HABILITATION A DIRIGER DES RECHERCHES

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Titre des travaux : « De la chimie physique expérimentale à la modélisation prédictive : intégration de la chimie théorique et de l'apprentissage automatique en chimie physique et catalyse hétérogène pour l'énergie et l'environnement »

Résumé

The following document presents a summary of the research work that will be discussed in my HDR manuscript and defense, following the four main research areas defined throughout the manuscript (**Table 1**). The following provides a coherent overview of my scientific trajectory, spanning experimental heterogeneous catalysis, atmospheric reaction kinetics, quantum-level modeling, and machine learning-assisted predictive analysis for energy and environmental applications.

Table 1. Structure of Research Work

Research area	Main focus
Research area 1	Experimental heterogeneous catalysis for energy and environmental applications
Research area 2	Experimental Kinetic Study of VOCs Reactions with Ozone in a Simulation Chamber
Research area 3	Transition from Experimental Chemistry to Quantum-Level Modeling: Applications of Force Fields, Molecular Dynamics, and Density Functional Theory
Research area 4	Data-Driven and Theoretical Analysis Coupled with Machine Learning for Energy, Environmental and Theoretical Applications

Research area 1: Experimental heterogeneous catalysis for energy and environmental applications

This first research area establishes the experimental foundation of HDR work. It focuses on heterogeneous catalysis as a central tool for addressing environmental and energy challenges, particularly pollutant mitigation and hydrogen production. The work combines catalytic testing, materials characterization, and mechanistic interpretation to understand how catalytic materials activate key reactions relevant to sustainable technologies.

Two complementary topics structure this area: soot oxidation on yttria-stabilized zirconia (YSZ), which is directly connected to particulate emission control, and catalytic hydrogen generation through sodium borohydride hydrolysis, which is relevant to hydrogen-based energy systems.

Research area 2: Experimental Kinetic Study of VOCs Reactions with Ozone in a Simulation Chamber

The second research area is dedicated to atmospheric chemistry, particularly the experimental kinetic study of volatile organic compounds reacting with ozone in simulation chambers. This axis extends experimental expertise from heterogeneous catalysis to gas-phase reactivity and atmospheric pollution mechanisms.

The work focuses on oxygenated aromatic compounds such as catechol and guaiacol, which are relevant atmospheric species emitted from combustion and biomass burning processes. Understanding their ozonolysis mechanisms is essential for evaluating atmospheric lifetimes, secondary pollutant formation, and potential contributions to secondary organic aerosols.

Research area 3: Transition from Experimental Chemistry to Quantum-Level Modeling: Applications of Force Fields, Molecular Dynamics, and Density Functional Theory

The third research area represents the scientific transition from experimental chemistry toward theoretical and computational chemistry. It was developed to support the interpretation of experimental observations at the molecular level and to provide a deeper understanding of interactions that cannot be fully resolved by experiments alone.

This research area integrates force field calculations, molecular dynamics, and density functional theory. These tools were applied to hydrogen-bonded systems, atmospheric clusters, adsorption processes, and catalyst-pollutant interactions, establishing a bridge between experimental measurements and quantum-level interpretation.

Research area 4: Data-Driven and Theoretical Analysis Coupled with Machine Learning for Energy, Environmental and Theoretical Applications

The fourth research area builds upon the experimental and theoretical foundations developed in the previous sections and introduces data-driven analysis coupled with machine learning. The objective is to move from descriptive interpretation toward predictive modeling, optimization, and rational design in chemistry, catalysis, energy, and environmental systems.

This area combines experimental datasets, theoretical descriptors, statistical analysis, and machine learning algorithms to identify hidden correlations, predict behavior, and optimize processes. It is organized into three subsections covering sustainable energy systems, environmental applications, and theoretical applications.

Overall Conclusion

Taken together, the four research areas define a coherent HDR trajectory. The work begins with experimental heterogeneous catalysis, extends to atmospheric kinetic studies, evolves toward quantum-level modeling, and culminates in data-driven and machine learning-assisted predictive analysis. This progression reflects a unified scientific vision: integrating experiment, theory, and artificial intelligence to address major challenges in energy, environmental chemistry, and molecular science.