République Algérienne Démocratique et Populaire

Ministère de l'Enseignement Supérieur et de la Recherche Scientifique

Ecole Nationale Polytechnique

LAVALEF

Département de Génie chimique

Laboratoire de Valorisation des Energies Fossiles

THESIS

Submitted by Amira OTHMANI

in Fulfillment of the Requirements for the Degree of Doctor of LMD

Valorization of Non-Living Microbial Biomass for the Adsorptive Removal of Cationic Dyes from Multicomponent Aqueous Systems: Mechanistic Study, DFT Adsorption Energy Analysis, Modeling, and Machine Learning-Based Optimization.

Under the supervision of Prof.: Ammar SELATNIA Professor

Presented and publicly defended on March 24th, 2026

Jury Composition:

President	REBAS Ouardia	Associate Professor	ENP
Examiner	KERCHICH Yacine	Professor	ENP
Examiner	BERRAMA Tarek Ibnou Ziad	Professor	USTHB
Examiner	AKSAS Hamouche	Professor	UMBB

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Thèse de Doctorat

Présentée par Amira OTHMANI

en vue de l'obtention du diplôme de doctorat (LMD)

Valorisation de la biomasse microbienne non vivante pour l'élimination adsorptive des colorants cationiques à partir de systèmes aqueux multicomposants : étude mécanistique, analyse de l'énergie d'adsorption par la théorie de la fonctionnelle de la densité (DFT), modélisation et optimisation basée sur l'apprentissage automatique.

Sous la direction du Pr. : Ammar SELATNIA **Professeur**

Présentée et soutenue publiquement le 24 Mars 2026

Composition du Jury:

Présidente	REBAS Ouardia	Maitre assistante	ENP
Examinateur	KERCHICH Yacine	Professeur	ENP
Examinateur	BERRAMA Tarek Ibnou Ziad	Professeur	USTHB
Examinateur	AKSAS Hamouche	Professeur	UMBB

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DEDICATION

To my beloved mother, **Fakia**,

the first light of my life, whose prayers built my strength,
whose love carried me when I could not carry myself.
Every breath of courage I took began with your faith in me.

To my father, **Salah**,

whose quiet strength and boundless patience taught me dignity, perseverance, and grace.
Your wisdom lives in every step I take.

To my sister, **Malak**,

my confidante and gentle soul,
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whose loyalty and warmth illuminated the darkest hours of this journey.
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To my husband, **Amir**,

the heart that beats beside mine,
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and for standing beside me through every storm and sunrise.

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You are the promise that makes every effort worthwhile,
the reason my heart never gives up.

To my family; near and far,

for their infinite love, for their faith when I doubted,
and for holding me up when I was weary.

And to every soul who was there when I needed strength,

your kindness became part of my story,
and your belief helped me reach this dream.

This work is the reflection of your love, of your prayers and the fruit of every silent sacrifice made for me.

With all my heart,
I dedicate this thesis to you.

Amira

ABSTRACT

الملخص

تتناول هذه الأطروحة دراسة تثمين الكتلة الحيوية للبكتيريا *Streptomyces rimosus*، وهي ناتج ثانوي لصناعة المضادات الحيوية، كمادة ماصّة صديقة للبيئة لإزالة الأصباغ الموجبة الشحنة (الأزرق الأساسي 41، الأحمر الأساسي 46، والأصفر الأساسي 28) من الأنظمة المائية متعددة المكونات. أظهرت التحاليل الفيزيائية-الكيميائية وجود مجموعات فعّالة مسؤولة عن الكفاءة العالية في الامتزاز. بيّنت الدراسات الحركية والإيزوثرمية أن العملية تلقائية، ماصّة للحرارة، وتخضع بشكل رئيسي للتفاعل الكيميائي السطحي. كما أوضحت حسابات نظرية دالة الكثافة (DFT) العلاقة بين طاقات الامتزاز والخواص الإلكترونية وآليات التفاعل الجزيئي. وقد مكّنت نماذج التعلّم الآلي المتقدمة، خصوصاً النموذج الهجين ثلاثي الطبقات DNN–NAS–PSO، من التنبؤ الدقيق وتحسين سلوك الامتزاز. تؤكد النتائج أن الكتلة الحيوية لـ *S. rimosus* تمثل مادة ماصّة فعّالة ومستدامة، وتقدّم مقاربة اقتصادية دائرية لمعالجة مياه الصرف الصناعي

الكلمات المفتاحية : الارتباط الحيوي؛ الكتلة الحيوية لـ *Streptomyces rimosus* ؛ الأصباغ الكاتيونية ؛ الأنظمة المائية متعددة المكونات ؛ نظرية دالة الكثاف (DFT) ؛التحسين باستخدام التعلم الآلي.

Résumé

Cette étude porte sur la valorisation de la biomasse de *Streptomyces rimosus*, sous-produit industriel de la production d'antibiotiques, comme biosorbant écologique pour l'élimination de colorants cationiques (Basic Blue 41, Basic Red 46 et Basic Yellow 28) à partir de systèmes aqueux multi-composants. La caractérisation physico-chimique a révélé la présence de groupements fonctionnels actifs conférant une forte affinité d'adsorption. Les études cinétiques et isothermes ont montré un processus spontané, endothermique et principalement de type chimisorptif. Les analyses de la Théorie de la Fonctionnelle de la Densité (DFT) ont permis de relier les énergies d'adsorption et les descripteurs électroniques aux observations expérimentales. Les modèles d'apprentissage automatique, notamment le réseau neuronal profond hybride DNN–NAS–PSO, ont permis une prédiction et une optimisation précises du processus d'adsorption. Cette recherche démontre le potentiel de *S. rimosus* comme biosorbant durable et efficace, contribuant à une approche circulaire pour le traitement des eaux usées industrielles.

Mots-clés : Biosorption ; Biomasse de *Streptomyces rimosus* ; Colorants cationiques ; Systèmes aqueux multi-composants ; Théorie de la Fonctionnelle de la Densité (DFT) ; Optimisation par apprentissage automatique

Abstract

This research investigates the valorization of *Streptomyces rimosus* biomass, an industrial by-product of antibiotic production, as an eco-friendly biosorbent for the removal of cationic dyes (Basic Blue 41, Basic Red 46, and Basic Yellow 28) from multicomponent aqueous systems. Comprehensive physicochemical characterization confirmed the presence of active functional groups responsible for high adsorption affinity. Adsorption kinetics and isotherms revealed a spontaneous, endothermic, and predominantly chemisorptive process. Density Functional Theory (DFT) analyses correlated adsorption energies and electronic descriptors with experimental performance, elucidating molecular-level interaction mechanisms. Advanced machine learning models, including a Tri-Hybrid DNN–NAS–PSO framework, provided accurate prediction and optimization of adsorption behavior. The study establishes *S. rimosus* biomass as a sustainable and efficient biosorbent, offering a circular-economy approach for industrial wastewater remediation.

Keywords: Biosorption; *Streptomyces rimosus* biomass; Cationic dyes; Multicomponent aqueous systems; Density Functional Theory (DFT); Machine learning optimization.

TABLE OF CONTENTS

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