles numériques existants. Cela représente une approche prometteuse pour améliorer la maintenance prédictive et la durabilité des structures exposées à des environnements agressifs.

Mots clés : Corrosion, Flambement, Simulation numérique, Poteaux en acier, Intelligence artificielle, Apprentissage automatique.

Synthèse de Nouvelles Molécules Hybrides Dérivées de la Quinazolin-4-One et Evaluation de Leurs Propriétés Antibactériennes, Etudes in Vitro et in Silico

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Abstract:

Les quinazolin-4-ones constituent une classe de composés hétérocycliques d'un grand intérêt en raison de leur large éventail d'activités biologiques, telles que les propriétés antifongiques [1], antivirales [2], antibactériennes [3], antioxydantes [4] et anticancéreuses [5], etc. Dans le cadre de cette étude, nous avons entrepris la synthèse de nouveaux hybrides quinazolin-4-one-acétamide, en associant deux pharmacophores bioactifs au moyen d'une réaction de N-alkylation. Les structures des composés obtenus ont été confirmées par les techniques spectroscopiques IR, RMN et HRMS. Les molécules synthétisées ont ensuite été évaluées in vitro contre cinq souches bactériennes pathogènes : Escherichia coli, Pseudomonas aeruginosa, Staphylococcus aureus, Salmonella enterica et Bacillus subtilis. Les composés ayant montré une activité antibactérienne prometteuse ont été soumis à des analyses in silico ciblant des protéines spécifiques à chaque souche bactérienne.

Keywords: quinazolin-4(3H)-one; N-alkylation; activité biologique; tests in vitro; docking moléculaire; simulation dynamique.

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Etude des Propriétés Antioxydantes de l'Urée, du Thiourée et De Certains de Leurs Dérivées : Analyse par Machine Learning

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Résumé

L'urée est un composé organique de formule chimique CO(NH2)2. Elle est similaire à la thiourée de formule SC(NH2)2, sauf que 1'atome d'oxygène est remplacé par un atome de soufre [1]. Il a été démontré que l'urée et le thiourée, possèdent des dérivées tels que : EnolUrée, 1'HydroxyUrée, HydroxyThiourée, EnolThiourée [2].

En effet, depuis la découverte de ces différents composés, des résultats des tests in vitro ont montré la capacité de chacun d'eux à participer à la défense antioxydante de 1'organisme par piégeage des radicaux libres. Ces derniers étant responsables des maladies dégénératives chez l'Homme [3]. Toute fois très peu de littératures ont été consacrées à l'étude théorique et à la comparaison des pouvoirs antioxydants de chacun des composés [4].

Dans les présents travaux, une étude comparative des propriétés antioxydantes de l'urée, de la thiourée et de certains de leurs dérivées a été réalisée par la méthode M06-2X/6-311++G (d, p) de la DFT.

Les résultats des différents calculs ont permis de :

- Dégager la thiourée comme la plus antioxydante d'entre les molécules,
- Constater que le mécanisme passant par l'élimination d'hydrogène atomique par rupture homolytique de liaison comme le plus probable pour le piégeage d'un radical par chacune des molécules.

En perspective, nous pensons intégrer des techniques d'intelligence artificielle dans la modélisation DFT et la prédiction ADMET afin réduire les coûts de calcul et accélérer la découverte de composés biologiquement actif

Mots clés: DFT, antioxydant, urée, ADMET. Machine learning

Exploring Of Novel Thymol-Based Amino-Thiazole Hybrids: Computational Evaluation Of Anticancer Activity

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Abstract:

Angiogenesis is a crucial process in the growth and proliferation of cancer, enabling tumor growth through the formation of new vasculature and the supply of nutrients and oxygen to growing malignant cells. This disease-promoting process can be targeted through the inhibition of tyrosine kinase enzymes. This study is designed to assess the anticancer potential of innovative amino-thiazole-based thymol derivatives using advanced computational methods. To achieve this, we utilized density functional theory (DFT) with the DFT/B3LYP/6-31G(d,p) basis set. This approach enabled us to effectively model and analyze various aspects of the compounds, including their molecular structures, reactivity patterns, stability, and key quantum chemical properties. The compound 5a exhibits a relatively high energy gap value of 3.886 eV, indicating significant stability and low chemical reactivity. A pivotal aspect of this investigation was the in-silico exploration of the biological properties of these compounds. Molecular docking studies shed light on their interaction profiles with crucial tyrosine kinase targets such as EGFR, VEGFR, PDGFR, and FGFR. Notably, the findings from molecular docking and subsequent molecular dynamics simulations underscored the potent anticancer activity of compounds 5b and 5d with values of -8.9 and -9.3 kcal/mol against EGFR and PDGFR, respectively. Encouragingly, predictions concerning ADMET properties revealed favorable compliance with Lipinski's rules and promising oral bioavailability for these compounds. As a future perspective, the integration of artificial intelligence (AI) tools such as machine learning-based predictive models could further accelerate the design and optimization of novel tyrosine kinase inhibitors.

Keywords: Angiogenesis; EGFR; VEGFR; PDGFR; FGFR; Computational methods.

Theoretical Study On The Interactions Of Pyrazoline Compounds With COVID-19 (Mpro) Master RNA

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Abstract

The regio-, stereo- and chemo-selectivity of the 1,3-dipolar cycloaddition reactions of nitrilimine with pyridazine-3(2H)-ones 1-2 were investigated by the DFT/B3LYP/6-31g(d) method, the study we developed shows that the theoretical approach is an efficient tool for the study of the selectivity (regio/chemio/stereo) of the 1,3-dipolar cycloaddition reactions and our study confirms correctly the experimental results. The direction of electron flow (charge transfer) was determined by natural population analysis (NPA) at the TSs.

The theoretical approach, described in this work, allowed us to propose the reaction mechanism of cycloaddition reactions; a study using other dipoles and dipolarophiles of the pyridazine family will be the subject of future publications.

Molecular interaction analysis of the inhibitors revealed that the six co-crystallized ligands; form very interesting H-bonds with protein donors of SARS-CoV-2. For the prediction of the interaction mode of ligands, the relative binding free energies would be sufficient (-10.6, -10.1, -10.0, -9.6, -9.3Kcal/mol). Indeed, it would also make it possible to classify by affinities of different ligands.

Keywords: pyridazine, nitrilimine, Cycloaddition, DFT, Docking.

Artificial Intelligence-Enhanced Prediction and Modeling of Magnetic Properties in Spinel Compounds

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Abstract

AB_2X_4 spinel compounds, known for their structural versatility and intricate magnetic interactions, are key materials for emerging technologies such as spintronics, magnetic sensors, and data storage devices. In this work, we apply artificial intelligence techniques to predict their physical and magnetic properties using models trained on curated materials databases. The approach relies on extracting relevant chemical and structural features to train machine learning algorithms, including Random Forests and Neural Networks, which can then generalize across a broad compositional landscape. This strategy significantly reduces the time and resources needed to screen new candidates, offering a powerful tool for the targeted discovery of spinel materials with optimized magnetic performance.

Keywords: Spinel compounds, AB_2X_4 structure, magnetic property prediction, machine learning, artificial intelligence, materials design.

Artificial Intelligence Enhanced Study of Artemisia herba alba Oil as a Sustainable Inhibitor for Mild Steel: characterization, electrochemical and surface analysis

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Abstract

This study explores the corrosion inhibition potential of Artemisia herba alba essential oil on mild steel in 1 M hydrochloric acid, combining experimental characterization with computational analysis. The oil was extracted via hydrodistillation, and its chemical composition was identified using GC-FID and GC-MS, revealing key constituents such as 1,8-cineole, camphor, α-pinene, and camphene. Electrochemical methods—including weight loss measurements, potentiodynamic polarization, and electrochemical impedance spectroscopy—along with SEM surface imaging, confirmed the effective protective behavior of AHAO on steel surfaces.

Looking toward future developments, this work highlights the transformative potential of Artificial Intelligence (AI) in corrosion science. By training machine learning models on experimental results and molecular descriptors, AI can predict inhibitor performance under varying environmental and compositional conditions. This approach promises to significantly reduce experimental burden while accelerating the identification of efficient, eco-friendly corrosion inhibitors.

Further integration of AI with quantum chemical tools such as Frontier Molecular Orbital (FMO) analysis offers a powerful framework for multiscale modeling, enabling deeper insights into adsorption mechanisms and molecular reactivity. This case study underscores the synergy between natural compounds and intelligent computational methods, paving the way for a sustainable, AI-assisted future in corrosion protection research.

Keywords: Artificial Intelligence; Artemisia Herba-alba; mild steel; corrosion inhibition; HCl 1M; density functional theory; frontier molecular orbitals.

COMMUNICATIONS PAR AFFICHE

Advancing Dye-Sensitized Solar Cells: The Role of Nanoarchitectures and Machine Learning in Photoanode Optimization

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Abstract:

Dye-sensitized solar cells (DSSCs) represent a promising alternative to conventional photovoltaic technologies, particularly for powering portable devices in indoor environments. Their efficiency largely depends on the performance of photoanodes, especially those based on metal oxides such as TiO_2 and ZnO.

This study examines the influence of material composition and morphology, with a particular focus on anatase TiO_2, renowned for its stability and high dye adsorption capacity. Advances in nanoarchitectures, such as nanotubes, mesoporous structures, and nanorods; along with theoretical tools like density functional theory (DFT) enable the optimization of structural and electronic properties.

Moreover, the integration of machine learning plays a key role in photoanode design. By leveraging experimental and simulated datasets, artificial intelligence facilitates the prediction of optimal structures, guides material selection, and significantly reduces development time and costs. These advancements pave the way for more efficient, scalable DSSCs tailored to market demands.

Keywords: DSSC, DFT, machine learning, TiO_2, anatse, mesoporous.

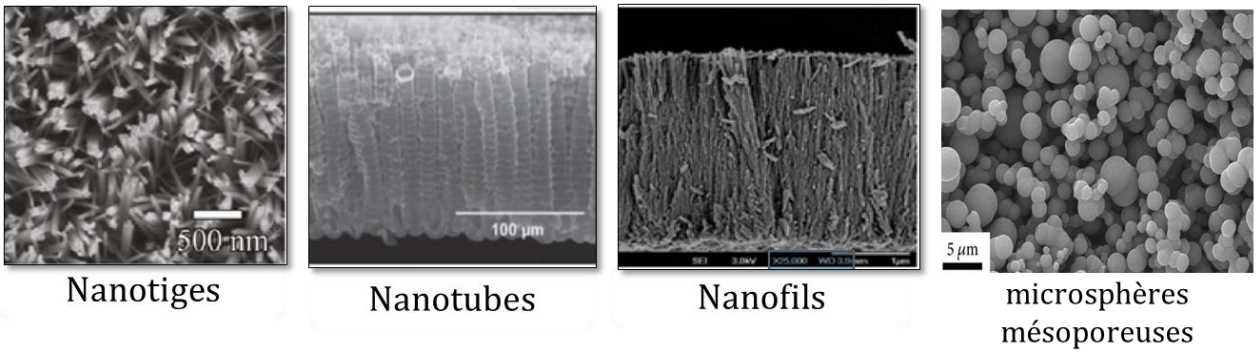

Fig. 1. Different Types of TiO_2 Nanostructures

Quantum Confinement in Silicon Quantum Dots: DFT Insights into Electronic Structure and Emerging Data-Driven Approaches

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Abstract:

The quantum confinement effect in silicon quantum dots (SiQDs) offers a pathway to tailor their electronic and optical properties, yet its microscopic origins remain incompletely understood. In this study, we employ advanced first-principles simulations to investigate size-dependent modulations in the band structure, density of states, and dielectric response of SiQDs ranging from 1 to 5 nm. Our analysis, based on hybrid DFT and quasiparticle corrections, reveals how spatial confinement induces discrete energy levels, exciton localization, and a transition from bulk-like to quantum-dominated behavior.

These results offer quantitative insight into the tunability of SiQDs for integration into photonic and photovoltaic technologies. Looking ahead, the combination of ab initio data with emerging machine learning approaches presents a promising strategy for mapping the broader design space of nanostructures, enabling rapid screening of size, shape, and surface chemistries beyond the reach of conventional simulations alone.

Keywords: Quantum Confinement, Silicon Nanostructures, Hybrid DFT, Exciton Localization, Data-Driven Materials Discovery

Applications of Artificial Intelligence to Water Quality Assessment and Prediction: A Bibliometric Analysis

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Abstract:

Water resources have been confronted with pollutants in several regions worldwide, making serious threats to global water security. Accurate monitoring and prediction of water quality are of great importance for identifying its major influencing factors. Numerous artificial intelligence (IA) algorithms have been used in recent years to monitor and predict water quality. These algorithms can, in fact, effectively handle non-linear relationships between water quality and influencing factors, providing further insights into water resource management. In this context, a bibliometric analysis of 1247 research articles on the applications of AI algorithms to water quality monitoring and prediction was conducted in this study. These articles were published over the 2019-2025 period in peer-reviewed journals indexed in the Scopus database. The results revealed the dominance of China in terms of the number of publications, followed by India, the United States, and Iran, with proportions of 25, 22, 16, and 12%, respectively. In Contrast, North Africa had comparatively lower proportions of related published articles, with a proportion of 1,8%. On the other hand, Random Forest (RF) was the most extensively applied algorithm in water quality monitoring and prediction, accounting for 26% of the published articles. Whereas Support Vector Machines (SVM), Artificial Neural Networks (ANN), and extreme gradient boosting (XGBoost) were applied in 22, 19, and 16% of the published articles, respectively. Our findings highlighted also a temporal increase in research on the combination of the Internet of Things (IoT) with AI algorithms. This study provides guidance for future related studies.

Keywords: Water Quality, Artificial Intelligence, Prediction, Monitoring, Bibliometric analysis.

Investigation of Structural and Optoelectronic Properties of π-Bridge-Modified Dyes for DSSCs Using Molecular Modeling and Machine Learning Approaches

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Abstract:

Optimizing energy consumption, particularly from fossil fuels, presents a major challenge in both conserving these finite resources and addressing the impacts of climate change. In this context, the development of sustainable energy sources most notably solar energy, represents a key strategy for improving energy efficiency across technological, industrial, and economic domains.

This work aims to enhance the performance of DSSCs through π-bridge modification in D–π–A dye molecules. Molecular modeling, based on density functional theory (DFT) and time-dependent DFT (TD-DFT) with the 6-31G(d,p) basis set, was employed to investigate key electronic and optical properties such as excitation energies, absorption spectra, oscillator strength, open-circuit photovoltage, and frontier molecular orbital energies (HOMO and LUMO) ...

Molecular modeling provides a powerful and cost-effective approach to predict and optimize the properties of dye materials prior to experimental synthesis, saving time and resources. In the future, integrating artificial intelligence tools, such as machine learning algorithms, could further support the screening and design of high-performance dyes by accelerating the identification of promising molecular structures.

Our results suggest that the studied molecules are promising candidates for dye solar cell (DSSC) applications.

Keywords: Solar cell, Molecular modeling, DSSC, DFT, Machine learning.

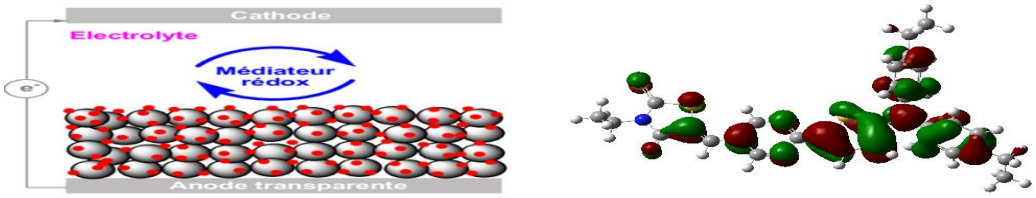

Fig. 1. (a) Operating Principle of DSSCs ; (b) Molecular orbital distribution.

QSAR-Based Study of Triazole Derivatives against *Mycobacterium tuberculosis*: Toward AI-Enhanced Molecular Modeling

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Abstract:

The increasing emergence of drug-resistant strains of *Mycobacterium tuberculosis* (MTB) calls for innovative strategies in drug discovery. In this study, the antibacterial activity of triazole derivatives was investigated using a computational approach combining 2D-QSAR modeling, Density Functional Theory (DFT), and the Petra/Osiris/Molinspiration (POM).

A set of molecular descriptors, including electronic parameters calculated using DFT and topological descriptors obtained from cheminformatics tools, were integrated into multiple linear (MLR) and multiple non-linear regression (MNLR) models. The non-linear QSAR model demonstrated strong predictive capacity, with a coefficient of determination $R^2 = 0.81$, highlighting its reliability in estimating antibacterial activity. The most influential descriptors identified were EHOMO, ELUMO, and PSA. Among the tested compounds, A, S, and T exhibited the highest predicted activity against MTB.

Pharmacophoric features responsible for bioactivity were explored through POM analysis, supporting the identification of promising structural motifs within the triazole scaffold.

Although classical statistical methods were used in this study, future integration of artificial intelligence (AI), machine learning (ML), and deep learning (DL) techniques into QSAR modeling, descriptor selection, and virtual screening is expected to enhance accuracy and accelerate the discovery of novel antimycobacterial agents.

This work establishes a solid computational foundation for the future application of AI-assisted methodologies in the rational design of bioactive molecules targeting MTB.

Keywords: AI, 2D-QSAR, DFT, POM, antitubercular activity.

Study Of Chemical Reactivity And Molecular Docking Of 2-Diazo-3,3,3-Trifluoro-1-Nitropropane With Phenyl Methacrylate: A Computational Approach With AI-Driven Perspectives

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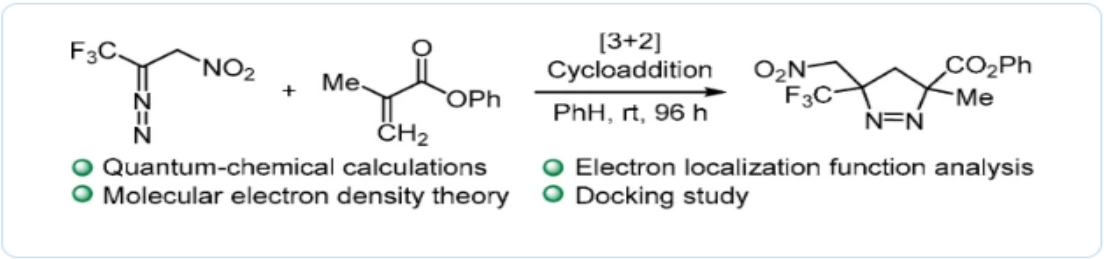
Abstract:

In this work, molecular electron density theory was applied to investigate the activation energies, reaction energies, and reactivity indices of the [3+2] cycloaddition reaction between 2-diazo-3,3,3-trifluoro-1-nitropropane and phenyl methacrylate. Through electron localization function (ELF) topological analysis, the reaction mechanism was elucidated in detail. Notably, the formation of the two key single bonds does not occur simultaneously. Instead, the C2–C5 bond forms first, acting as a prerequisite for the subsequent formation of the C1–N3 bond, indicating a stepwise process. This sequential bond formation offers deeper insight into the mechanistic intricacies of the cycloaddition reaction. Furthermore, docking studies performed on the resulting products revealed strong interaction energies with proteins, particularly involving oxygen and nitrogen atoms. These interactions were exemplified through binding with the COVID-19 protease, suggesting potential bioactivity and relevance in antiviral drug discovery. Overall, the study provides a comprehensive understanding of both the reaction mechanism and the biological implications of the cycloaddition products.

Future investigations could benefit from the integration of artificial intelligence techniques, such as machine learning and deep learning, to enhance computational efficiency and predictive capabilities in reaction modeling and drug discovery.

Keywords: [3+2] cycloaddition reaction, quantum-chemical calculations, Electron Localization Function (ELF), Molecular Electron Density Theory (MEDT), Docking, Artificial intelligence (AI).



Integrating Artificial Intelligence into Molecular Docking for the Identification of Antidiabetic Agents from Asparagus officinalis

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Abstract:

This study explores the antidiabetic potential of phytochemicals derived from Asparagus officinalis through molecular docking analyses, supported by artificial intelligence (AI)-driven tools. Using AutoDock Vina, we assessed the binding affinity and interaction dynamics of major bioactive compounds saponins, quercetin, and kaempferol with key human proteins involved in diabetes pathophysiology: β-glucosidase, NR4A1 nuclear receptor, and GLUT4 transporter. Ligands were selected based on their prevalence in A. officinalis and their pharmacological relevance. Protein structures were obtained from the Protein Data Bank (PDB IDs: 1OGS, 2QW4, 7WSM), and ligands were sourced from PubChem.

Docking simulations evaluated binding energies, RMSD values, and protein–ligand conformational stability. Among the tested compounds, saponins showed the strongest affinity for β-glucosidase

(ΔG = −13.2 kcal/mol), suggesting robust inhibitory activity that could delay carbohydrate breakdown and glucose absorption. Quercetin and kaempferol displayed strong interactions with their respective targets, aligning with mechanisms such as GLUT4 activation, α-glucosidase and DPP-IV inhibition, and AMPK stimulation. [1]

The integration of AI-assisted modeling tools enhanced the precision of target prediction and compound prioritization, significantly streamlining the drug screening workflow. In future perspectives, the adoption of advanced artificial intelligence methods such as machine learning and deep learning could further accelerate in silico screening, optimize ADMET profiling, and reduce the cost and time required for antidiabetic drug development from plant-based sources. [2].

Keywords: Asparagus officinalis, Molecular Docking, Antidiabetic Activity, Phytochemicals, Protein–Ligand Interactions, Artificial Intelligence, Machine Learning, Deep Learning

Table 1: Binding Affinities and Targets

Compound	Target Protein	PDB Code	Best Affinity (kcal/mol)	Key Effect
Saponins	β-glucosidase	1OGS	−13.2	Enhanced β-cell function
Quercetin	NR4A1 ligand domain	2QW4	−9.7	Insulin secretion & glucose uptake
Kaempferol	GLUT4 transporter	7WSM	−8.9	Promotes GLUT4 translocation & uptake

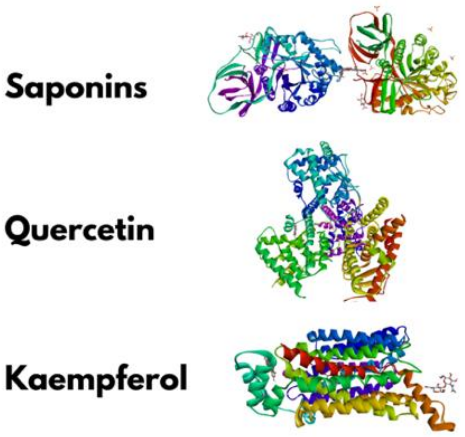

Fig. 1. Docked Complexes of Key Antidiabetic Compounds

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Valorization of Natural Atlantones via 1,3-Dipolar Cycloaddition: Mechanistic Study and Biological Properties

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Abstract:

The 1,3-dipolar cycloaddition reaction constitutes a privileged synthetic strategy for the construction of five-membered heteroaromatic rings, notably isoxazoles, pyrazoles, and triazoles, which are renowned for their structural diversity and wide-ranging applications in medicinal and materials chemistry. Heterocyclic compounds incorporating an isoxazoline motif, particularly those of natural origin, display a broad spectrum of biological activities, including anticancer, analgesic, and anti-inflammatory properties.

In the present study, we carried out both experimental and theoretical investigations of the 1,3-dipolar cycloaddition reaction between nitrile oxides and atlantone derivatives isolated from the essential oil of Atlas cedar (Cedrus atlantica). Regioselectivity and chemoselectivity analyses were performed using a combination of spectroscopic techniques (^{1}H and ^{13}C NMR) and density functional theory (DFT) calculations to elucidate the underlying reaction mechanisms. Additionally, the resulting cycloaddition products were subjected to a preliminary assessment of their potential biological activities.

Keywords: isoxazoline, Cedrus atlantica, Atlantone, DFT.

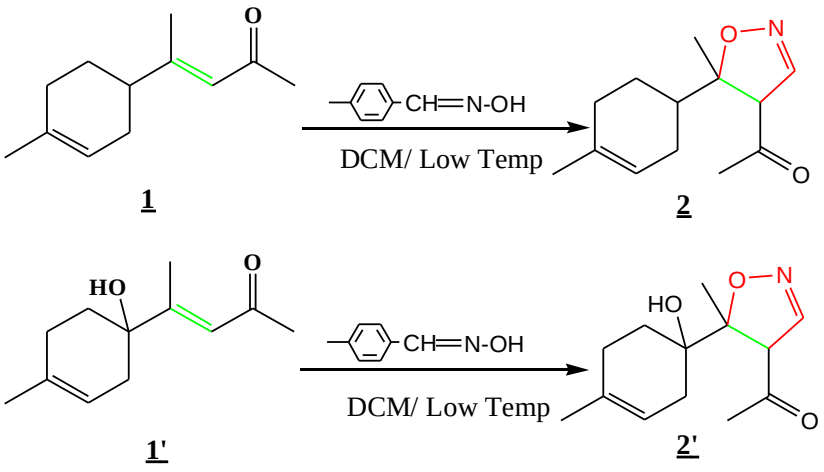

Fig.1. [3+2] Cycloaddition of Atlantone Derivatives **1** and **1'**

Hémisynthèse de nouvelles isoxazolines à partir de l'(E)-α-atlantone : études des activités antimicrobiennes, ADME-Tox, docking moléculaire et simulations de dynamique moléculaire

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Resumé:

La réaction de cycloaddition 1,3-dipolaire a toujours été considérée comme l'une des principales voies utilisées pour synthétiser des systèmes hétérocycliques pentagonaux, tels que l'isoxazole1,2, le pyrazole3 et le triazole4. Ces composés hétérocycliques présentent un grand intérêt en raison de leur application dans divers domaines5. De plus, les composés hétérocycliques d'origine naturelle, en particulier ceux portant un motif isoxazoline, présentent une large gamme d'activités biologiques, telles que l'activité anticancéreuse6 et anti-inflammatoire7.

Dans ce travail, de nouvelles isoxazolines ont été hémisynthétisées par la cycloaddition 1,3-dipolaire des oxydes de nitrile avec le (E)-α-atlantone, un composé sesquiterpénique isolé de l'huile essentielle de l'espèce Cedrus atlantica8. La réaction se déroule de manière sélective pour aboutir à deux cycloadduits dont les structures ont été déterminées par les méthodes spectroscopiques usuelles IR, RMN et SM. De plus, les cycloadduits hémisynthétisés ont été testés pour leurs activités antibactériennes et antifongiques9. En outre, des études in silico ont été menées, incluant le Docking moléculaire, la dynamique moléculaire, ainsi que des tests ADMET et une évaluation de la pharmaco-modulation.

Mots clés : Cedrus atlantica, atlantones, cycloaddition 1,3-dipolaire, sélectivité, antibactérien.

Remerciements : Ce travail est soutenu par l'Agence Universitaire de la Francophonie (AUF) dans le cadre du projet DRM-6588.

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Theoretical analysis of $TiCl_4$-catalyzed cycloaddition reactions: Catalytic influence and prospective application of Artificial Intelligence in MEDT research

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Abstract:

Molecular Electron Density Theory (MEDT) at the DFT/B3LYP/SDD calculation level is being used to investigate cycloaddition reactions between cyclopenta-1,3-diene and benzyl acrylate, as well as benzyl 2-fluoroacrylate, with and without the TiCl4 catalyst. This approach allows for a full examination of reaction energy profiles, providing insights into mechanism and stereochemical selectivity. The results show stereoselectivity, favoring certain stereoisomers, with the TiCl4 catalyst increasing reaction selectivity, consistent with experimental observations. This study also opens the way for the prospective application of Artificial Intelligence in MEDT research, aiming to further improve predictive accuracy and mechanistic exploration within DFT-based investigations.

Keywords: Cyclopenta-1,3-diene, MEDT, benzyl acrylate, benzyl 2-fluoroacrylate, TiCl4, selectivity, AI.

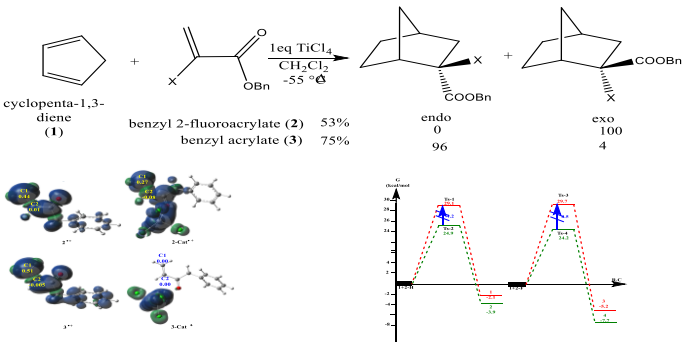

Fig. 1. $TiCl_4$ catalyzed DA reaction of Cyclopenta-1,3-diene with Benzyl 2-Fluoroacrylate and Benzyl Acrylate.

Novel Copper and Nickel Complexes-Based Sulfonamide Schiff Base Ligand: Structural Study and Antioxidant Activity

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Abstract:

Schiff base ligands incorporating sulfonamide moieties have attracted increasing attention due to their versatility and wide range of applications in coordination and medicinal chemistry. In this study, a novel Schiff base ligand was synthesized via the condensation of a sulfonamide bearing a primary amine group with salicylaldehyde, yielding a stable and well-defined compound. This ligand was subsequently used for the complexation of divalent transition metal ions, specifically copper (II) and nickel (II) (figure 1), leading to the formation of both mono- and binuclear metal complexes.

The structures of the resulting complexes were determined by a range of experimental techniques, including IR, UV-Visible spectroscopy, as well as elemental (CHN) and thermal (TGA/TDA) analyses. The molecular structures of the copper and nickel complexes were further elucidated by single-crystal X-ray diffraction.

In addition, the antioxidant activity of the ligand and its metal complexes was assessed by three complementary methods: DPPH, FRAP and TAC. The results showed that metal complexation significantly influences antioxidant activity, highlighting the potential role of these compounds in the development of new bioactive agents.

Keywords: Schiff base, Sulfonamide, Coordination, X-Ray; Antioxidant, DPPH, FRAP.

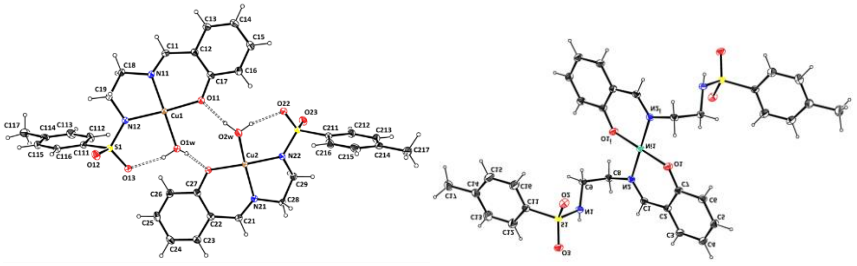

Fig. 1. Structures of copper and nickel complexes.

Experimental and Computational Study of β-Himachalene-Derived Cyclopropane Reactions: Reactivity and AI Perspectives in ADMET Analysis

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Abstract:

As part of the valorization of compounds derived from Atlas cedar essential oil, we conducted a combined theoretical and experimental study on the epoxidation and [2+1] cycloaddition reactions of β-Himachalene-Derived Cyclopropane. The cycloaddition with dichlorocarbene and the epoxidation with meta-chloroperbenzoic acid (m-CPBA) both yielded two main products in quantitative amounts. The structures of these products were confirmed by proton (^{1}H) and carbon (^{13}C) NMR spectroscopy. Reaction mechanisms were analyzed using density functional theory (DFT) at the wB97XD/6-311+G(d,p) level. Theoretical energy profile analysis revealed a clear stereoselectivity, consistent with experimental observations. ADMET predictions indicated that most of the synthesized compounds possess favorable pharmacokinetic properties, particularly in terms of lipophilicity and polarity. However, some molecules showed moderate limitations in solubility and molecular flexibility. These findings support the potential of these compounds as antiviral agents against HIV, pending further biological validation.

To improve ADMET in future work, we plan to integrate deep learning models based on structural and electronic descriptors. The use of artificial intelligence is expected to enhance ADMET accuracy, reduce computational cost, and accelerate the discovery of effective antiviral compounds.

Keywords: WB97XD/6-311+G(d,p), Epoxidation, Dihalocyclopropanation, Molecular Docking, ADMET.