جامعة عبد المالك السعدي
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Université Abdelmalek Essaadi

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

ANNOUNCEMENT OF DOCTORAL THESIS DEFENSE

M. RAISSOUNI Jaber

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

Doctoral program: Biology, Chemistry and Geology (BCG)
Discipline: Chemistry
Specialty: Physical Chemistry of Materials and Environment / Data sciences and AI

On 24/06/2026 at 10H00 at the Meetings Hall, Faculty of Sciences of Tetouan, UAE
Under the Theme

Quantum-AI and Data Science Algorithms for Modeling Experimental and Theoretical Insights into the Adsorption of Industrial Dyes and Pharmaceutical Antibiotics on Green Materials for Sustainable Environmental Protection

Front of the jury composed of :

First Name & Last Name	Establishment	Designation
Pr. EL AMRANI Mohamed EL Amin	FS of Tetouan, UAE	President
Pr. RAIHANE Mustapha	FST of Marrakech, UCA	Reviewer
Pr. CHAFIK Tarik	FST of Tangier, UAE	Reviewer
Pr. CHTOUN El Hossain	FS of Tetouan, UAE	Reviewer
Pr. ACHAK Ouafae	FST of Tangier, UAE	Examiner
Dr. MAHHA Yahdih	APDS-Laâyoun	Guest
Pr. AIT AGHZZAF Ahmed	ENS of Tetouan, UAE	Co-Supervisor
Pr. ALVAREZ RODRIGUEZ Esperanza	University of Santiago de Compostela, Spain	Co-Supervisor
Pr. DRAOUI Khalid	FS of Tetouan, UAE	Supervisor

Host Research Structure: Laboratory of Engineering Materials and Sustainable Energy, Faculty of Sciences, Abdelmalek Essaadi University, Tètouan

Abstract

This thesis develops and validates an integrated Quantum-AI + data-science framework that advances adsorption research from empirical curve-fitting toward mechanistic, predictive, and deployable solutions across materials science, agriculture, pharmaceuticals, climate mitigation, and industrial process optimization. The work couples systematic laboratory experiments (isotherms, kinetics, thermodynamics, XRD, XRF, FTIR, SEM/EDS, TGA, Zeta), high-throughput Monte-Carlo compositional sensitivity, electronic-structure calculations (DFT; Hirshfeld /ELF /LOL /RDG), molecular sampling, and a broad ML toolbox to identify dominant drivers and deliver virtual optimization.

Materials and contaminants studied include natural and modified clays (Stevensite/Ghassoul, smectite, illite, kaolinite, chlorite) and hydrogels; target adsorbates span dyes and antibiotics. Across these systems, adsorption is multi-factorial but typically dominated by one or two primary controls (e.g., masse, concentration, functional groups of polymers and clays minerals), while secondary factors (surface area, pH, modifications, temperature, contact time) act mainly through interactions.

Methodologically, the thesis contrasts classical empirical isotherm modelling (Langmuir 1916, Freundlich 1906) and Design-of-Experiments (DOE/DSD) with modern ML/AI: (1) DOE offers interpretable, causal screening but scales poorly with high dimensionality; (2) Classical Langmuir/Freundlich provide compact parametric descriptions suitable for mechanistic hypothesis testing but fail on heterogeneous, nonlinear, multiscale systems; (3) ML (including ANN and ensemble methods) captures complex, nonlinear interactions and enables virtual optimization and rapid screening, but requires careful regularization and interpretability techniques (Monte-Carlo sensitivity) to recover mechanistic insight. Together, DOE supplies structured experimental design, ML supplies high-precision prediction/optimization, and mechanistic quantum calculations supply physical interpretability forming a complementary triad.

A comprehensive ML suite of fourteen algorithms was evaluated and benchmarked: Neural Boosted, K-Nearest Neighbors (KNN), Boosted Tree, Support Vector Machines (SVM), Bootstrap Forest, Decision Tree, Generalized Regression Ridge, Generalized Regression Elastic Net, Generalized Regression Lasso, Partial Least Squares (PLS), Generalized Regression Pruned Forward Selection, Fit Stepwise, Generalized Regression Forward Selection, and Fit Least Squares. Models regularly achieved exceptional predictive performance ($R^2 \approx 0.99–0.999$) when coupled with Monte-Carlo feature selection and cross-validation.

Practical demonstrations cover clay-based remediation (RhB, SDZ, AMX and MON). Bibliometric analysis confirms the novelty of integrating clays with ML/AI: despite ~831k adsorption records, ML+clay studies are vanishingly rare, highlighting the thesis's frontier role.

Collectively, the Quantum-AI + data-science workflow substantially reduces experimental burden, delivers mechanistic interpretability, and enables cost-effective, scalable strategies for sustainable environmental protection and industrial decision support. Future work emphasizes field validation, life-cycle assessment, and development of user-friendly decision tools to accelerate technology transfer.

Keywords : Adsorption/Desorption; Deep Learning; Monte Carlo; DoE; DFT; Optimization; Clay; Biopolymers; Bionanocomposites.