Nanoscaled ferroelectric (pseudo)-binary oxide thin film for energy storage supercapacitors

Luís S. Marques,[1,2*] Corneliu Ghica,[3] Bertrand Vilquin,[4] José P. B. Silva[1,2]

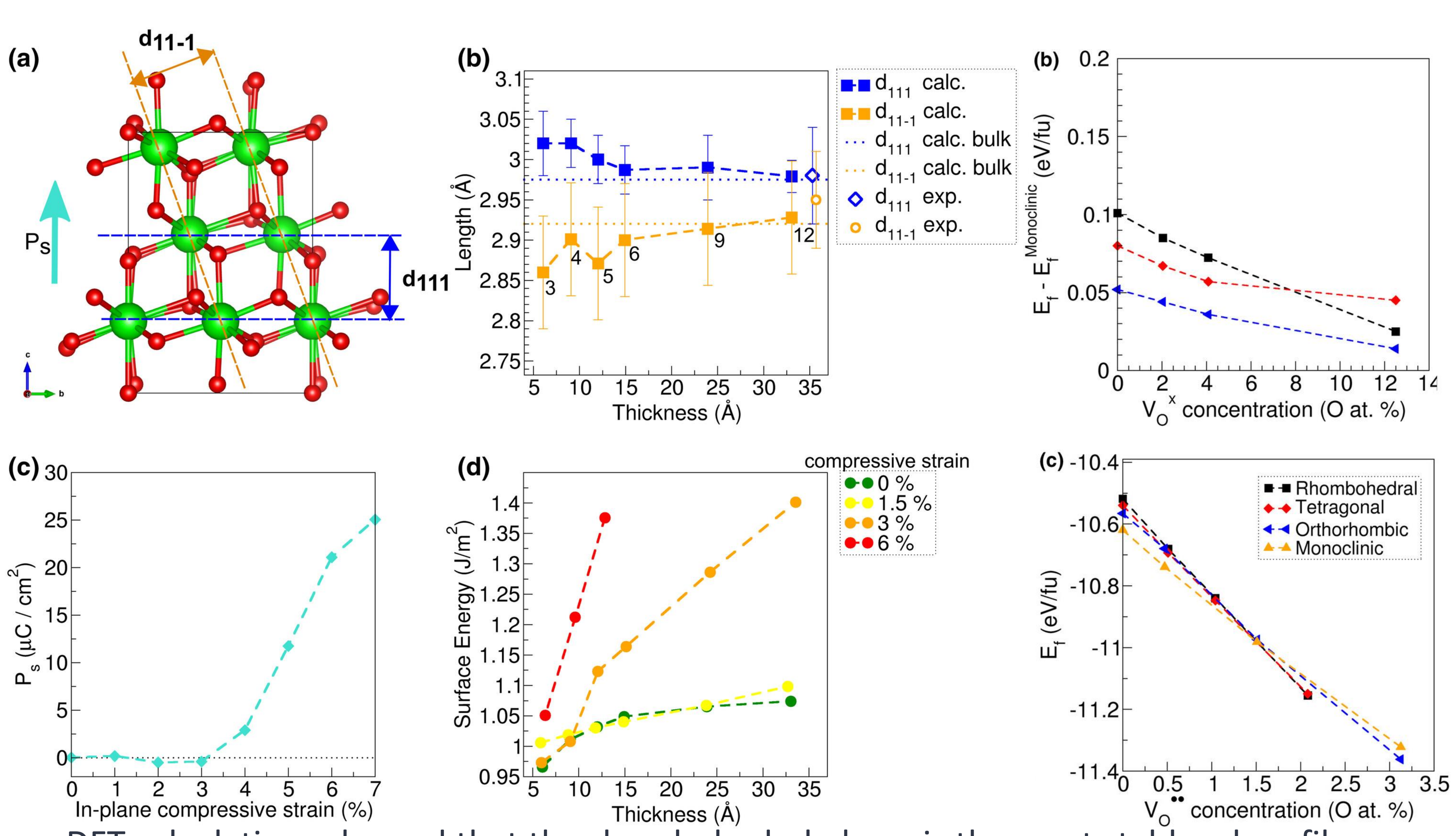
[1]Physics Center of Minho and Porto Universities (CF-UM-UP), University of Minho, Campus de Gualtar, 4710-057 Braga, Portugal
[2]Laboratory of Physics for Materials and Emergent Technologies, LapMET, University of Minho, 4710-057 Braga, Portugal
[3]National Institute of Materials Physics, 077125 Magurele, Romania
[4]Ecole Centrale de Lyon, INSA Lyon, CNRS, Universite Claude Bernard Lyon 1, CPE Lyon, INL, UMR5270, 69130 Ecully, France
*presenting author e-mail: lsam@fisica.uminho.pt

The Project

The NanOx4EStor project (Nanoscaled Ferroelectric (Pseudo)-Binary Oxide Thin Film Supercapacitors for Flexible and Ultrafast Pulsed Power Electronics) aims to develop innovative, cost-effective, high-throughput methods for fabricating advanced dielectric capacitors. These capacitors, based on wake-up-free (pseudo-)binary oxide thin films, are produced through physical vapor deposition (PVD) processes and optimized for superior ferroelectric and energy storage (ES) properties using (i) strain, (ii) interface, and (iii) dead-layer engineering techniques.

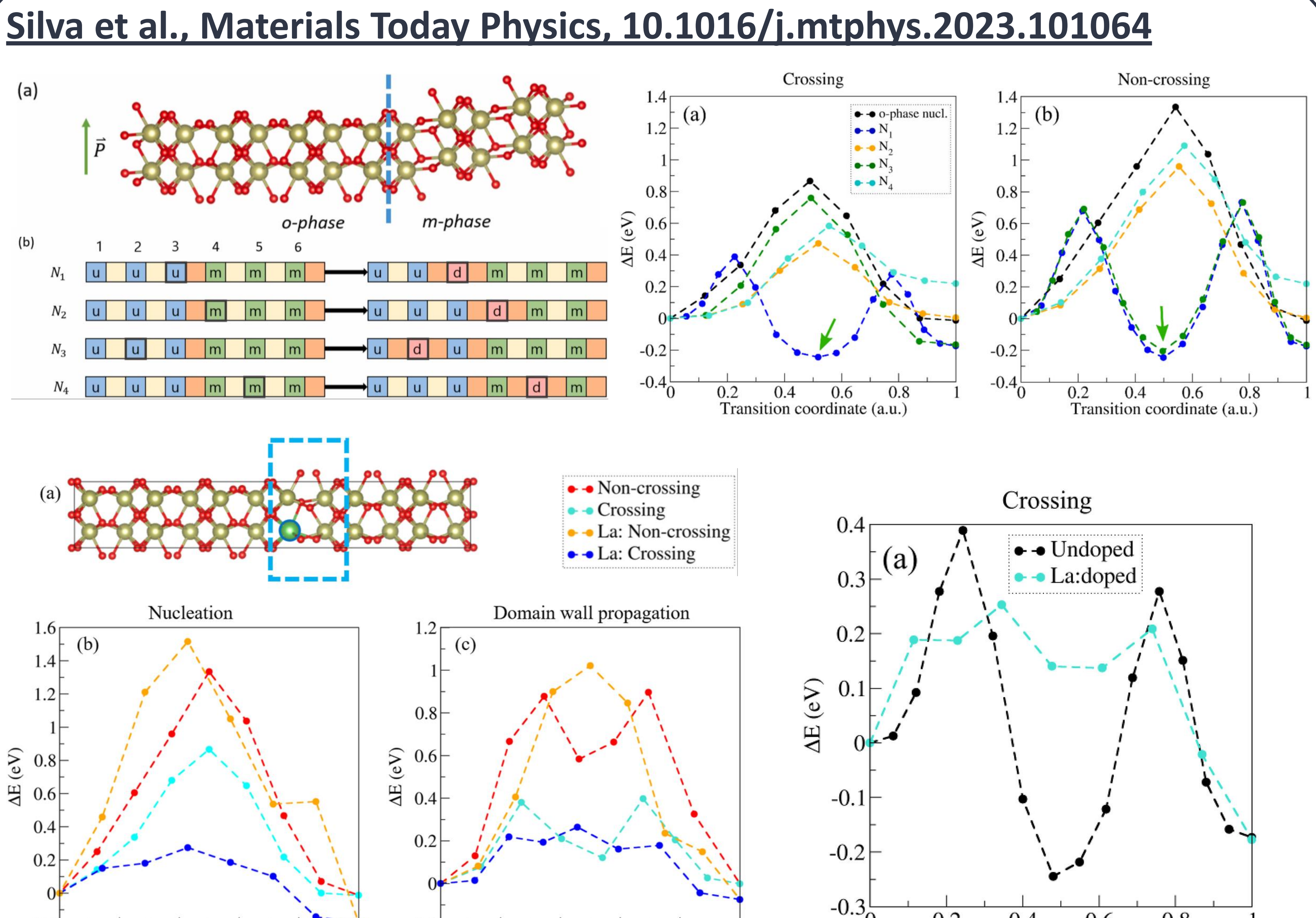
Simulation work

Lenzi et al., Energy Environ. Mater., 7: e12500



- DFT calculations showed that the rhombohedral phase is the most stable when films are grown in a O-poor environment. V_O^{**} have a drastic effect on relative phase stability.
- Charged and neutral V_O contribute to the large spontaneous polarization observed in this phase.

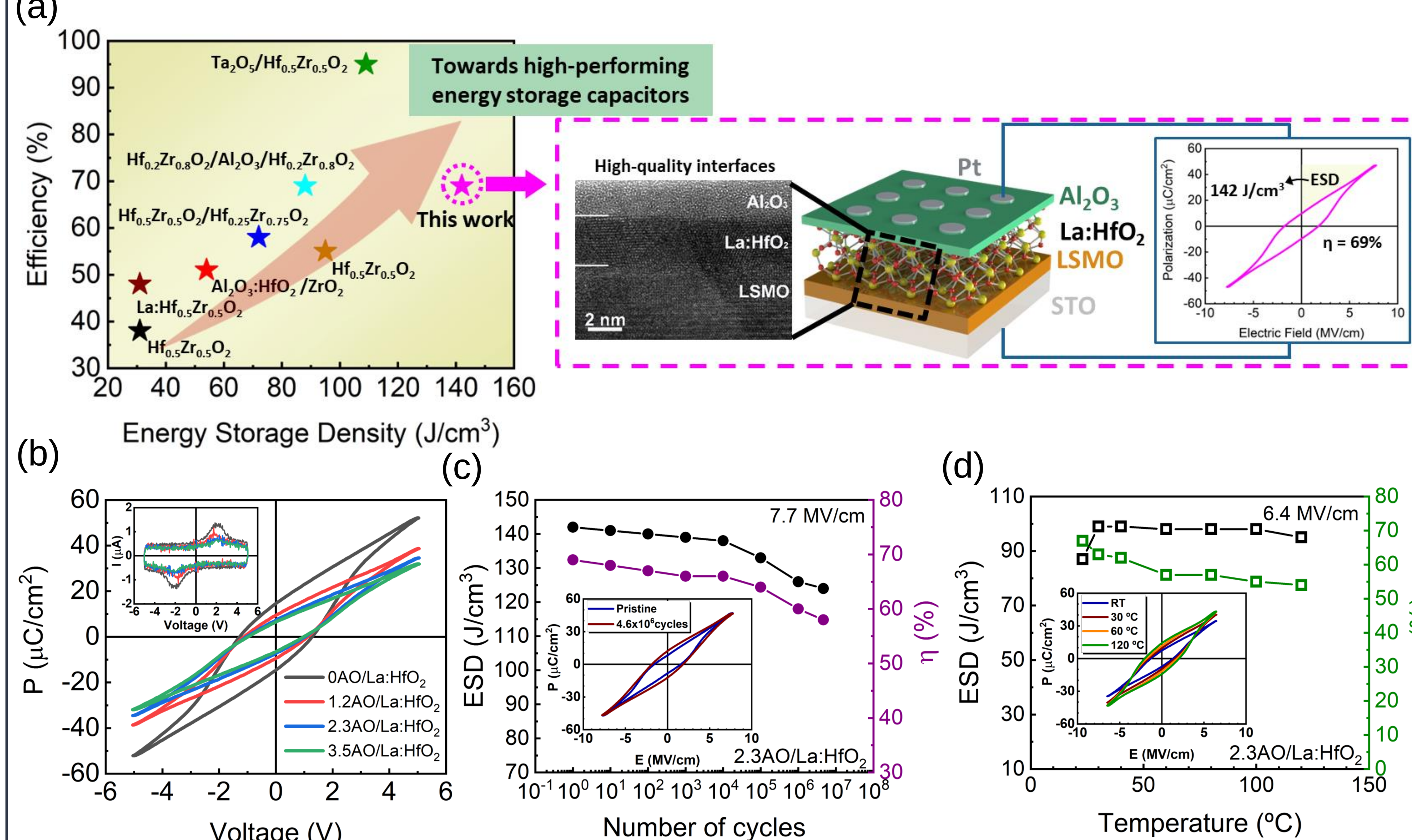
Silva et al., Materials Today Physics, 10.1016/j.mtphys.2023.101064



- m/o-phase interfaces lower the coercive field in La-doped HfO_2 thin films for different switching mechanisms and pathways.
- The presence of La dopants significantly reduces nucleation and domain wall motion energy barriers.
- The joint effect of La-doping and o/m-phase interfaces contributes to a lower coercive field in La-doped HfO_2.

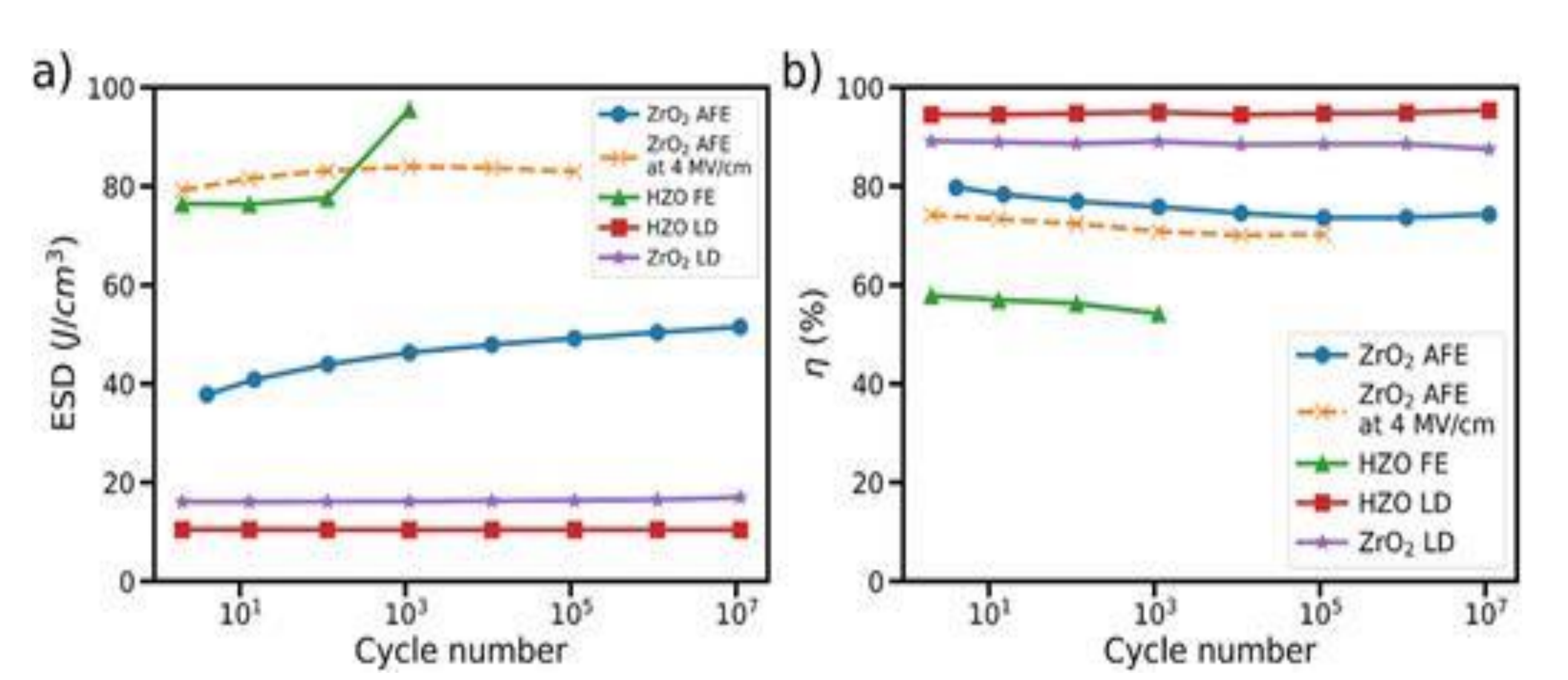
Experimental work

Silva et al., Submitted



- The insertion of a 2.3 nm dielectric Al_2O_3 in a sub-10 nm ferroelectric La:HfO_2-based 2D capacitor enhances the energy storage density and efficiency up to 142 J/cm³ and 69%, respectively, at 7.7 MV/cm.
- The devices exhibit good endurance (10^6 cycles) and thermal stability (up to 120 ºC).

Magagnin et al., APL Materials, 10.1063/5.0220110



- Antiferroelectric ZrO_2 thin film strikes a balance between ferroelectric and linear dielectric behavior, showing reduced losses compared to the ferroelectric sample but an energy storage density as high as 52 J/cm³ at 3.5 MV/cm.
- This value can be further increased up to 84 J/cm³ at a higher electrical field (4.0 MV/cm), with an efficiency of 75%, among the highest values reported for fluorite-structured materials.

Achievements

The NanOx4EStor consortium has published 13 ISI papers (and 3 other are submitted) in the first 2.5 years of the project in high visibility journals including Advanced Functional Materials, Advanced Science, Applied Physics Reviews, Materials Horizons, APL Materials, among others, with a cumulative I.F. above 125.
In addition, 32 conference publications were presented at prestigious international conferences and symposia, and 2 symposium/minicolloquia at European conferences (E-MRS 2023 Fall meeting and CMD-31) were organized.

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