# 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

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|---|---|
| **Family name** | MENEZO |
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| **Lab name** | LOCIE |
| **Lab web site** | https://www.univ-smb.fr/locie/ |
| **Polytech name** | PAC |
| **University name** | USMB |
| **Country** | France |

## PhD information

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| **Title** | Solar-Activated Nanoparticles for Conductive Cement in Energy-Active Envelopes: A Molecular Dynamics Study |
| **Main topics regards to CSC list (3 topics at maximum)** | IV-1. Nanotechnologie et Nanotechnique (Nanotechnology and Nanotechnique)<br>IV-2. Nanomatériaux (Nanomaterials)<br>IV-11. Matériaux d'information, de stockage et de capteurs (Information, storage and sensor materials) |

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| **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 conductive cementitious matrices incorporating solar-activated nanoparticles represents a promising research direction for the development of energy-efficient and adaptive building materials. While traditional concrete is primarily valued for its mechanical strength, modern applications increasingly demand multifunctional capabilities, such as energy harvesting, self-sensing, or thermal regulation. These emerging functions can be achieved by embedding nanostructures with tailored electrical, photothermal, or optoelectronic properties into the cement matrix [1–3].
Carbon nanotubes (CNTs), graphene derivatives, titanium dioxide ($TiO_2$) nanoparticles, etc., have demonstrated strong potential for enhancing both the mechanical and functional performance of cementitious materials [4–6]. In particular, carbon-based nanostructures can improve electrical conductivity, increase thermal sensitivity, and act as charge carriers or piezoresistive sensors within cement-based composites [7–9]. Furthermore, $TiO_2$ exhibits photocatalytic and photothermal effects when exposed to solar radiation, which can be exploited to activate new behaviors in cementitious matrices, such as self-cleaning, pollutant degradation, or thermal energy conversion [10,11].
This research will be conducted entirely through molecular dynamics (MD) simulations aimed at modeling and predicting the physical and chemical interactions between calcium-silicate-hydrate (C-S-H) gels and embedded nanoparticles at the atomic scale. MD simulations offer a powerful approach to capture the complex nanoscale mechanisms that govern the mechanical reinforcement, fracture behavior, and multifunctional properties of cementitious composites. Special attention will be given to the role of light-activated nanoparticles incorporated within the cement matrix, which can trigger photocatalytic and photothermal effects under solar irradiation. These effects not only enhance traditional properties such as strength and durability but also enable advanced functionalities like self-cleaning, pollutant degradation, and dynamic modulation of electrical conductivity and sensing capabilities. Understanding the impact of solar resource variability is therefore crucial to improving the performance of solar-based systems [12]. By simulating these interactions at the atomic level, this study aims to optimize the design and dispersion of active nanoparticles to achieve tailored mechanical, physical, and photoresponsive properties well before experimental implementation.
The proposed research will focus on three main aspects within a single comprehensive study. First, it will simulate the interactions between calcium-silicate-hydrate (C-S-H) structures and hybrid nanostructures, such as carbon nanotube-titanium dioxide, graphene–titanium dioxide, multi-walled carbon nanotubes, graphene oxide, and metal oxide nanoparticles like zinc oxide and alumina composites. This will enable evaluation of interfacial energies, atomic bonding characteristics, and their influence on mechanical properties like stiffness and fracture toughness. Second, the research will model the effects of solar activation by introducing temperature gradients that mimic localized heating due to solar radiation, examining how this thermal input affects nanoparticle dispersion, atomic mobility, and the overall thermal conductivity of the cementitious composite. Finally, the study will investigate the long-term behavior of the nanoparticle within the C-S-H matrix under repeated thermal cycling, assessing their durability and potential performance in building materials designed for energy harvesting or thermal regulation applications.
This project aims to create a scientific framework for the design of solar-responsive, energy-storing, and conductive cementitious materials, providing the theoretical foundation for future experimental validation and practical applications in smart building envelopes.

References :


1. Almotlaq, T., Huang, B., Saafi, M., & Ye, J. (2024). Enhancing the self-sensing and energy storage capabilities of cementitious composites through marine sand doping. *Construction and Building Materials*, *428*, 136218. https://doi.org/10.1016/j.conbuildmat.2024.136218
2. Wang, X., Ding, S., Ni, Y.-Q., Zhang, L., Dong, S., & Han, B. (2024). Intrinsic self-sensing concrete to energize infrastructure intelligence and resilience: A review. *Journal of Infrastructure Intelligence and Resilience*, *3*(2), 100094. https://doi.org/10.1016/j.joir.2024.100094
3. Li, W., Qu, F., Dong, W., Mishra, G., & Shah, S. P. (2022). A comprehensive review on self-sensing graphene/cementitious composites: A pathway toward next-generation smart concrete. *Construction and Building Materials*, *346*, 127284. https://doi.org/10.1016/j.conbuildmat.2022.127284
4. Thostenson, E. T., Ren, Z., & Chou, T.-W. (2001). Advances in the science and technology of carbon nanotubes and their composites: A review. *Composites Science and Technology*, *61*(13), 1899–1912. https://doi.org/10.1016/S0266-3538(01)00094-X
5. Lushnikova, A., & Zaoui, A. (2018). Influence of single-walled carbon nanotubes structure and density on the ductility of cement paste. *Construction and Building Materials*, *172*, 86–97. https://doi.org/10.1016/j.conbuildmat.2018.03.231
6. Janus, M., Mądraszewski, S., Zając, K., Kusiak-Nejman, E., Morawski, A. W., & Stephan, D. (2019). Photocatalytic activity and mechanical properties of cements modified with $TiO_2$/N. *Materials*, *12*(22), 3756. https://doi.org/10.3390/ma12223756
7. Lushnikova, A., Plé, O., De Souza Gomes, Y., Jia, X., & Yang, W. (2023). Strength and electrical properties of cementitious composite with integrated carbon nanotubes. *Materials, 16*(13), 4771. https://doi.org/10.3390/ma16134771
8. Yoo, D. Y., You, I., & Lee, S. J. (2018). Electrical and piezoresistive sensing capacities of cement paste with multi-walled carbon nanotubes. *Archives of Civil and Mechanical Engineering, 18*(2), 371–384. https://doi.org/10.1016/j.acme.2017.09.007
9. Thomoglou, A. K., Falara, M. G., Gkountakou, F. I., Elenas, A., & Chalioris, C. E. (2023). Smart cementitious sensors with nano-, micro-, and hybrid-modified reinforcement: Mechanical and electrical properties. *Sensors, 23*(5), 2405. https://doi.org/10.3390/s23052405
10. Pereira Lessa, F., Lima Jr, O., Margalho, É., & et al. (2025). Application of nano-$TiO_2$ and micro-ZnO on cementitious surfaces for self-cleaning façades by spray coating and dip coating: A comparative study. *Journal of Building Pathology and Rehabilitation, 10*, 16. https://doi.org/10.1007/s41024-024-00522-3
11. Tang, S., Mu, B., Li, Y., & et al. (2024). Advances in $TiO_2$-enhanced photocatalytic building materials: Applications in cement and asphalt for environmental purification. *Low-carbon Materials and Green Construction, 2*, 26. https://doi.org/10.1007/s44242-024-00059-1
12. Heyine M.S., Yahya A.M.,Deher D.H, Gaillard L., Ménézo C., Mahmoud A.K. (2022). Performance evaluation of 50 MWp solar plant under different climatic conditions. *International Journal of Power Electronics and Drive Systems (IJPEDS)*. 13(1), 561–575. https://doi.org/10.11591/ijpeds.v13.i1.pp561-575