

# PEPR\* DIADEM

## Overall description

**D**iscovery **A**cceleration for the  
**D**eployment of **E**merging **M**aterials

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Mario Maglione / CNRS  
Alexandre Legris / CNRS*

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\*Priority Equipment and Research Program



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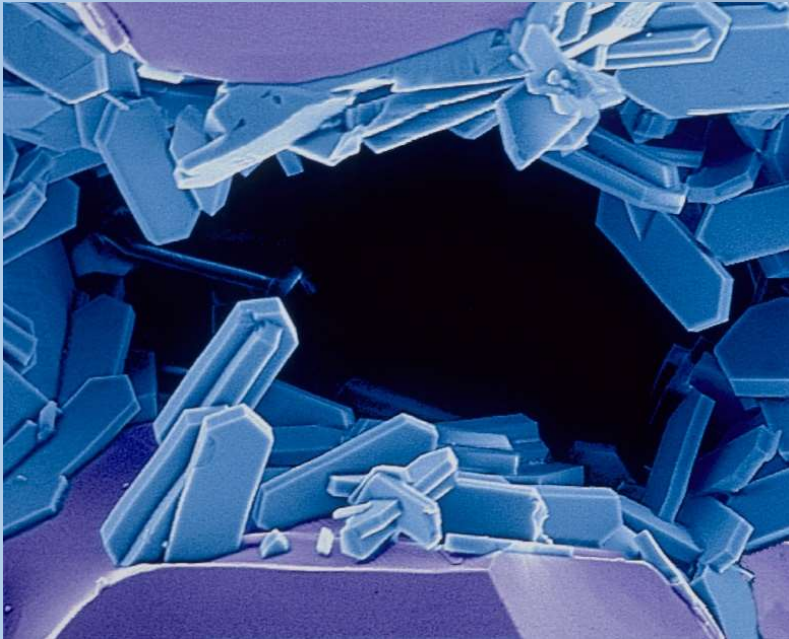


# ACCELERATED MATERIALS DISCOVERY

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# MATERIALS DISCOVERY

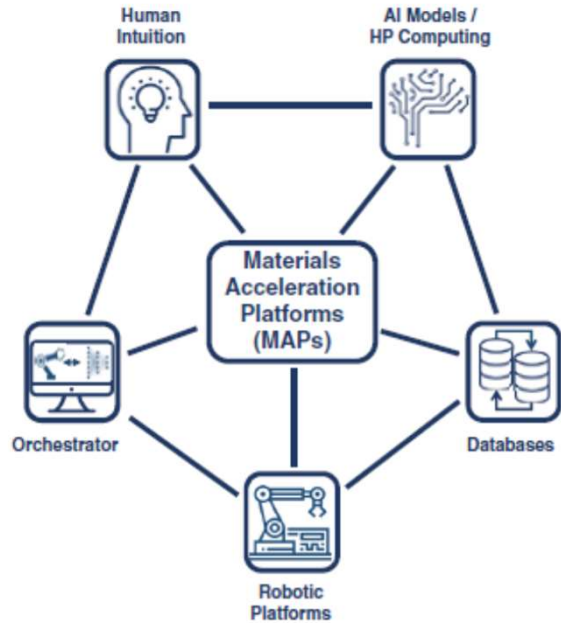


## CHALLENGES

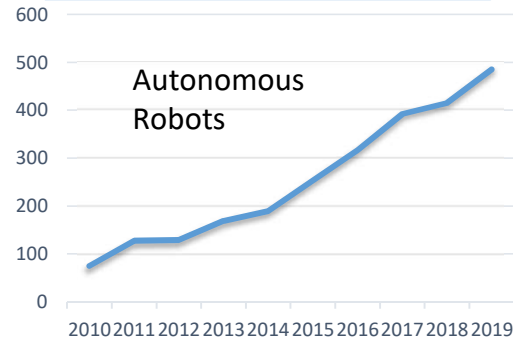
- Numerous technologies rely on the materials discovery: energy, transport, health, digital transition....
- The deployment of novel materials is delayed (more than a decade of try and errors) as their complexity increases
- The Green Deal context and sustainable growth requirements : life cycle assessment, energy sobriety, decrease of the impact on critical resources

Artificial Intelligence can help facing these challenges

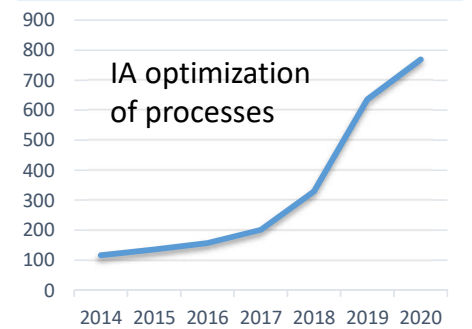
# ACCELERATION FROM THE LAUNCH OF THE MATERIAL GENOME INITIATIVE IN US



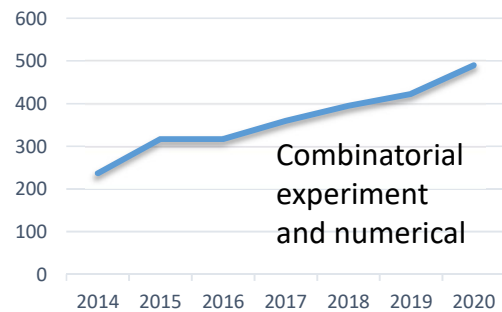
2553 Patents



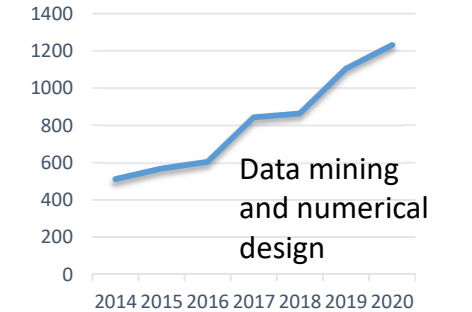
2347 Publications



2539 Publications

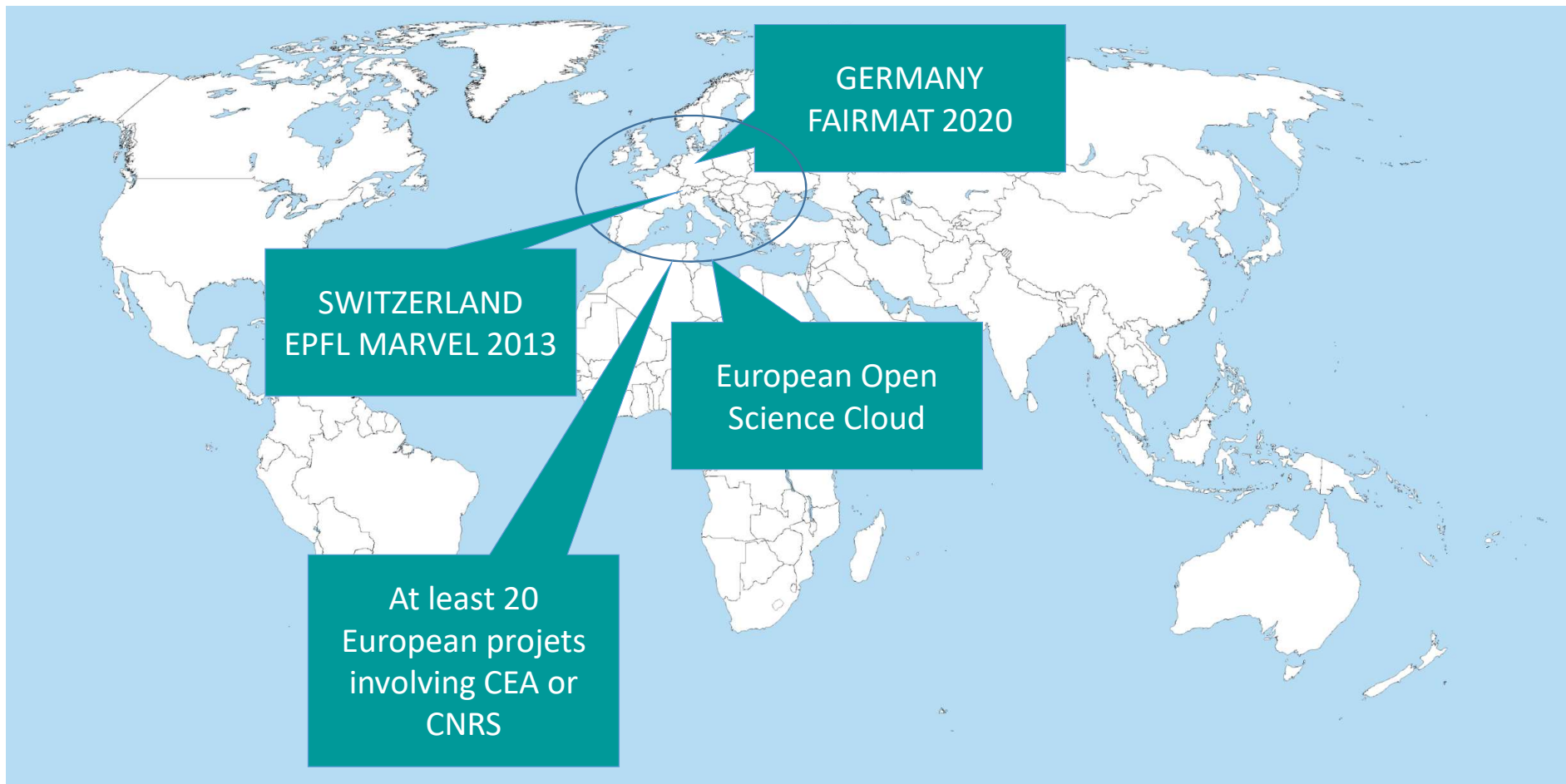


5726 Publications

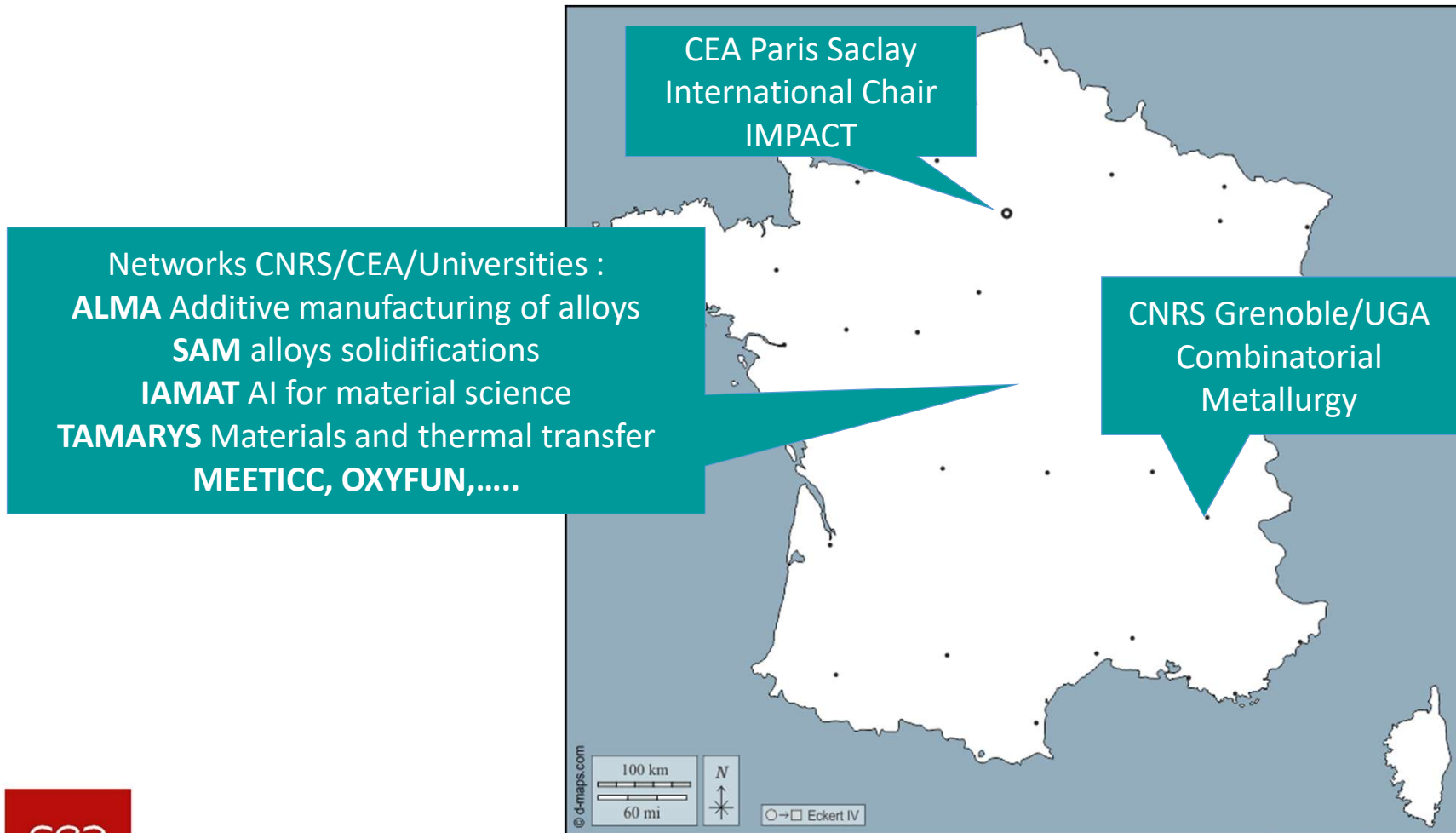




## EUROPEAN PROJECTS



# NATIONAL PROJECTS



# ORGANISATION AND PRINCIPLES OF DIADEM

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## GUIDELINES AND SPECIFICITIES

### CHALLENGES

- Accelerated materials discovery for the main transitions : energy (batteries, hydrogen, nuclear for the future...), environnement, digital (électronics...), health
- Substitution of critical materials and/or toxics
- Diversity of materials and processes (this is a DIADEM specificity)

### GOALS

- Build in France a network of platforms aiming at accelerated discovery of materials
- Open these platforms to the scientific community through open Call for Projects and beyond DIADEM (end 2030)
- National building of a synergy between materials science and artificial intelligence
- Take part into international initiatives



## PEPR DIADEM TOOLS

### Platforms

- Numerical Design
- High Throughput Synthesis and Shaping
- High Throughput Characterization
- Data Bases & AI Tools

### Targeted Projects (started)

- Methodological Demonstrators
- Platforms Building

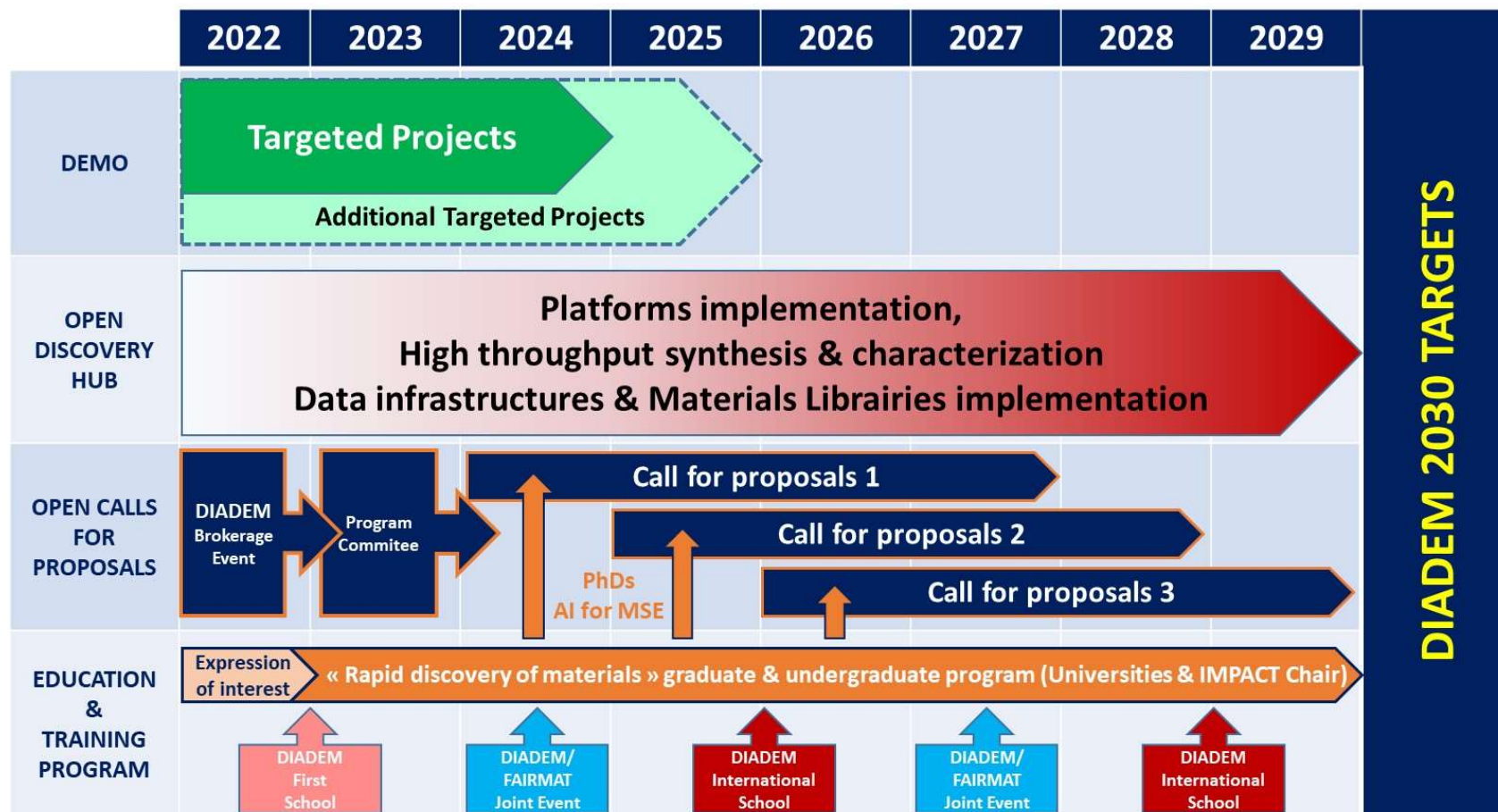
### Projects calls (*3 runs 2024-2025-2026*)

- 30 to 40 projects 750 k€ to 1M€ each
- Open to all French labs
- Possible opening to international cooperation and companies

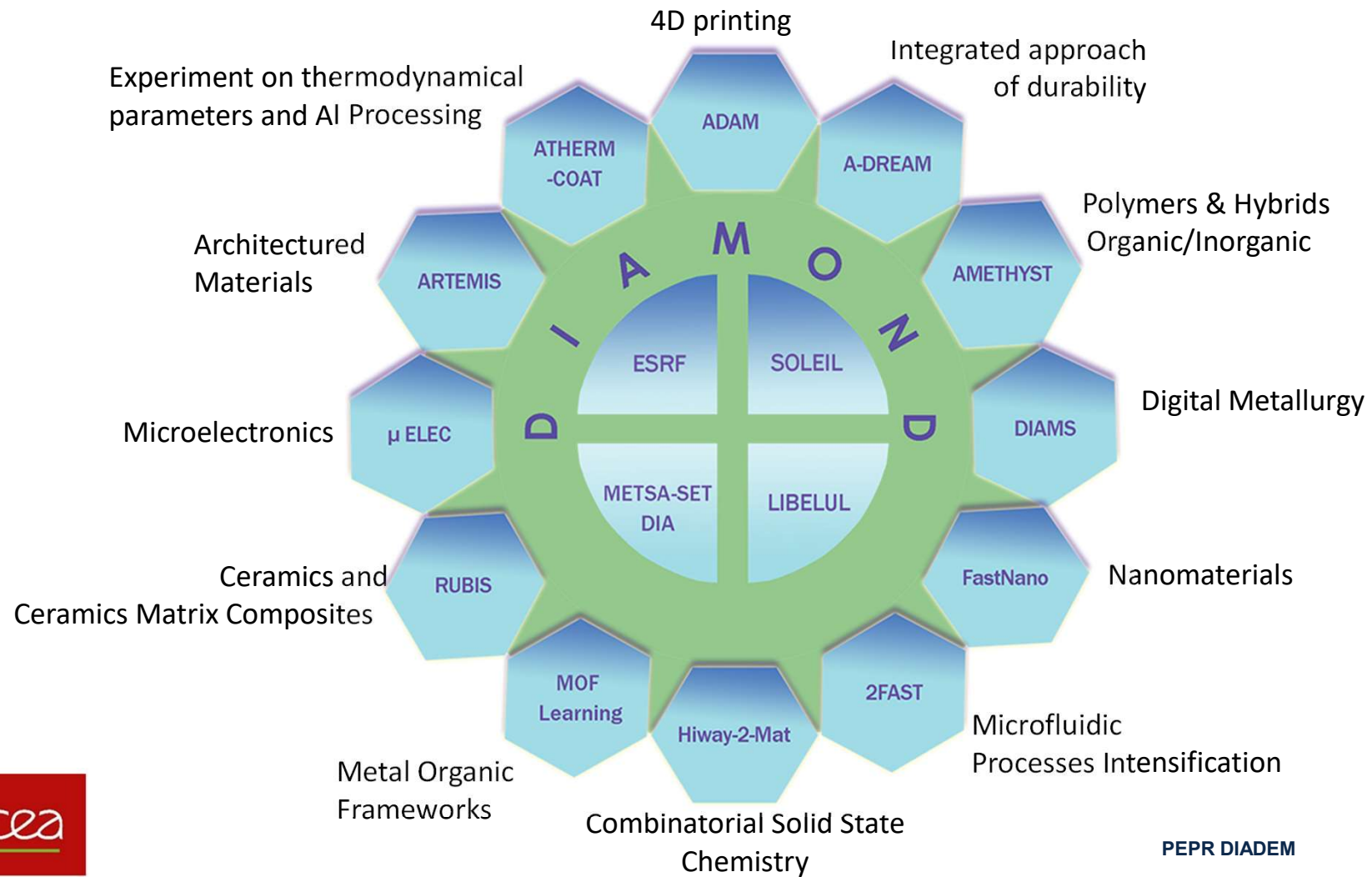
### Education calls (*5 projects*)

- Education tools
- International schools

# GLOBAL PLANNING OF THE PEPR DIADEM



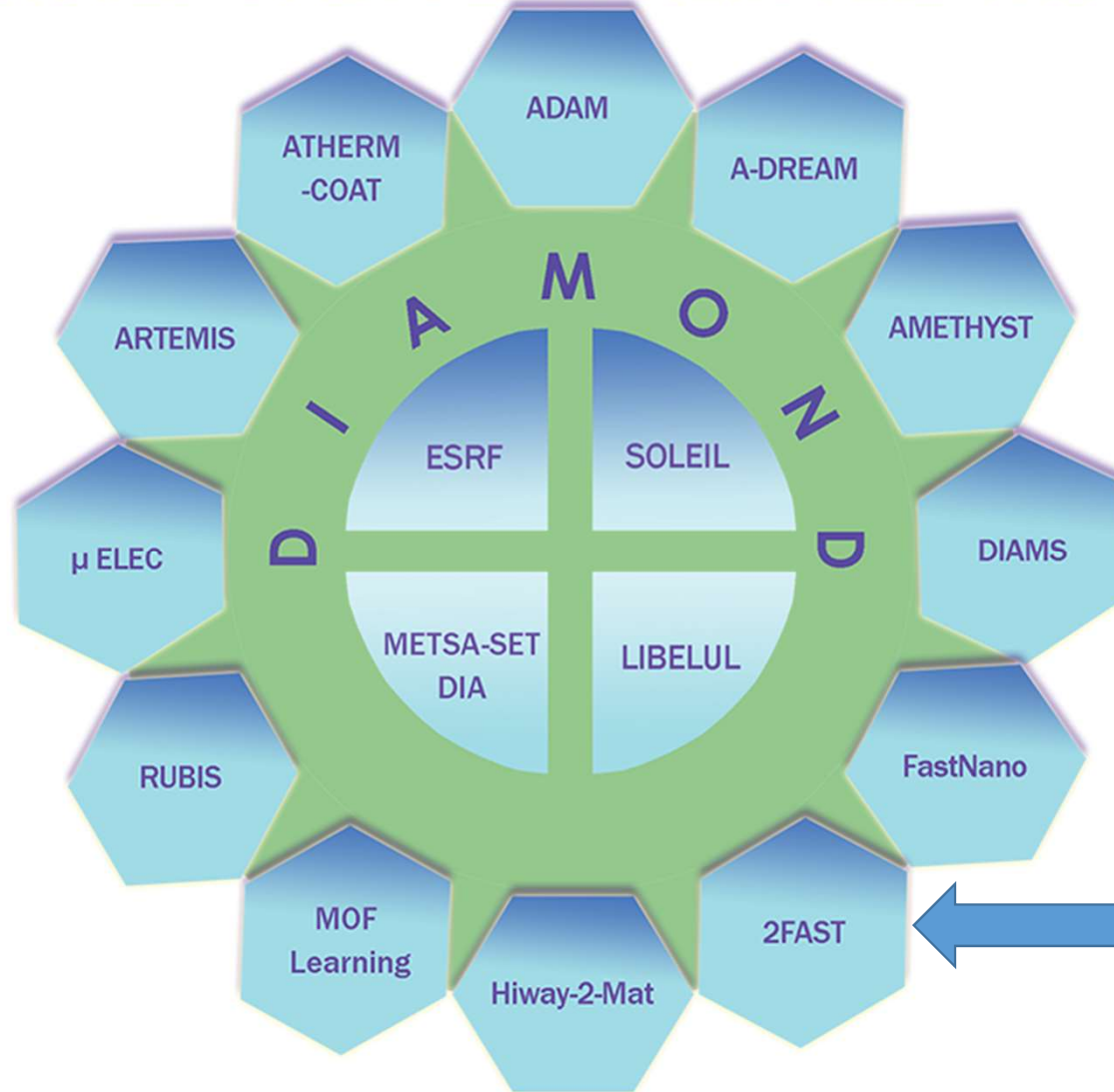
# UNDERGOING 17 DEMONSTRATOR PROJECTS AI ASSISTED OPEN PLATFORMS ARE THE DIADEM CORE



**Budget  
45 M€**

PEPR DIADEM

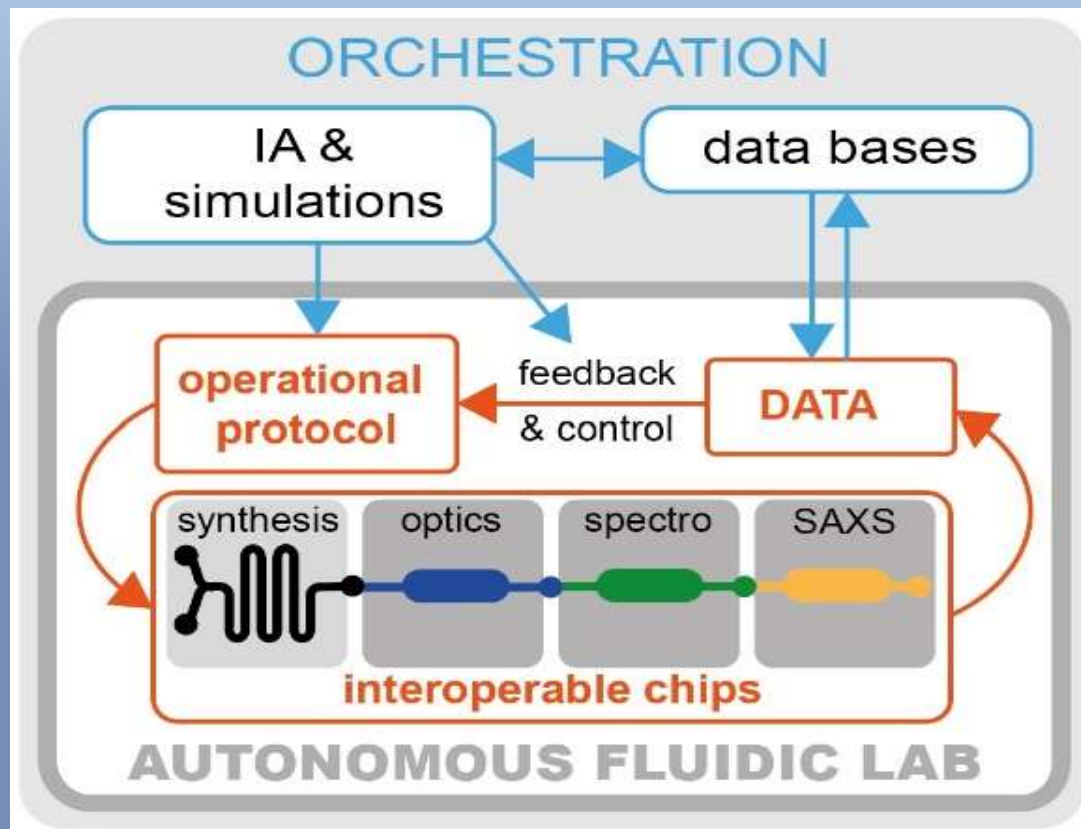
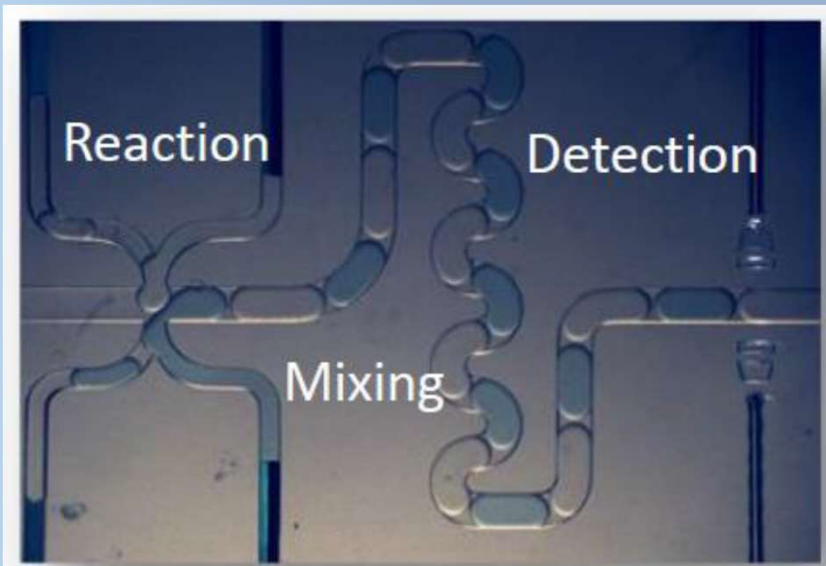
# UNDERGOING 17 DEMONSTRATOR PROJECTS AI ASSISTED OPEN PLATFORMS ARE THE DIADEM CORE



# MICROFLUIDICS PROCESS INTENSIFICATION



ISEC, LIONS  
ICMCB, LGC, LOF

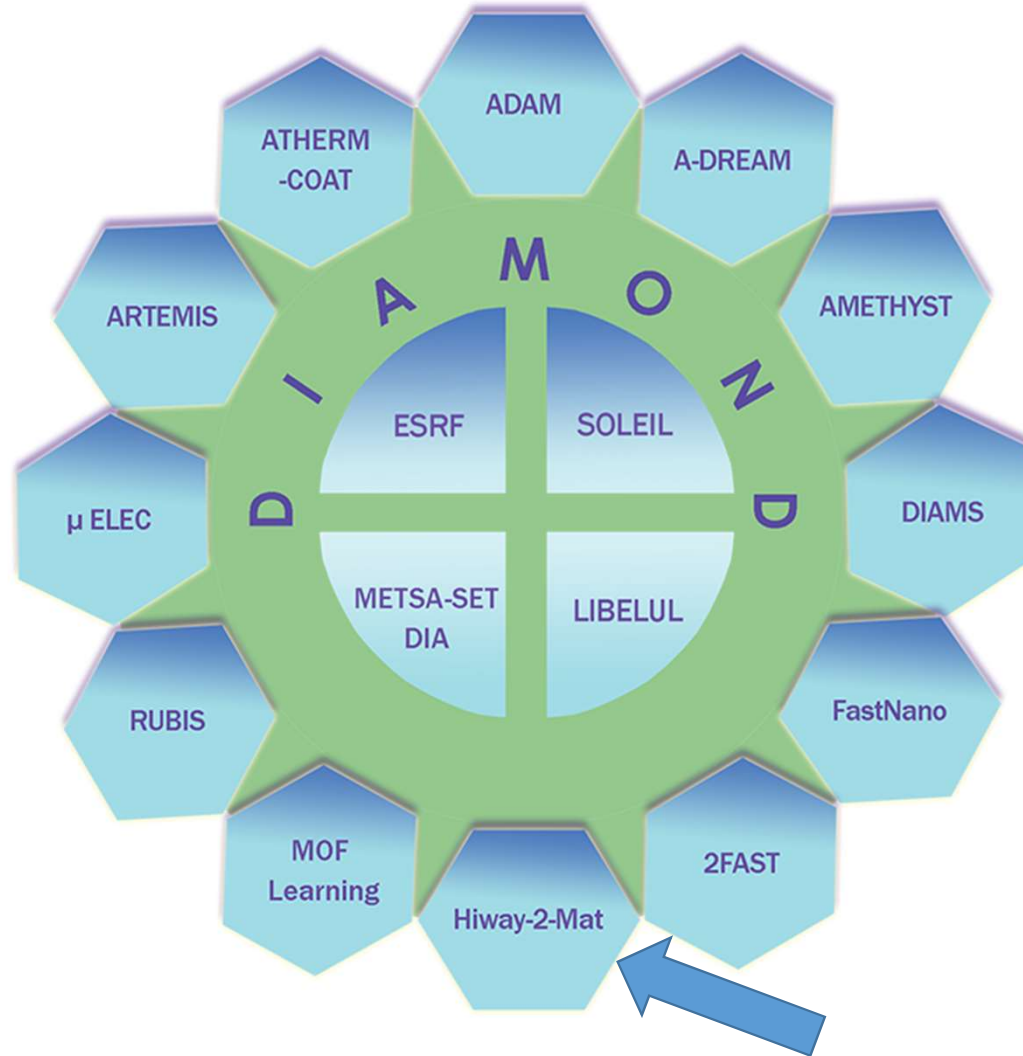


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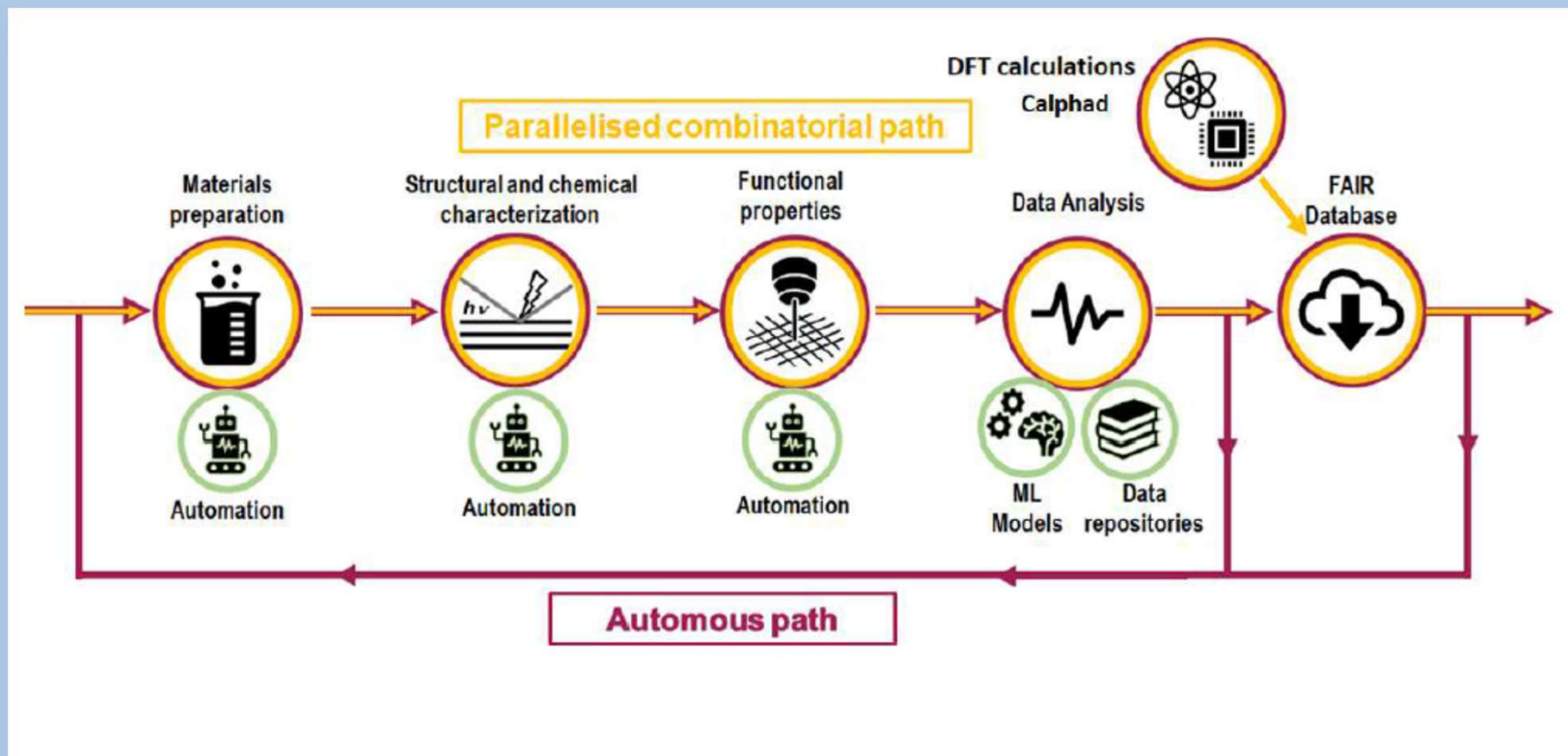




# UNDERGOING 17 DEMONSTRATOR PROJECTS AI ASSISTED OPEN PLATFORMS ARE THE DIADEM CORE



# COMBINATORIAL SOLID STATE CHEMISTRY: HIWAY-2-MAT



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# COMBINATORIAL SOLID STATE CHEMISTRY: HIWAY-2-MAT

Automated structural analysis and deep learning looking for novel hybrid perovskites for photovoltaics

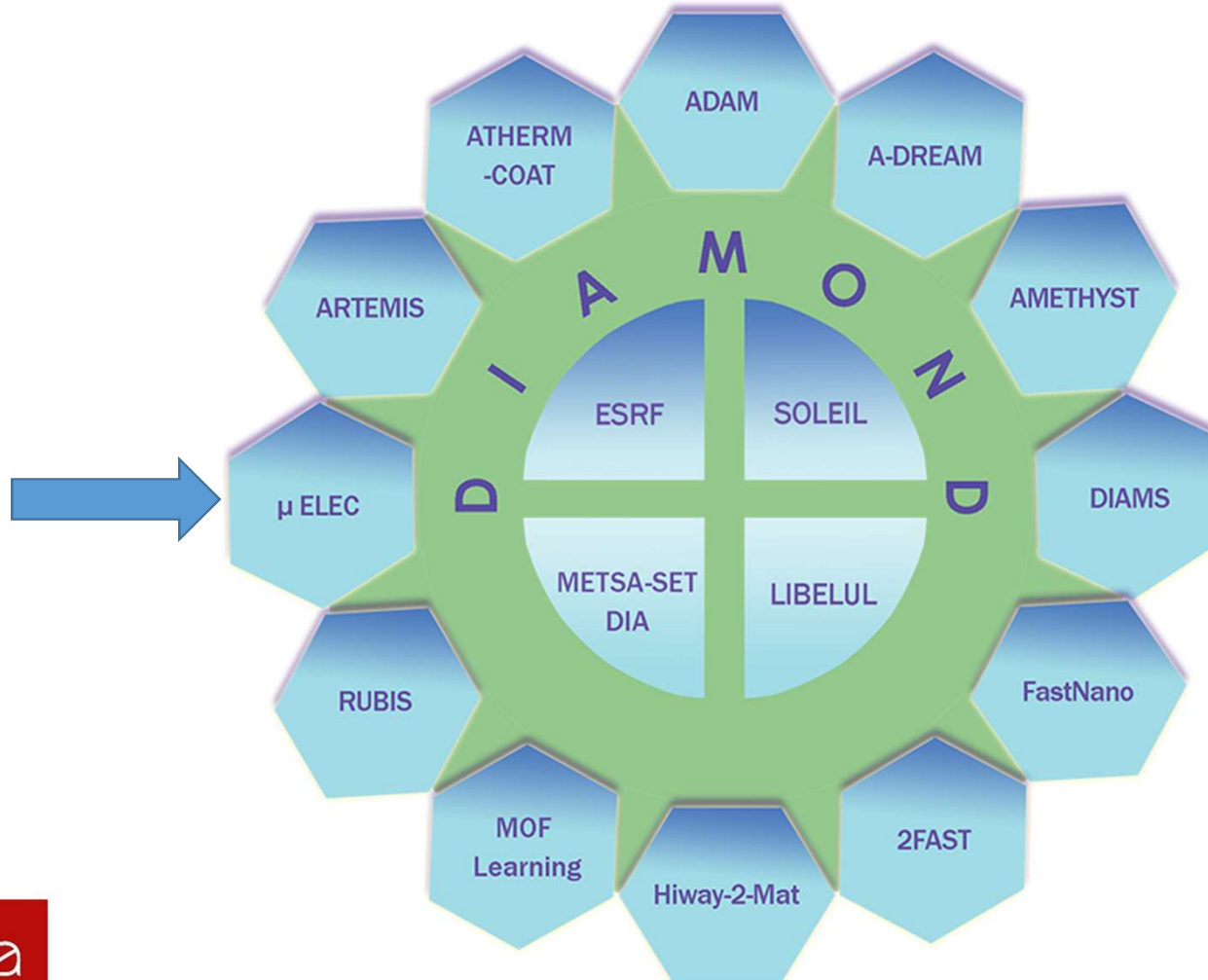


“Perovskite or Not Perovskite? A Deep Learning Approach to Automatically Identify New Hybrid Perovskites from X-ray Diffraction Patterns” F. Massuyeau, T. Broux, F. Coulet, A. Demessence, A. Mesbah, R. Gautier, *Advanced Materials*, 34, 41, (2022) (doi/10.1002/adma.202203879)

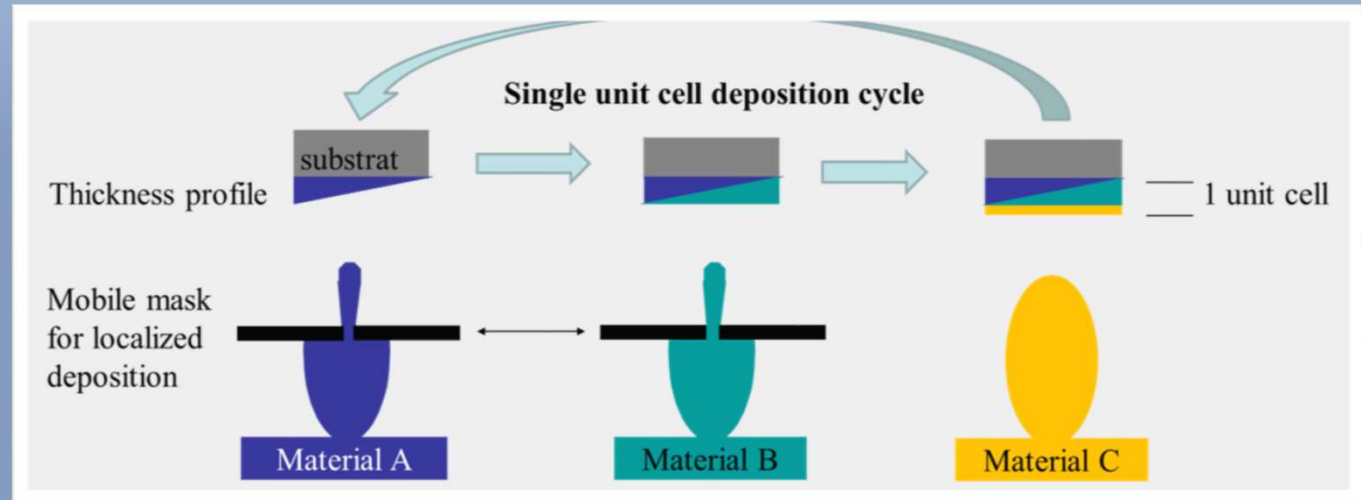
Romain.Gautier@cnsr-imn.fr



# UNDERGOING 17 DEMONSTRATOR PROJECTS AI ASSISTED OPEN PLATFORMS ARE THE DIADEM CORE



# COMBINATORIAL PLD DEPOSITION @GREMAN TOURS



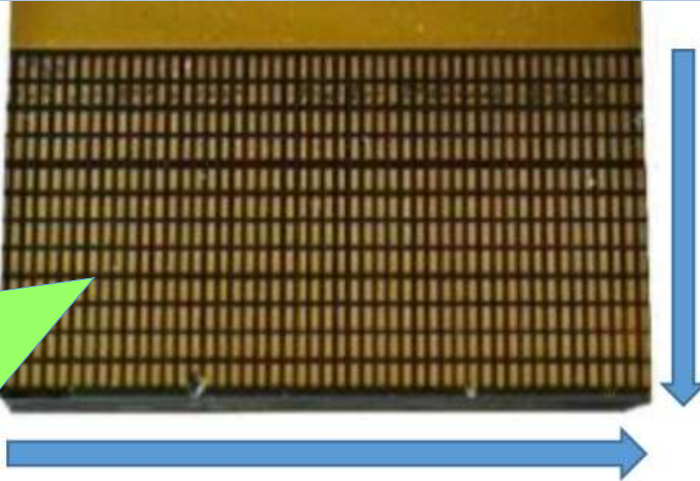
Jerome Wolfman <wolfman@univ-tours.fr>





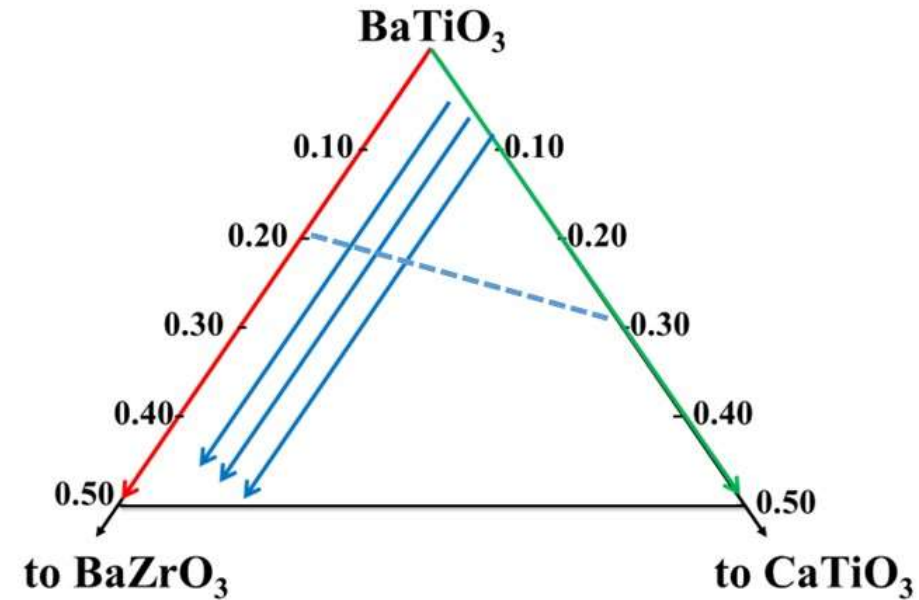
# COMBINATORIAL PLD DEPOSITION 500 SAMPLES ON A SINGLE SUBSTRATE

-High throughput synthesis  
-Robot structural and functional



Fixed Zr over 12 capacitors

High entropy oxide  $(\text{Ba,Ca})(\text{Ti,Zr})\text{O}_3$   
Zr content increasing along a line

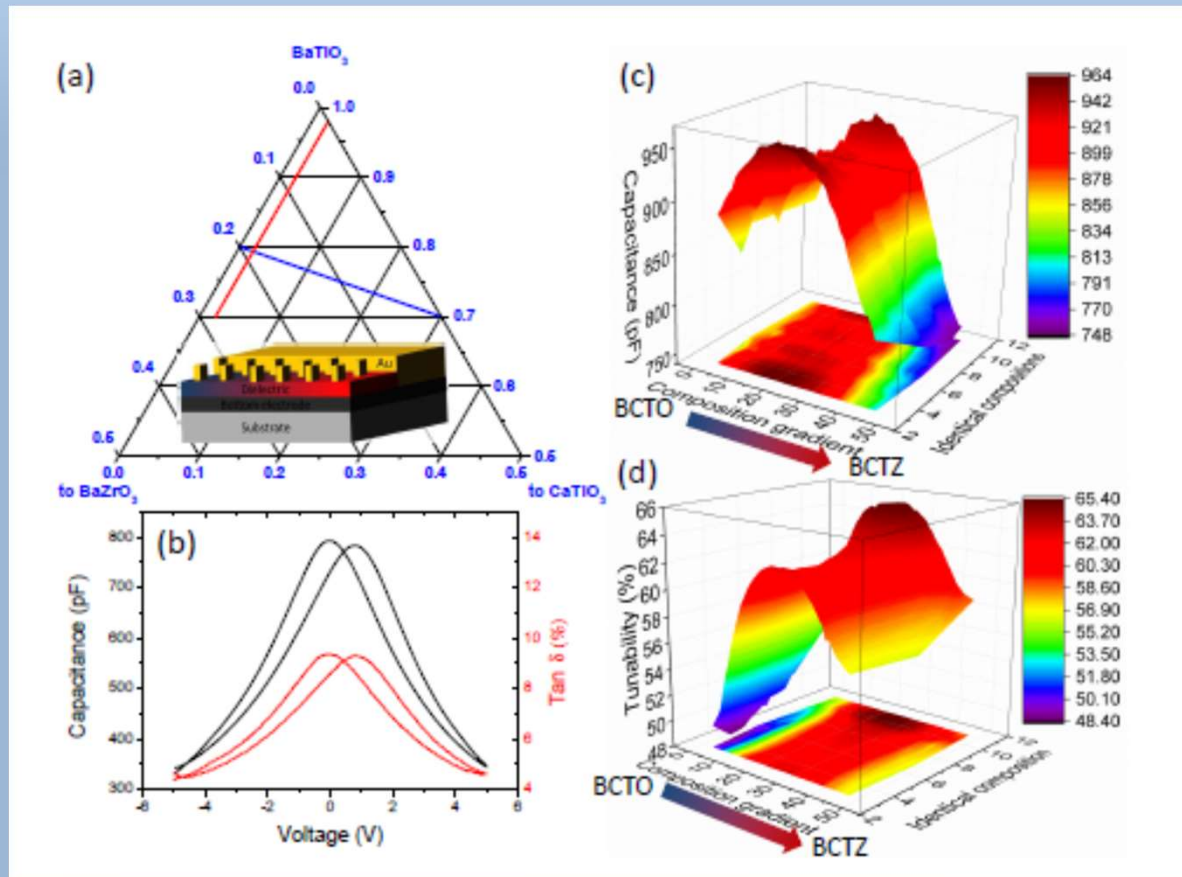


**Tunability Investigation in the  $\text{BaTiO}_3$ - $\text{CaTiO}_3$ - $\text{BaZrO}_3$  Phase Diagram Using a Refined Combinatorial Thin Film Approach.**

Daumont, C.; Simon, Q.; Payan, S.; Gardes, P.; Poveda, P.; Maglione, M.; Negulescu, B.; Jaber, N.; Wolfman, J

J. Coatings **2021**, 11, 1082

# MAXIMISE THE DIELECTRIC NON-LINEARITY



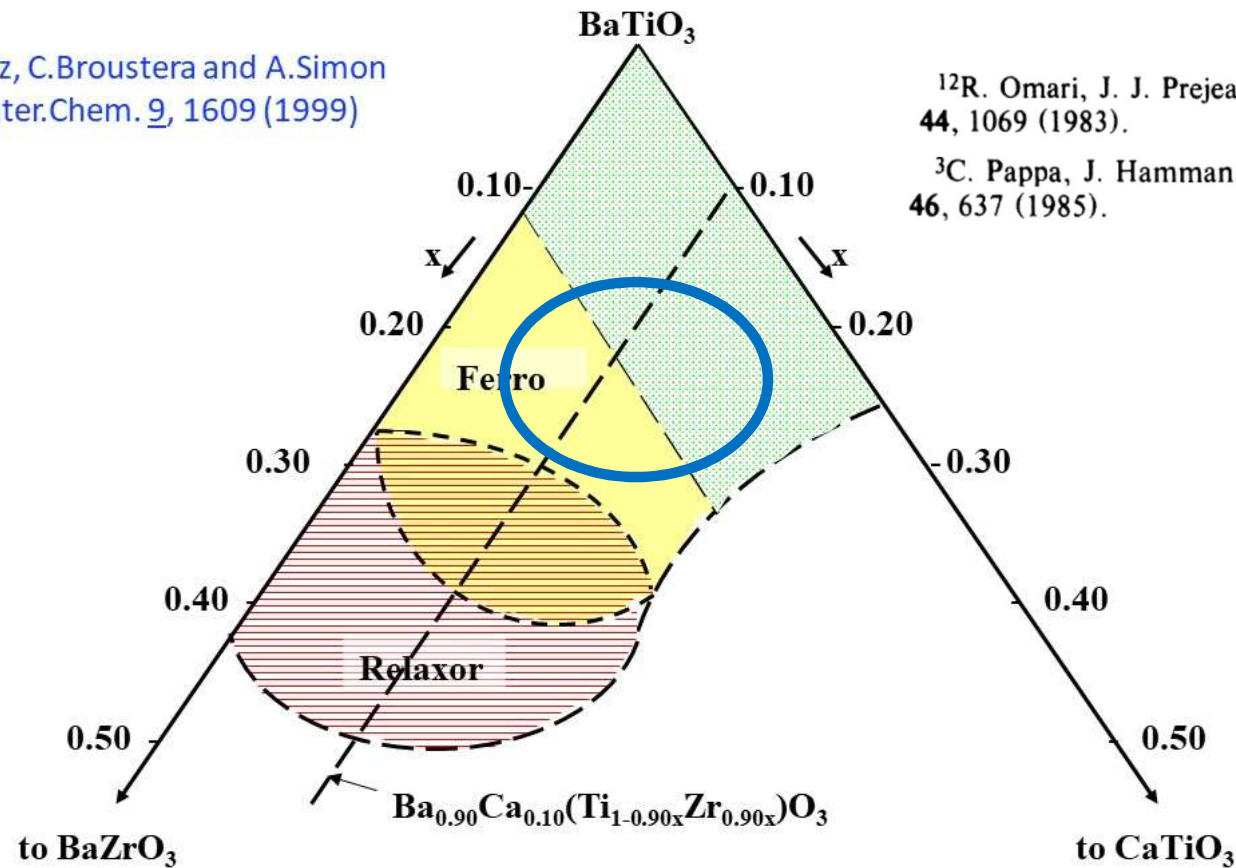
C Daumont et al  
JAP 119, 094107 (2016)

# EXTREME NON-LINEARITY AT THE CROSS-OVER FROM ORDER TO DISORDER

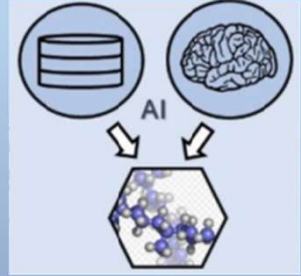
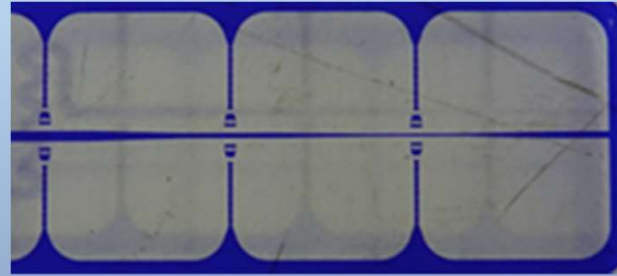
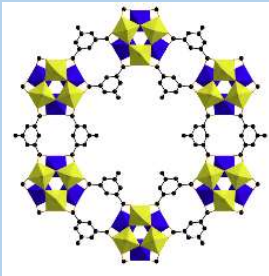
J.Ravez, C.Broustera and A.Simon  
J.Mater.Chem. 9, 1609 (1999)

<sup>12</sup>R. Omari, J. J. Prejean, and J. Souletie, J. Phys. (Paris)  
**44**, 1069 (1983).

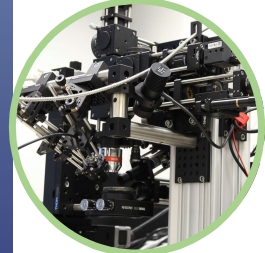
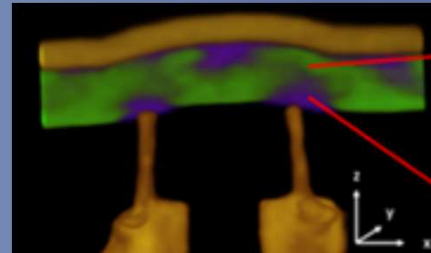
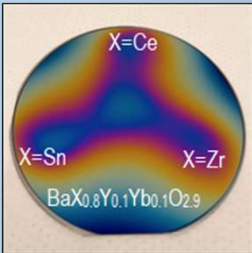
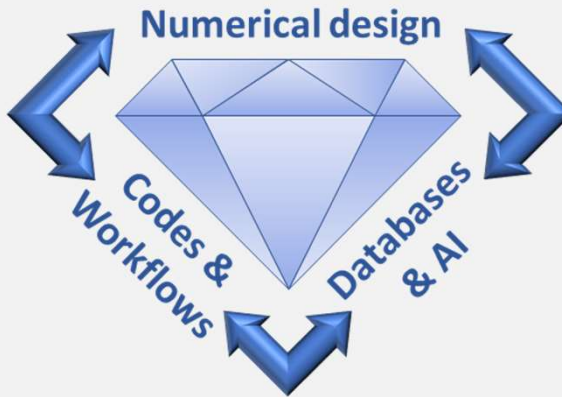
<sup>3</sup>C. Pappa, J. Hamman, and C. Jacoboni, J. Phys. (Paris)  
**46**, 637 (1985).







# DIADEM... MATERIALS... DIFFERENTLY



M.Maglione GDR MEETICC 01/06/2023







## BUDGET SUMMARY

Action	Budget	%	Comment
Targeted projects and platforms	45.6 M€	54.2%	including 34 M€ (40%) For equipments
Project calls	32 M€	38 %	30 to 40 projects
Education/Formation	3 M€	3,6 %	5 projects
Internationalisation, Scientific meetings Management	3,5 M€	4.2%	Including Schools Workshops