



Pole for Doctoral Studies  
Center for Doctoral Studies Sciences and Techniques and Medical Sciences

## ANNOUNCEMENT OF DOCTORAL THESIS DEFENSE



**M. NOR Mohammed**

**Will present their research work with the aim of earning a  
Doctorate**

**Doctoral program: Engineering Sciences and Techniques  
Discipline: Chemistry**

**Specialty: Applied Chemistry, Process Engineering and Chemo-  
Informatics**

**On 01/07/2026 at 09H00 at the Conference Hall, Faculty of  
Sciences and Techniques of Al Hoceima, UAE  
Under the Theme**

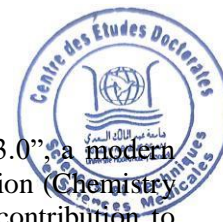
**Advancing Chemical Applications: Exploring and Synthesis  
Novel DESs and Cellulose Derivatives Applied to Water  
Treatment, Developing and Investigating the Impact of LLMs  
and In Silico Methods in Applied Chemistry**

**Front of the jury composed of :**

First Name & Last Name	Establishment	Designation
Pr. AHARI Mhamed	FST of Al Hoceima, UAE	President
Pr. EL MASSAOUDI Mohamed	ESEF of Oujda, UMP	Reviewer
Pr. EL OUARGHI Hossain	ENSA of Al Hoceima, UAE	Reviewer
Pr. ROHAND Taoufik	FST of Al Hoceima, UAE	Reviewer
Pr. EL MIZ Mohamed	FP of Nador, UMP	Examiner
Pr. SALHI Amin	FST of Al Hoceima, UAE	Examiner
Pr. EL BARKANI Soufian	FP of Nador, UMP	Co-Supervisor
Pr. AMHAMDI Hassan	FST of Al Hoceima, UAE	Supervisor

*Host Research Structure:* Applied Chemistry Research Team , FST of Al Hoceima

## Abstract



This dissertation is a contribution in the paradigm shift towards “Chemistry 3.0” a modern chemistry integrating experimental investigation (Chemistry 1.0) with in silico simulation (Chemistry 2.0) and AI-driven data processing (Chemistry 3.0). It presents a multidisciplinary contribution to applied chemistry through the exploration of novel cellulose derivatives, deep eutectic solvent and the development of new methodological tool called ChemNOR.

The experimental part of this work focuses on the rational designing process (by integrating in silico and AI based techniques to fetch and predict the “reactivity and stability of candidate reagents) in the synthesis, and characterization of novel DES and cellulose based adsorbents. Then, it investigates their efficacy in two applications : water treatment, where modified HEC (EDTA-HEC; BEC-S, BEC-M and BEC-Ph) and HPC (BPC-S, BPC-M and BPC-Ph) derivatives based on are employed for the efficient elimination of contaminants (cationic metals ( $\text{Cu}^{2+}$ ,  $\text{Co}^{2+}$ ) and  $\text{MB}^{+}$ ) towards the adsorption methods that were described experimentally and computationally , and to find original and novel materials of natural origin based on cellulose , The structures of the new products have been confirmed by FTIR, and NMR technique that were used to study the grafting process and its effect on the crystallinity. In addition, the morphological changes and the elemental composition of the surfaces were studied using an SEM to evaluate the adsorption performance, along with thermal profile investigation trough ATG/DTA to study the stability of the novel polymers. And in green chemistry, by using relatively green solvent as DMSO and novel DESs (1-benzylpyridin-1-ium bromide : urea and N-Benzyl-N,N-diethylethanaminium bromide : urea) that were fully elaborated using dataset analysis of reported DESs to tune low melted point’ DESs. Providing innovated models as reference for such application-specific performance metrics. In addition, this work leverages in silico methods, including MD simulations and DFT calculations. These computational approaches are not used in isolation but are integral to the workflow of synthesizing all the adsorbents and DESs, by aiding in the analysis of DES combinations by predicting their thermodynamic properties and interaction energies, and providing atomistic insights into the solvation mechanisms and polymer functionalization processes.

A pioneering contribution of this thesis is the development of software tools (ChemNOR package and “ChemNOR it!” apps) after a critical investigation of LLMs as tools for applied chemistry. We explore their capabilities and limitations in tasks related to chemical sciences, including automated literature fetching from ChemPUB database, predictive retrosynthetic analysis, reaction optimization, and hypothesis generation and spectroscopic insights about the desired product. This research provides an assessment of Gemini ‘s LLMs, API and Hive’ database protocols for their reliable use by numerous users to day with +2600 cumulative downloads.

As a last word mixed with honor and humble, our work demonstrates a pioneer contribution in Chemistry 3.0 paradigm. It successfully bridges experimental material science with advanced computational guidance and AI-assisted strategy, offering novel advancements in green solvent and polymer engineering while simultaneously pioneering the integration of LLMs into the modern chemist's toolkit.

**Keywords:** cellulose, in silico, AI assisted chemistry, water treatment, process engineering, Chemoinformatic.