# Advanced first-principles and machine learning modeling of polyanionic glasses and glass-ceramics for energy storage applications

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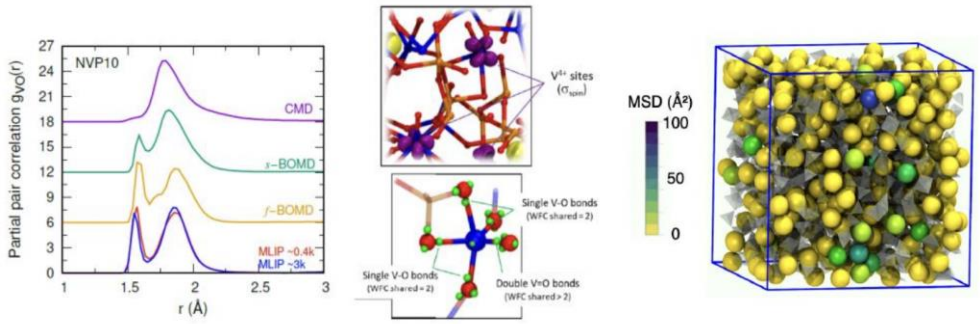
Understanding how the atomic structure of glass-based materials influences ionic transport is crucial for designing better electrode materials for sodium-ion batteries (1). This PhD project focuses on **transition metal (TM)**-containing **polyanionic glasses** and **glass-ceramics**, assessing how short-to-medium range structures and glass polyhedral arrangements affect Na-ion dynamics. A key objective is to explore the **glass/crystalline interface** and its impact on ionic mobility, structural stability, and crystallisation mechanisms.

Building on recent findings in **Na-TM-P-O glass systems** (2-3), the project investigates how structural and bonding features, as well as compositional factors, influence Na-ion mobility, stability, and thermodynamic behaviour. A particular focus is given on **identifying the key structural** and **bonding features governing crystallisation**, ultimately aiding the development of tailored glass-ceramics.




Preliminary results have shown how MLIP can achieve first-principles accuracy in describing the local environment of V in Na-V-P-O glasses. MLIP allows capturing the **local spin topology** and **bonding fingerprints** of V environments, which may affect the heterogeneous Na-ion dynamics observed in these materials [3].

A major aspect of this project is the **screening** and **development of machine-learning interatomic potentials** (MLIP) for modeling these complex systems (4,5). Using **first-principles molecular dynamics**, the research leverages insights from **electronic structure, local magnetic properties, bonding fingerprints, and dispersion forces** to refine MLIP-accelerated MD simulations for large-scale modeling. Additionally, **ML tools** will be applied to uncover structure-property correlations by analysing simulation and (available) experimental datasets. To reveal the **chemical-physical origins of material properties**, **ML-based feature importance analysis tools** will be applied to identify the most relevant structural, chemical, or physics-driven descriptors distinguishing different glass and glass-ceramic functionalities. This will provide a deeper understanding of the atomic-scale mechanisms driving material behaviour, helping to **optimize compositions** and **guide material design**.

The computational work will have access to **high-performance computing** (HPC) **resources** at the University of Strasbourg and national HPC centres under **the GENCI-DARI** allocations.

The project will be carried out in close collaboration with Prof. A. Pedone's Research Group at the University of Modena and Reggio Emilia, fostering an active exchange of expertise and methodologies (5).

[1] M. S. Whittingham *Chem. Rev.* **114**, 11414 (2014).
[2] S.D. Wansi Wendji *et al. J. Non-Cryst. Solids* **655**, 123420 (2025).
[3] S.D. Wansi Wendji *et al. ChemRxiv, 10.26434/chemrxiv-2025-0hrw6* (2025).
[4] S.Urata *et al. J. Am. Ceram. Soc.* **107**, 7665 (2024).
[5] I. Batatia *et al. Arxiv*, 10.48550/arXiv.2401.00096 (2024).