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Matériaux à base de phosphate, Matériaux hybrides, Diffraction des rayons X sur monocristal, Spectroscopie infrarouge à transformée de Fourier, Analyse thermique, Inhibition de la corrosion, Activité catalytique, Adsorption, Théorie fonctionnelle de la densité.

**SYNTHESIS, STRUCTURAL CHARACTERIZATION, AND
PHYSICOCHEMICAL STUDY OF NEW MIXED AND HYBRID ORGANIC-
INORGANIC MATERIALS BASED ON PHOSPHATES AND TRANSITION
METALS AND THEIR APPLICATIONS.**

Abstract:

This thesis demonstrates the synthesis of phosphate-based materials using a slow evaporation technique, forming well-crystalline hybrid organic-inorganic and purely inorganic compounds confirmed by single crystal and powder X-ray diffraction. Hybrid materials, incorporating functional organic moieties into inorganic phosphate frameworks, exhibited tailored morphologies, high surface areas, enhanced thermal stability, and synergistic functionalities through FTIR, SEM-EDS, TGA-DTA, and BET analysis. These hybrids achieved exceptional corrosion inhibition in acidic environments via protective organic-inorganic films and high catalytic efficiency in the selective redox conversion of aminophenol isomers, with kinetics confirming bifunctional active sites and rapid electron transfer. Purely inorganic phosphates, characterized via DRX, FTIR, TGA-DTA, SEM-EDX, and BET, displayed defined crystallinity, morphology, and porosity, enabling high methylene blue dye adsorption from water. Isotherm modeling, kinetics, and thermodynamic analyses quantified removal efficiency, in parallel, simulations based on density functional theory (DFT) provided atomic-scale insights into the interaction mechanisms between the adsorbed species and the material surface, highlighting the role of surface hydroxyl groups, phosphate oxygen atoms, and metal centers through hydrogen bonding and electrostatic interactions. In conclusion, this work highlights the multifunctionality of phosphate-based systems, demonstrating how the integration of synthesis, advanced characterization, and theoretical modeling enables the rational design of materials for corrosion reduction, catalysis, and environmental remediation.

Key Words:

Phosphate-based materials, Hybrid materials, Single crystal X-ray diffraction, Fourier transform infrared spectroscopy, Thermal analysis, Corrosion inhibition, Catalytic activity, Adsorption, Density functional theory.