

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.

Supervisor information	
Family name	MENEZO
First name	Christophe
Email	christophe.menezo@univ-smb.fr (director) anna.lushnikova@univ-smb.fr (co-director)
Web reference	https://www.univ-smb.fr/locie/christophe-menezo-enseignant-chercheur-membre-dulocie/ https://www.univ-smb.fr/locie/anna-lushnikova-enseignante-chercheuse-membre-dulocie/
Lab name	LOCIE
Lab web site	https://www.univ-smb.fr/locie/
Polytech name	Polytech Annecy-Chambéry
University name	Université Savoie Mont Blanc
Country	France

PhD information	
Title	Solar-Control Transparent Building Envelopes: An Ab Initio Molecular Dynamics Study
Main topics regards to CSC list (3 topics at maximum)	IV-1. Nanotechnologie et Nanotechnique Nanotechnology and Nanotechnique IV-11. Matériaux d'information, de stockage et de capteurs Information, storage and sensor materials IV-6. Calcul des matériaux et simulation pour la conception

	Calculation of materials and simulation for design
Required skills in science and engineering	Materials science, molecular dynamics, physics and chemistry; appreciated programming knowledge, civil engineering and energy

Subject description (two pages maximum including biblio)

The design of transparent building envelopes capable of controlling solar radiation represents a promising research direction for the development of energy-efficient and climate-adaptive buildings. While conventional glazing provides daylight and visual comfort, it is also one of the principal pathways for unwanted solar heat gain, significantly increasing cooling demand during warm periods [1-3]. The development of advanced transparent materials capable of selectively reducing solar heat transmission while maintaining high visible-light transmittance has therefore become a key challenge for sustainable buildings.

Recent advances in nanotechnology have opened new opportunities for engineering multifunctional transparent coatings and smart glazing systems. Thermochromic materials such as vanadium dioxide (VO_2), electrochromic oxides (WO_3 , NiO), transparent conductive oxides (ITO, FTO, ZnO), titanium dioxide (TiO_2), graphene-based materials, and hybrid nanostructures have demonstrated strong potential for controlling solar radiation while preserving optical transparency [4-7]. Depending on their composition and nanostructure, these materials can selectively reduce near-infrared transmission, improve thermal comfort, provide self-cleaning capabilities, and enhance the durability of transparent façades.

Despite significant experimental progress, the atomic-scale mechanisms governing the interactions between functional nanomaterials and transparent substrates remain poorly understood. In particular, the interfacial bonding, structural stability, thermal response, and electronic properties of these systems strongly influence their long-term performance and durability. Understanding these mechanisms is therefore essential for designing next-generation transparent building envelopes with optimized solar-control properties.

This research will be conducted entirely through ab initio molecular dynamics (AIMD) simulations. AIMD provides a powerful computational approach to investigate atomic interactions, chemical bonding, charge redistribution, thermal stability, and structural evolution without relying on empirical force fields. This methodology is particularly suitable for studying semiconductor oxides, transparent conductive materials, thermochromic compounds, and hybrid nanostructures intended for solar-control applications [8,9].

The proposed research aims to establish an atomistic framework for the design of transparent building-envelope materials capable of reducing unwanted solar heat gains while preserving daylight transmission. By simulating the interactions between transparent substrates and functional nanomaterials, this study will provide fundamental insight into the mechanisms controlling solar selectivity, thermal stability, and long-term durability before experimental implementation.

The proposed research will focus on three complementary aspects within a single comprehensive study.

First, the project will investigate the interactions between transparent substrates, such as silica-based glass or aluminosilicate glass, and functional nanomaterials including VO₂, TiO₂, ZnO, WO₃, graphene, graphene oxide, transparent conductive oxides, and hybrid nanostructures. The simulations will evaluate interfacial energies, atomic bonding characteristics, charge transfer, structural stability, and their influence on the durability of transparent coatings.

Second, the research will simulate the effects of solar exposure by introducing temperature conditions representative of building façades subjected to solar irradiation. Particular attention will be devoted to atomic mobility, thermal expansion, phase stability, defect formation, and the evolution of structural and electronic properties. For thermochromic materials such as VO₂, the simulations will also provide insight into the atomistic mechanisms responsible for temperature-dependent changes in solar-control performance [10].

Finally, the study will investigate the long-term behaviour of transparent nanostructured systems under repeated thermal cycling representative of daily and seasonal environmental conditions. The simulations will evaluate atomic diffusion, interfacial degradation, defect generation, and structural evolution, providing guidelines for designing durable solar-control materials suitable for long-term building applications.

This project aims to establish a scientific framework for the atomistic design of advanced transparent building envelopes capable of controlling solar heat gains while maintaining high optical transparency. The results will provide theoretical guidelines for the development of durable and multifunctional glazing systems and will support future experimental validation toward next-generation energy-efficient building façades.

References

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2. Jiang, C., He, L., Xuan, Q., Liao, Y., Dai, J.-G., Lei, D., et al. (2024). *Phase-change VO₂-based thermochromic smart windows*. *Light: Science & Applications*, 13, 255.
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10. Heyine, M. S., Yahya, A. M., Daher, D. H., Gaillard, L., Ménézo, C., & Mahmoud, A. K. (2022). *Performance evaluation of a 50 MWp solar plant under different climatic conditions*. *International Journal of Power Electronics and Drive Systems*, 13(1), 561–575.