

French Polytech network form for PhD Research Grants from the China Scholarship Council

This document describes one of the PhD subjects proposed by the French Polytech network. The network is composed of engineering schools/universities. The document also provides information about the supervisor.

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PhD information	
Title	Molecular Dynamics Study of Vegetal fibers-Resin-Lime Interfaces for Sustainable Bio-Based Textile Reinforced Mortar Composites
Main topics regards to CSC list (3 topics at maximum)	IV-7. Matériaux pour l'environnement et l'écologie (Materials for environment and ecology) IV-10. Bio-matériaux et matériaux polymères (Biomaterials and polymer materials)

Required skills in science and engineering	Materials science, molecular dynamics, physics and chemistry; appreciated programming knowledge
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Subject description (two pages maximum including biblio)

Historic masonry buildings represent a major architectural and cultural heritage that must be preserved. Their vulnerability to structural stresses and environmental aggressions – such as moisture, salts, or thermal cycles – requires the development of innovative reinforcement solutions that are both durable and compatible with the original materials [1,2].

Among such solutions, Textile Reinforced Mortar composites, which combine a lime-based matrix with natural fibers such as flax and jute have emerged as promising alternatives to conventional materials. These bio-based composites help reduce the carbon footprint of interventions while preserving compatibility and integrity with historic masonry materials [3,4].

However, vegetal fibers present significant limitations, particularly reduced durability in the alkaline environment of lime-based matrices. Recent research has shown that coating flax fibers with graphene nanoplatelet-based nanocomposites dispersed in waterborne polyurethane significantly improves their mechanical properties and resistance to moisture [5]. These protective coatings enhance fiber-matrix adhesion and limit fiber degradation, both crucial factors for ensuring the performance and durability of bio-based lime composites.

Despite these experimental advances, several uncertainties remain regarding the behavior of interfaces within these complex systems. In particular, the adhesion mechanisms between natural fibers and lime matrix, as well as the actual effectiveness of protective coatings – especially graphene/polyurethane nanocomposites – in improving interfacial cohesion and long-term durability, are still poorly understood. Furthermore, the complex chemical and physical interactions at the fiber-matrix-coating interface and their evolution under mechanical and environmental stresses cannot be fully captured by macroscopic or microstructural experiments alone.

The main objective of this proposed research is to address these knowledge gaps by employing molecular dynamics (MD) simulations to model and understand, in detail, interfacial interactions in these innovative composites. Several previous studies on cementitious and clay-based matrices [6-8] have demonstrated the effectiveness of MD in capturing phenomena at the atomic scale. Research on natural fibers such as cellulose has also shown the relevance of atomistic simulations in exploring fiber-related mechanisms [9-10]. Through MD simulations, this work aims to explore the atomic-scale adhesion mechanisms between lime and vegetal fibers, the protective role and adhesion behavior of resin coatings – particularly nanocomposite coatings – on fibers, and the overall response of the lime-fiber-resin system to aggressive agents such as water or chlorides, as well as to mechanical loading such as tension and shear. The influence of the matrix microstructure, including its porosity and crystallinity, on mechanical performance and durability will also be considered.

Molecular dynamics will thus serve as a key tool to generate new insights into interface phenomena at the nanoscale. This fundamental knowledge will help guide applied research, including the selection of optimal fibers and resins, the design of protective treatments or coatings, and the formulation of more durable, high-performance composites. Ultimately, this approach seeks to integrate molecular dynamics into the

development of innovative, bio-based Textile Reinforced Mortar solutions specifically tailored for the sustainable reinforcement of historic masonry structures, while simultaneously reducing experimental costs and time.

References :

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