Materials for Energy from AI-driven approaches at ENS and in France

A. Marco Saitta

Laboratoire de Physique de l'Ecole Normale Supérieure (LPENS)
Dir GDR IAMAT – CoPil DIAMOND / PEPR DIADEM – PEPR Batteries

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Outline

- AI & ab initio for energy, hydrogen, carbon dioxide storage
- Materials for energy storage, supercapacitors
- Supercapacitors modeling: ab initio calculations, molecular dynamics
- AI and Machine Learning Interatomic Potentials
- French/European ecosystem for AI & Materials

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Accelerated Design

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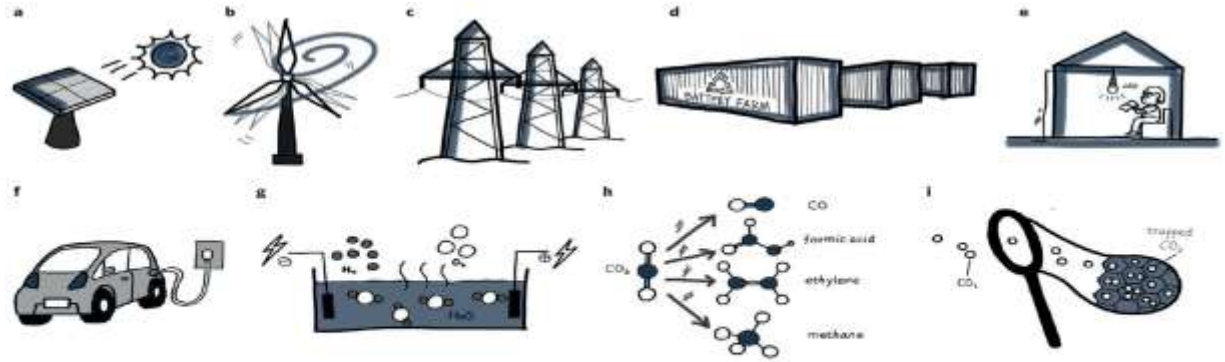
Materials for energy storage

- Energy transition, energy storage, new materials
- Principle of energy-storage materials (ESM): two “states”, one as “storage configuration”, the other one as “release” configuration
- Need to efficiently predict transition mechanisms with a specific control, under a multitude of possible external conditions



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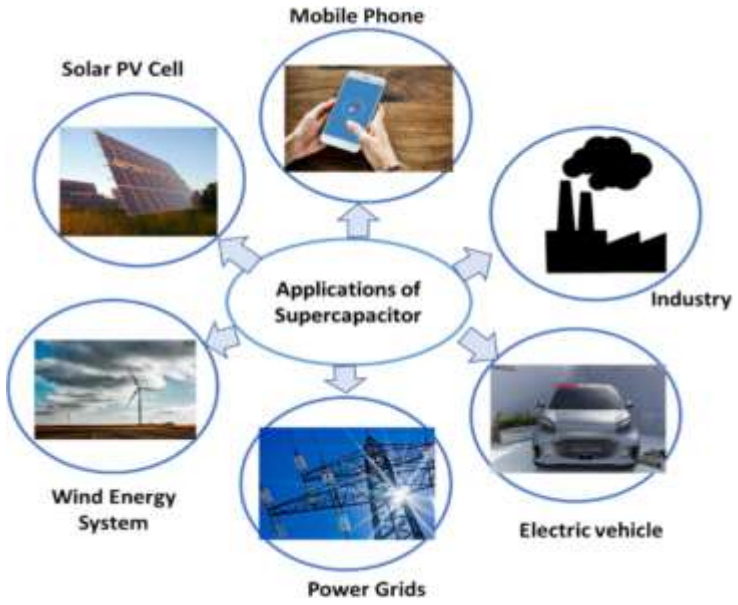
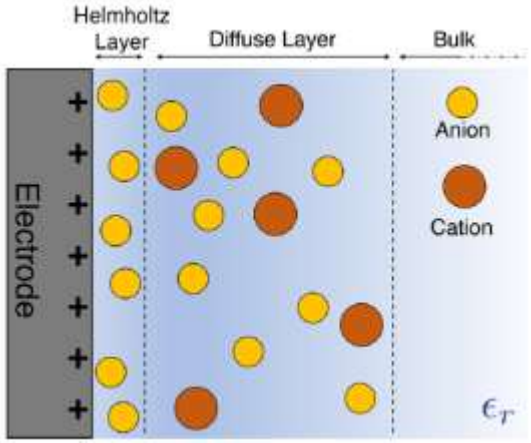
Batteries & supercapacitors

- Batteries: Store energy chemically (Faradaic reactions). High energy, slow delivery.
- Supercapacitors: Store energy electrostatically (physical charge separation).



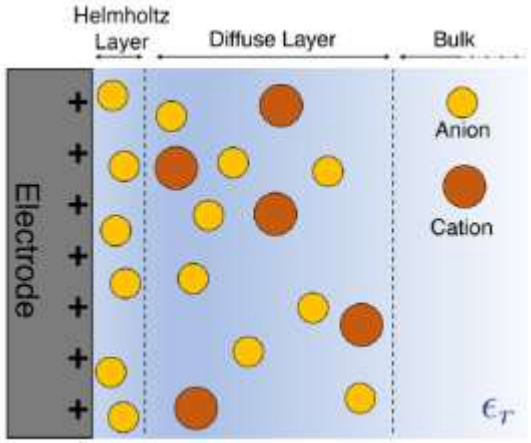
Supercapacitors

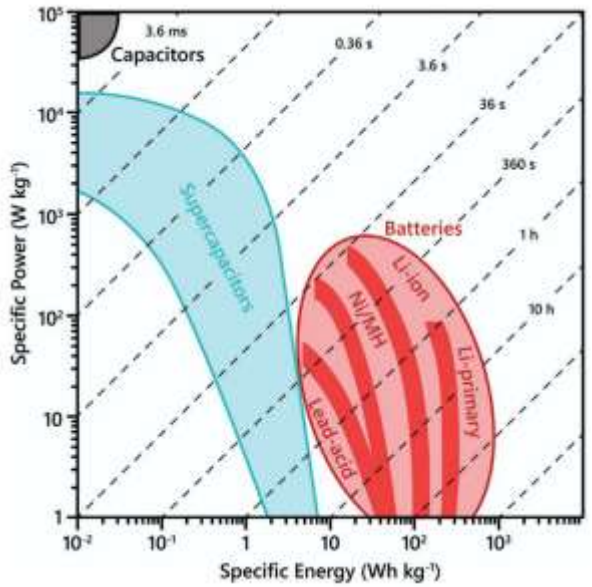
- Supercapacitors store energy using either ion adsorption or fast surface redox reactions
- They complement batteries when high-power density or uptake is needed

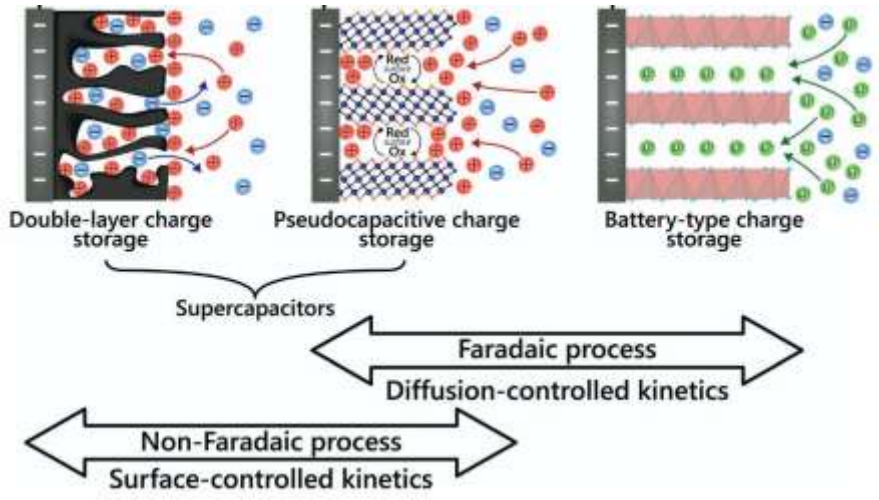


Supercapacitors

- Electric Double Layer (EDLC): Ions form a "double layer" at the electrode/electrolyte interface (Helmholtz layer).
- Pseudocapacitance: Fast, reversible surface redox reactions (adds energy density).
- Rapid Charge/Discharge: Seconds vs. hours. Cycle Life: >1,000,000 cycles (vs. ~1,000 for Li-ion).

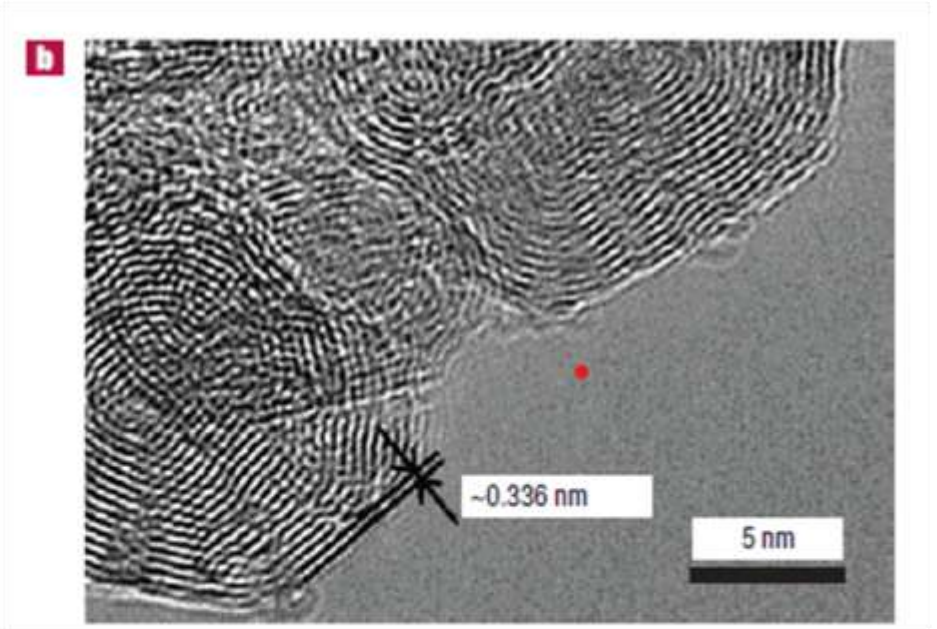


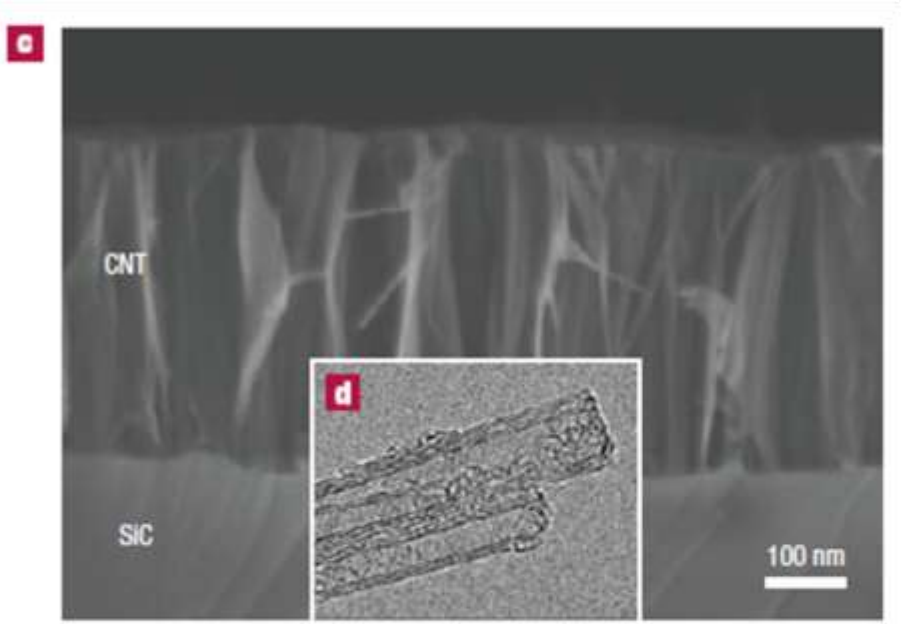




Nanoporous graphitic electrodes for supercapacitors

- Ion desolvation in subnanometer pores increases capacitance
- Need for design of high-energy density electrodes





Simon, P. & Gogotsi, Y. Materials for electrochemical capacitors. *Nat. Mater.* **7**, 845–854 (2008).

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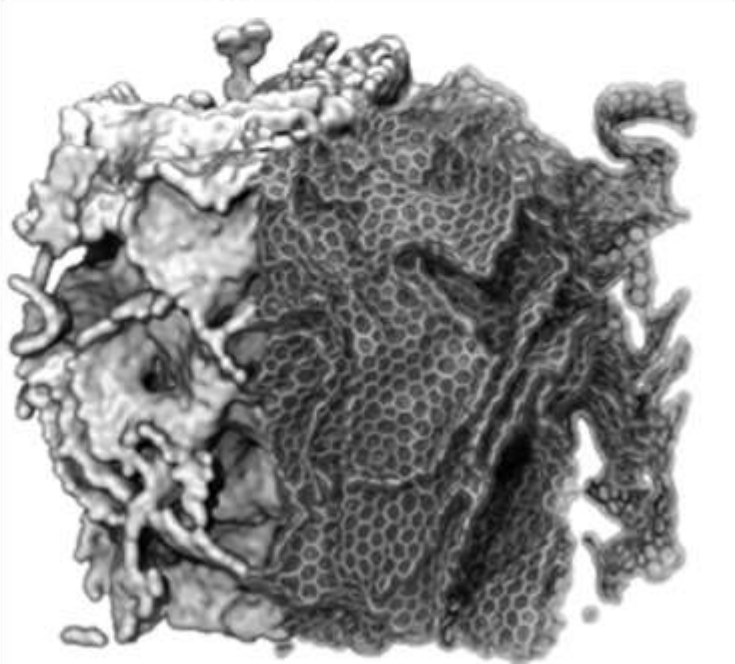
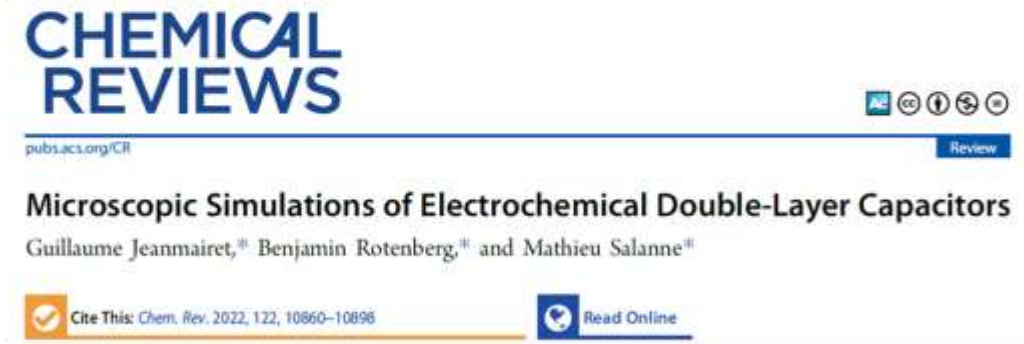
Computational modeling of supercapacitors

- Classical molecular dynamics
- A special ad hoc development for constant applied voltage
- Ions might be coarse-grained
- What about the graphitic electrodes?





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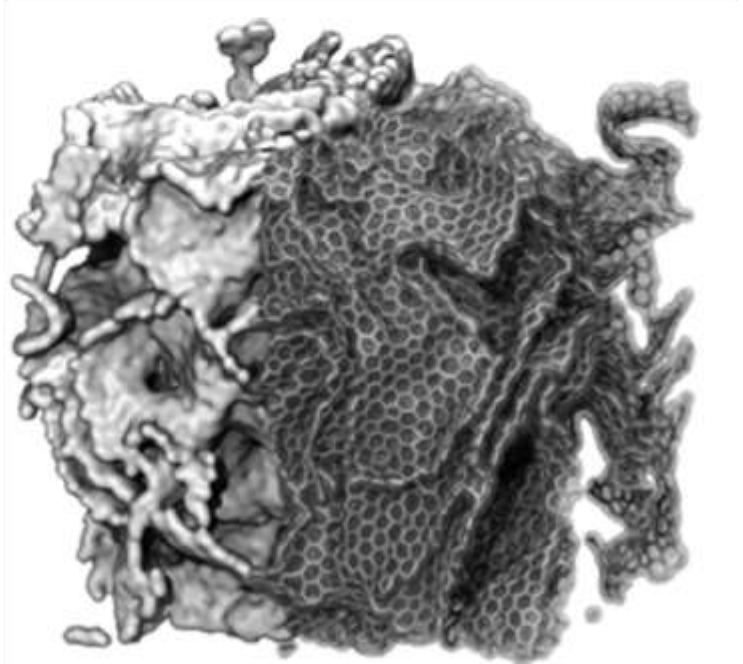
Graphitic electrodes modeling, the dilemma

- Thousands (at best) of C atoms, structural disorder → Classical MD
- Defects, C-C interactions, carbon versatility → Ab initio/DFT



CHEMICAL REVIEWS
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Review

Microscopic Simulations of Electrochemical Double-Layer Capacitors

Guillaume Jeanmairet,* Benjamin Rotenberg,* and Mathieu Salanne*

Cite This: Chem. Rev. 2022, 122, 10860–10898
Read Online

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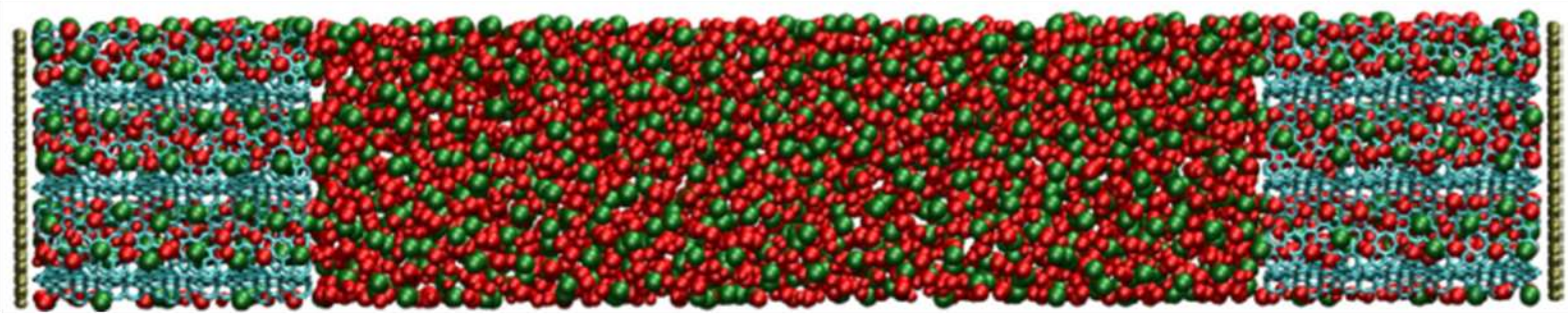
Graphitic electrodes modeling, the choice (so far)

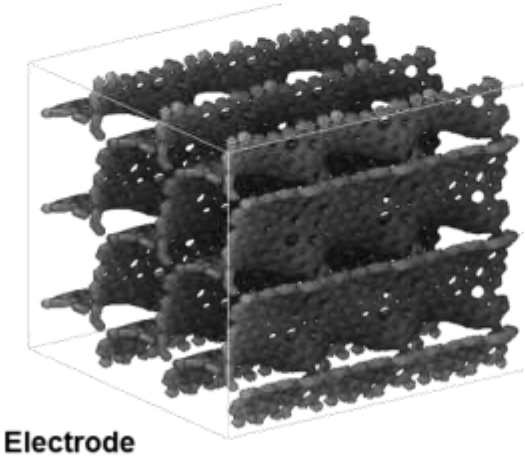


Carbon–carbon supercapacitors: Beyond the average pore size or how electrolyte confinement and inaccessible pores affect the capacitance

Special Collection: The Chemical Physics of the Electrode-Electrolyte Interface

El Hassane Lahrar; Patrice Simon; Céline Merlet

J. Chem. Phys. 155, 184703 (2021)
https://doi.org/10.1063/5.0065150 **Article history**



Electrode

Carbon electrodes are kept completely rigid

DFT and HPC in materials science

MATERIALS ARE KEY TO SOCIETAL WELL BEING

We need novel materials for:

- **Energy harvesting, conversion, storage, efficiency**
- **Environmental protection and reparation**
- **High-tech and high-value industries**
- **Information and communication technologies**
- **Health care and biomedical engineering**
- **Pharmaceuticals** (crystallization, stability, polytypes)
- **Monitoring, provenance, and safety of foods**
- **Fundamental science** (graphene and 2D materials, topological insulators, entangled spins for quantum computing, high-T_c)
- **Experimental science** (detectors, sensors, magnets)

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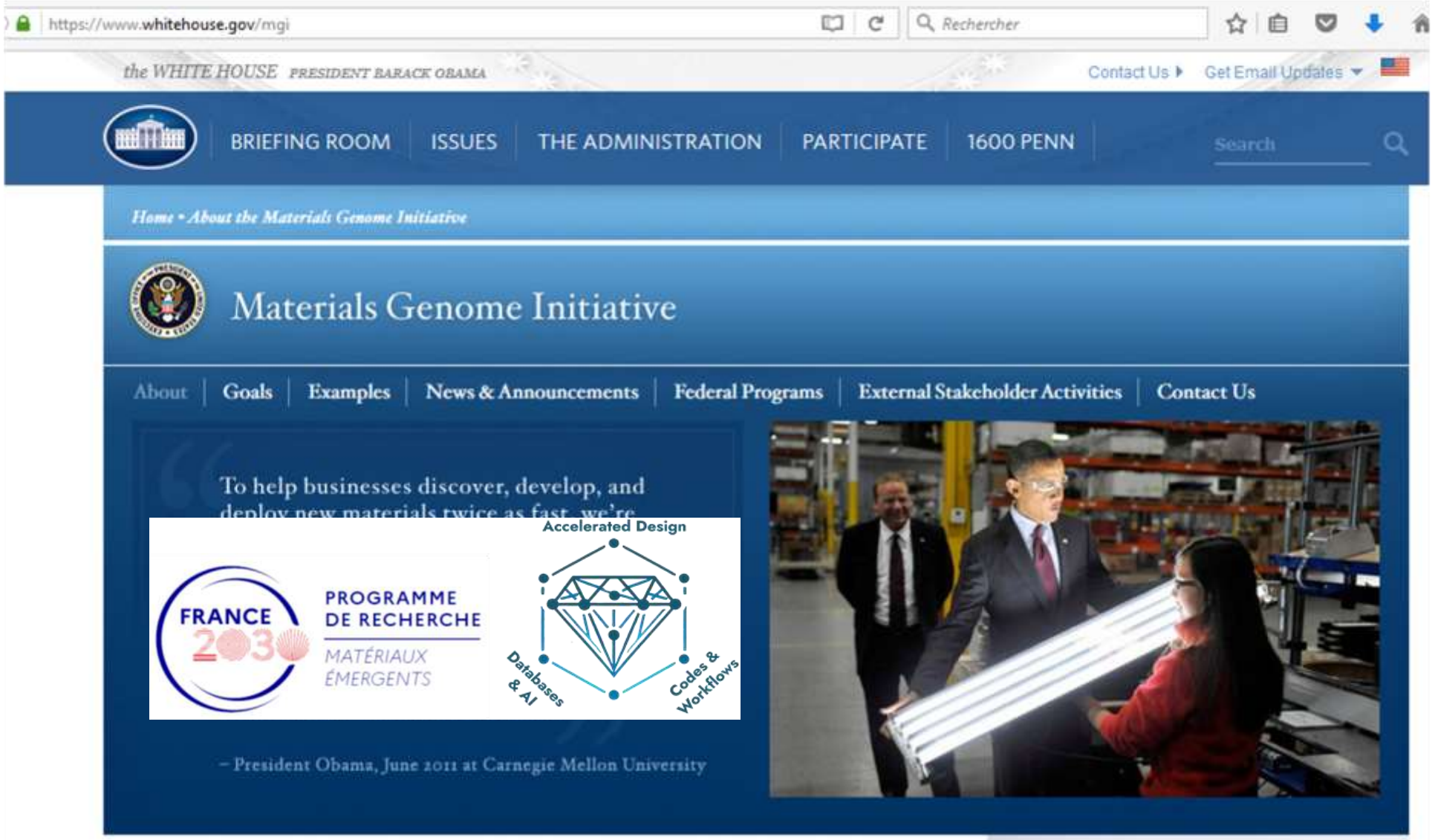
DFT and HPC in materials science



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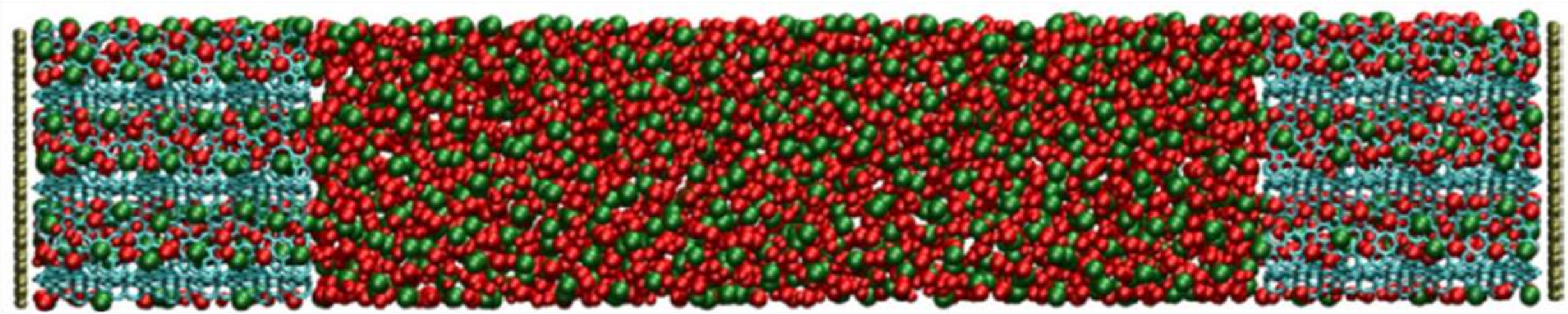

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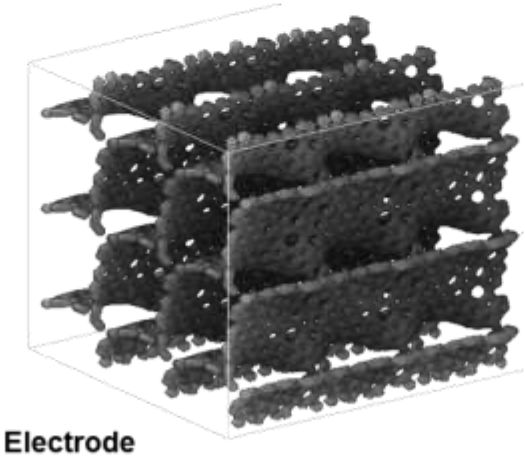

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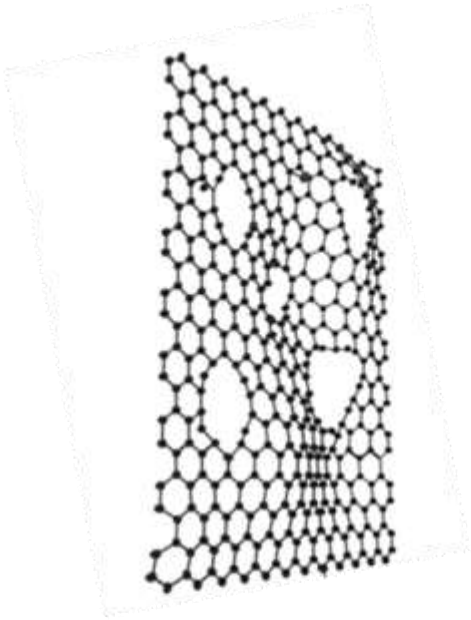
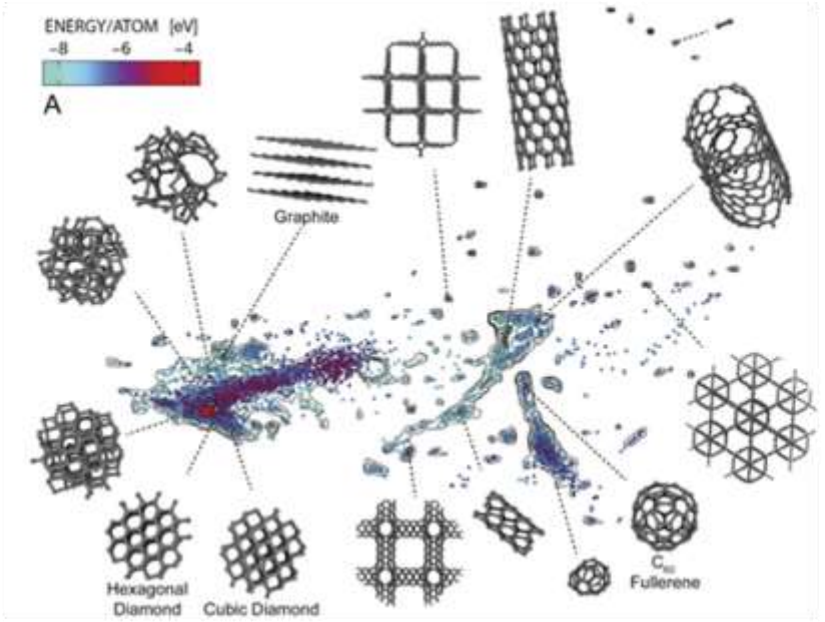
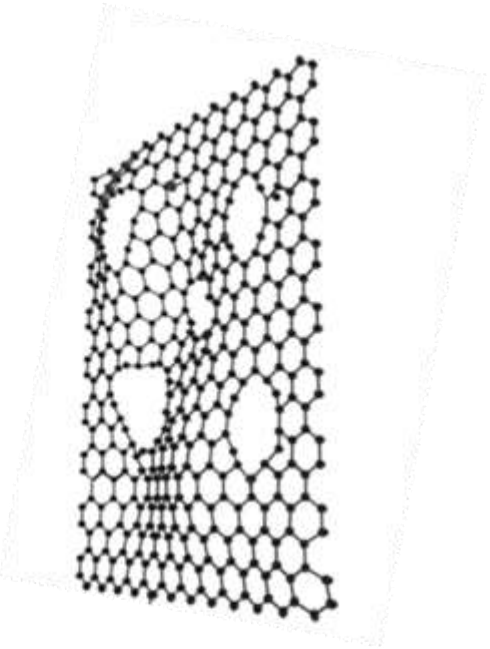
Graphitic electrodes modeling with MLIPs

- Foundation model (MACE), trained on "all" carbon conformations







PhD thesis of Zacharie Waysenson

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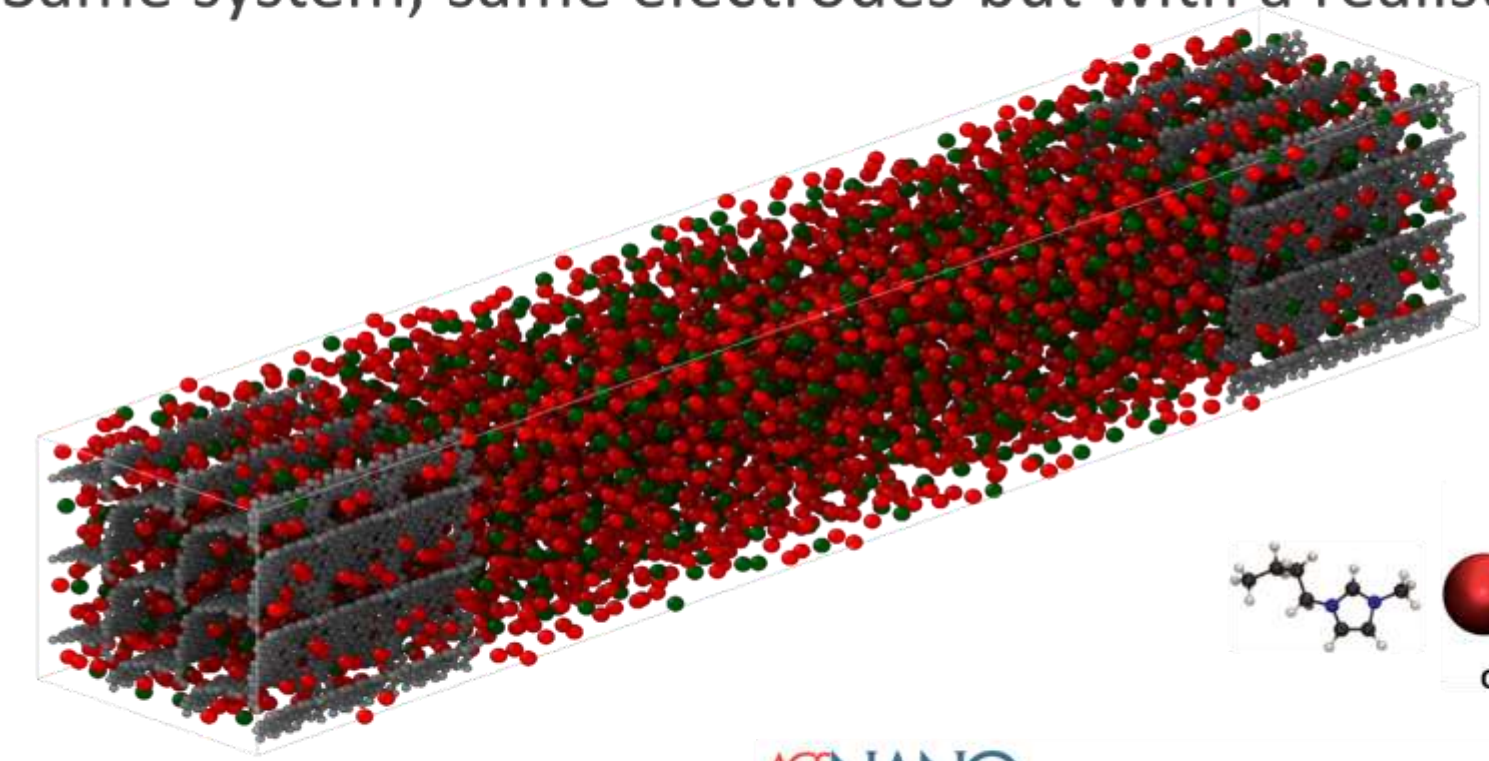
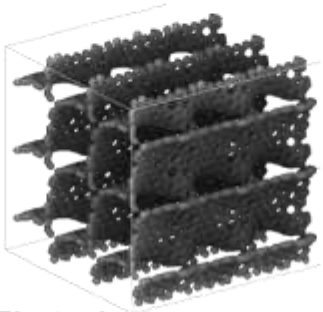
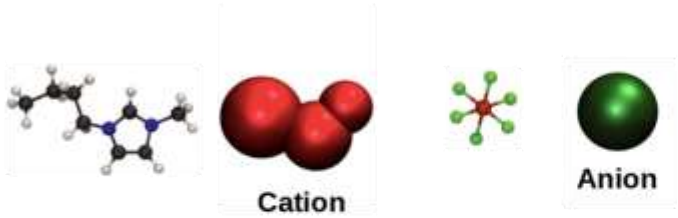
Supercapacitors with (ordered) flexible electrodes

- Same system, same electrodes but with a realistic MLIP enabling flexibility





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Electrode Flexibility Enhances Electrolyte Dynamics during Supercapacitor Charging

Zacharie Waysenson, Arthur France-Lanord, Alessandra Serva, Patrice Simon, Mathieu Salanne, and A. Marco Saitta*

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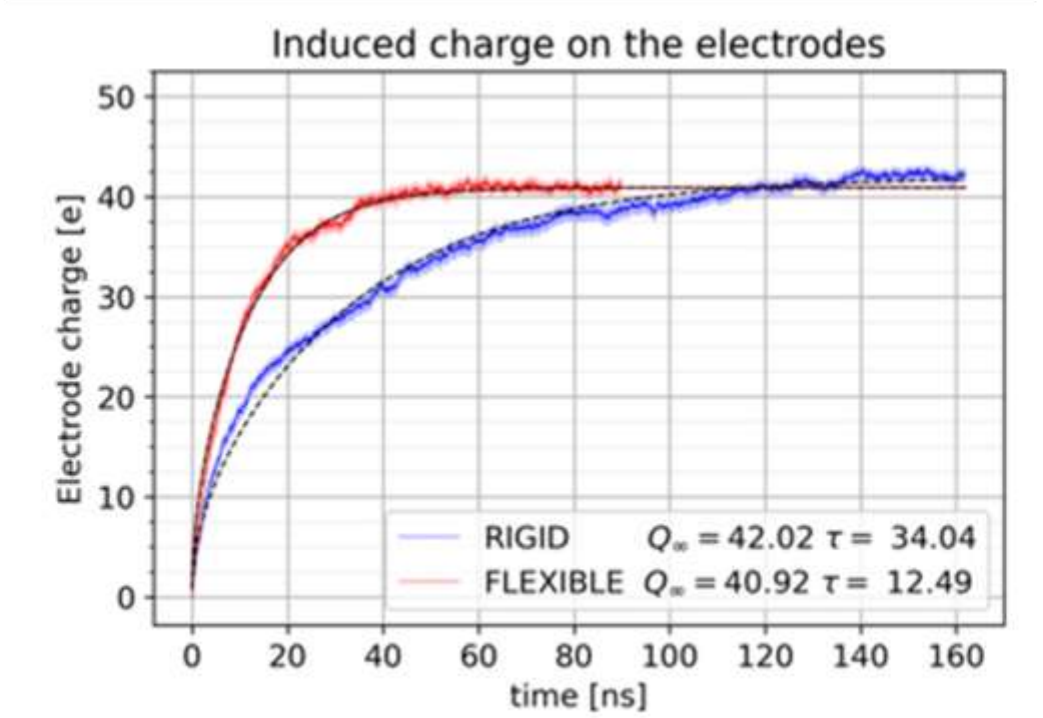
Supercapacitors with (ordered) flexible electrodes

- Same system, same electrodes but with a realistic MLIP enabling flexibility
- Charging time reduced by a factor 3 !



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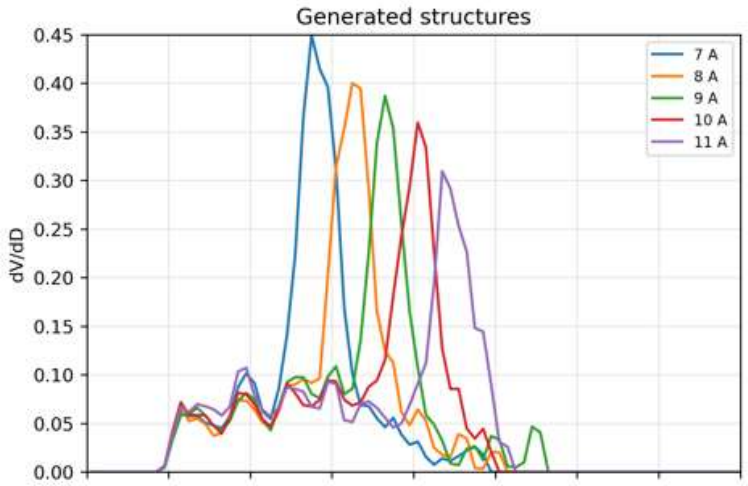
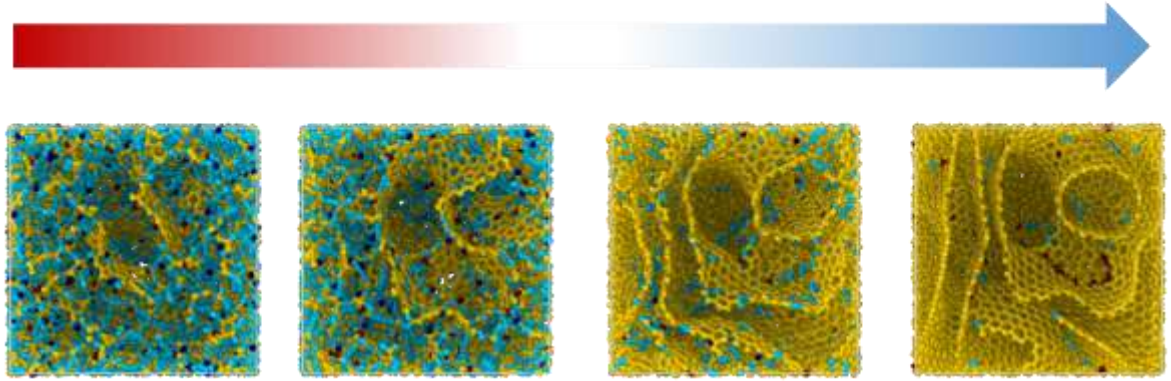
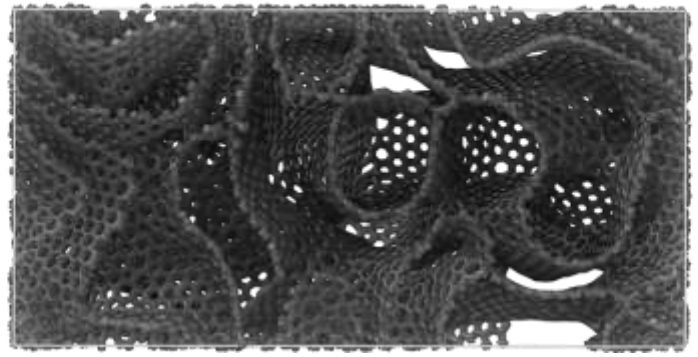
Supercapacitors with realistic disordered electrodes?

- MLIP-driven design of disordered electrodes
- Fine-tuning the morphology
- Optimizing the ion-accessible surface



- Quench MD





PhD thesis of Zacharie Waysenson (work in progress)

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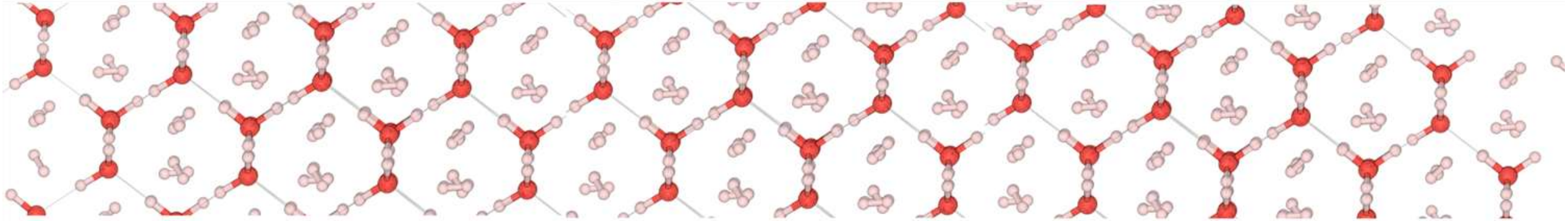
Optimization of Hydrogen Storage in Clathrates and Ices through Advanced Molecular Simulations



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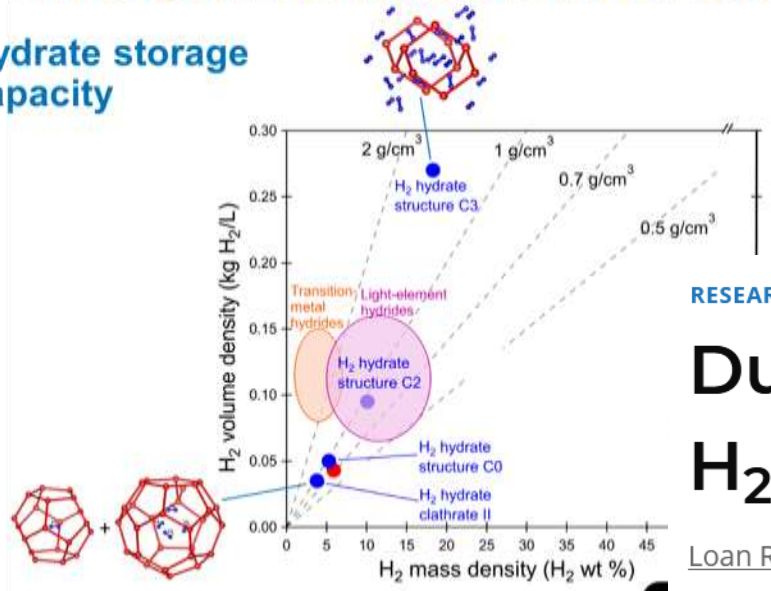
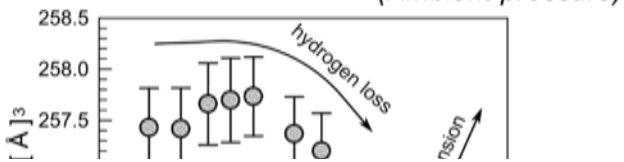
OPTIMIZATION OF HYDROGEN STORAGE IN CLATHRATES AND ICES THROUGH ADVANCED MOLECULAR SIMULATIONS

Hydrate storage capacity



H_2 gradual desorption in the C2 phase

(Ambient pressure)



RESEARCH ARTICLE | PHYSICS

Dual quantum locking: Dynamic coupling of H_2 and H_2O sublattices in hydrogen-filled ice

Loan Renaud, Tomasz Poreba, Simone Di Cataldo, +6, and Livia Eleonora Bove Authors Info & Affiliations

Edited by Russell Hemley, University of Illinois at Chicago, PNAS ember 23, 2025; accepted January 16, 2026

February 10, 2026 | 123 (7) e2526369123 | https://doi.org/10.1073/pnas.2526369123

Adsorption and **desorption** of gas in the structures

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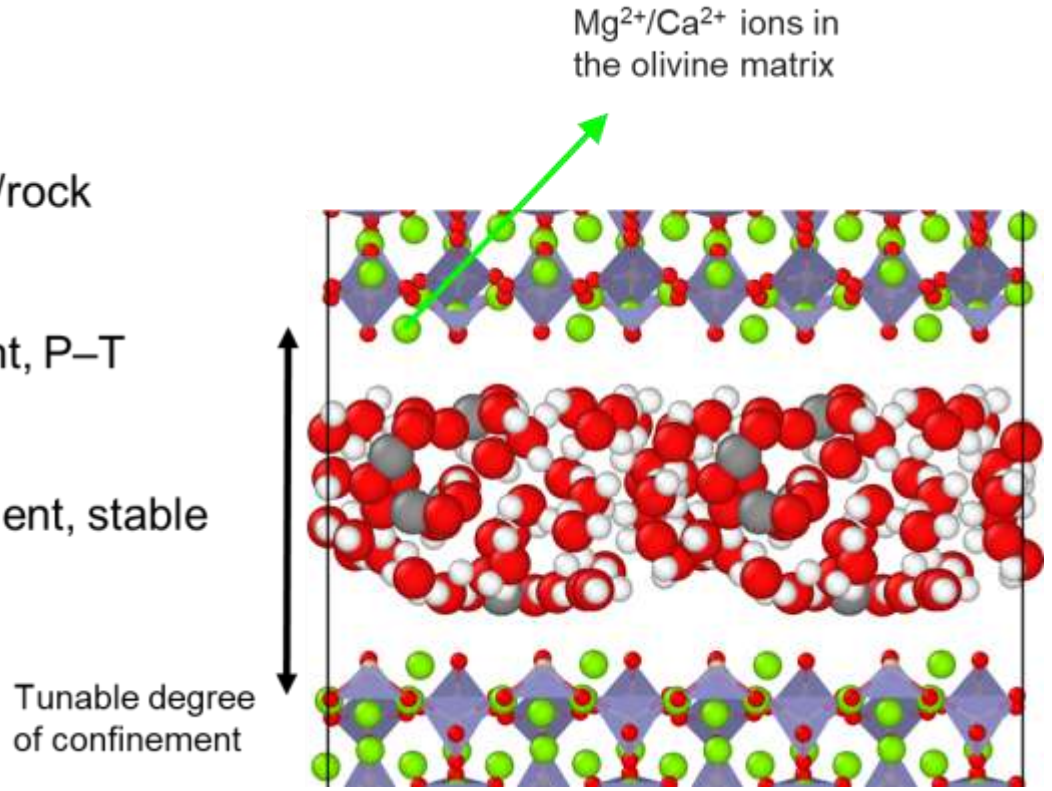
NATURE-CO_2 : **N**atural **A**bility of **T**rapping and **U**sing **RE**sources for **CO_2**

- Understand CO_2 speciation and mineralization mechanisms at water/rock (Mg_2SiO_4) interfaces
- Explore effects of nanoconfinement, P–T conditions, and surface chemistry
- Identify optimal conditions for efficient, stable CO_2 trapping



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- Supercapacitors modeling: ab initio calculations, molecular dynamics
- AI and Machine Learning Interatomic Potentials
- **French/European ecosystem for AI & Materials**

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DIscovery Acceleration for the Deployment of Emerging Materials

DIADEM, a pioneer PEPR* at the crossroads of Materials Science and Artificial Intelligence

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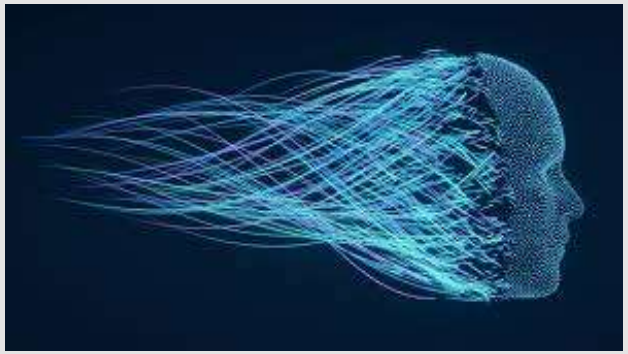
*Programme et Equipements Prioritaires de Recherche

Les matériaux sont stratégiques pour les grandes transitions

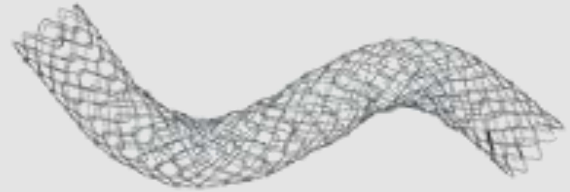
DIADEM : DIscovery Acceleration for the Deployment of Emerging Materials

La convergence entre Science des Matériaux & Science des données

Transitions écologique et énergétique vers un futur décarboné



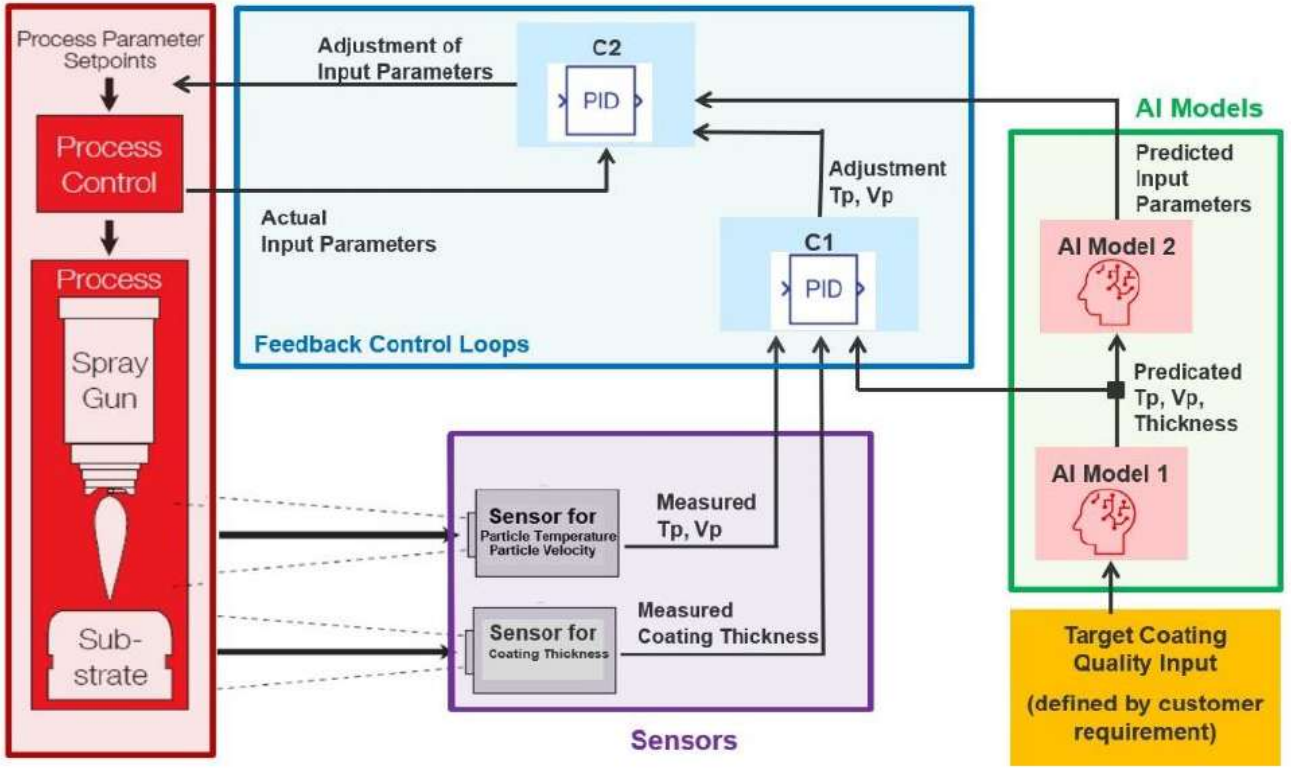
Transition vers un numérique frugal



Innovation technologique pour la médecine du futur

DIADEM …
… le recours à l'IA pour deux principales problématiques

Accélérer le **design de nouveaux matériaux** grâce aux plates-formes d'accélération et aux laboratoires autonomes (DIADEM Discovery Hub)

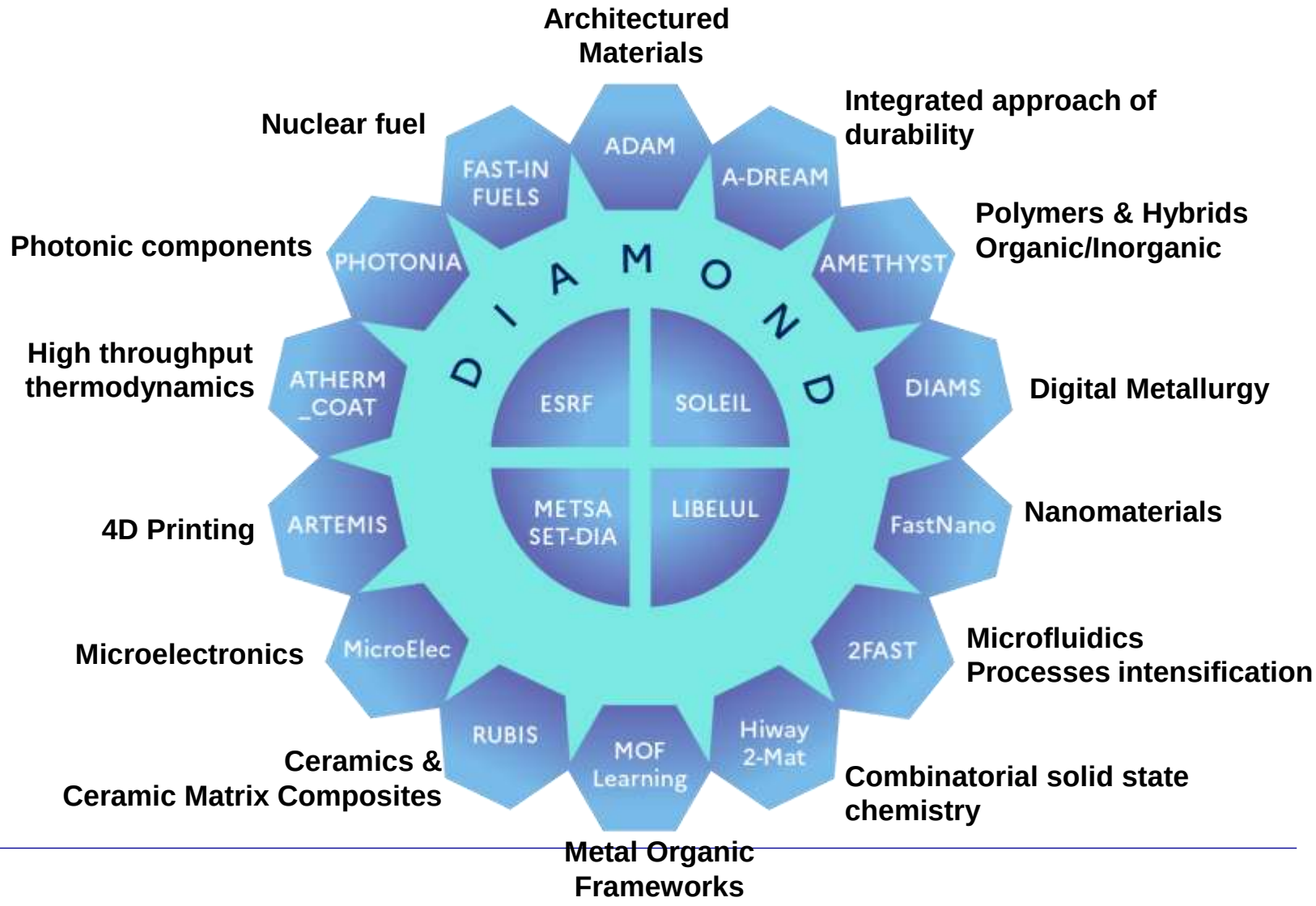


Accélérer le **déploiement de procédés** grâce à des jumeaux numériques (procédés émergents 1D,2D,3D,4D & conventionnels)

DIADEM pioneering strategy

DIADEM main features
85 M€ / 8 years

19 platforms
33 selected projects
1 DIADEM ACADEMY
6 transverse working groups
1 National Infrastructure
(DIADEM DISCOVERY HUB)



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Machine Learning Interatomic Potentials (MLIP)

https://deepmind.google/discover/blog/millions-of-new-materials-discovered-with-deep-learning/

Google DeepMind About Research Technologies Discover

Millions of new materials discovered with deep learning

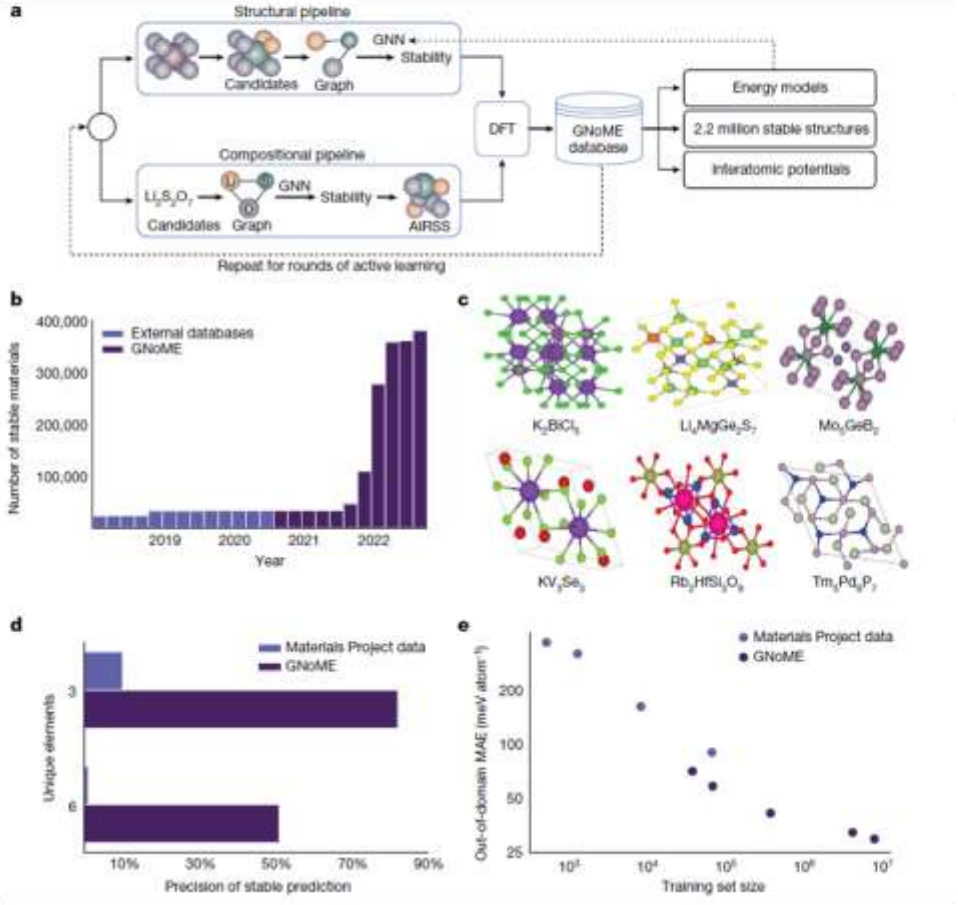
29 NOVEMBER 2023

Amil Merchant and Ekin Dogus Cubuk

Share

AI tool GNoME finds 2.2 million new crystals, including 380,000 stable materials that could power future technologies

Modern technologies from computer chips and batteries to solar panels rely on inorganic crystals. To enable new technologies, crystals must be stable otherwise



nature

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Article | Open access | Published: 29 November 2023

Scaling deep learning for materials discovery

Amil Merchant, Simon Batzner, Samuel S. Schoenholz, Muratahan Aykol, Gowoon Cheon & Ekin Dogus Cubuk

Nature 624, 80–85 (2023) | Cite this article

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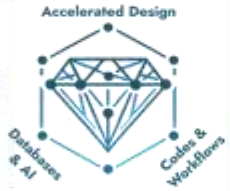
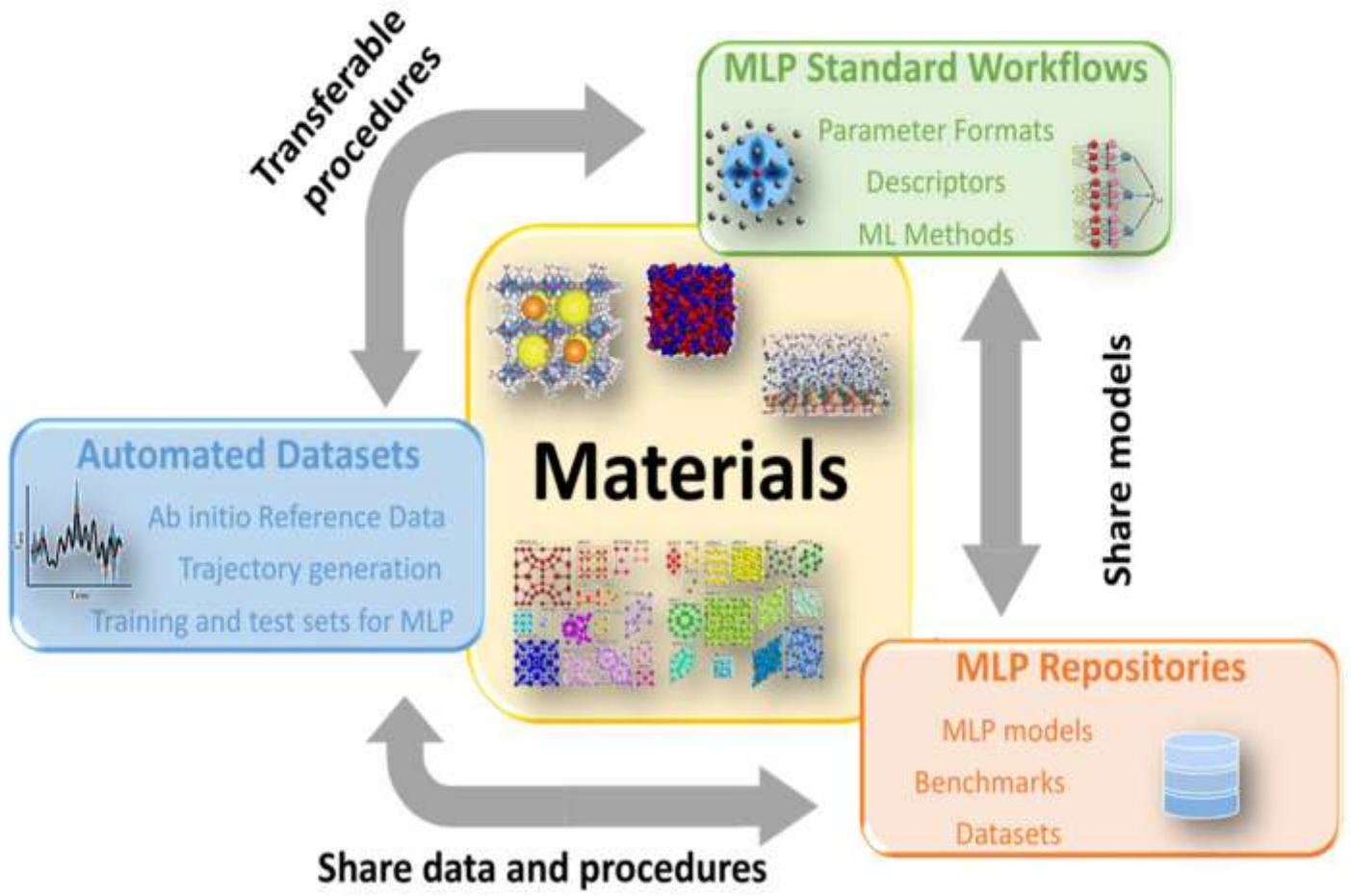
FRANCE 2030 PROGRAMME DE RECHERCHE MATÉRIAUX ÉMERGENTS





Akshay Ammothum Kandy (postdoc)

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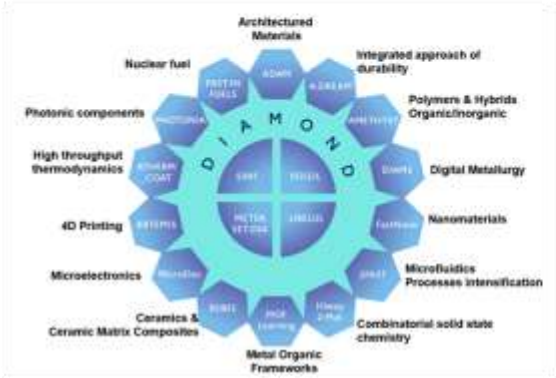
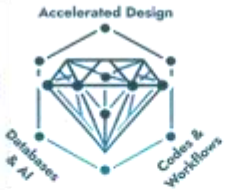
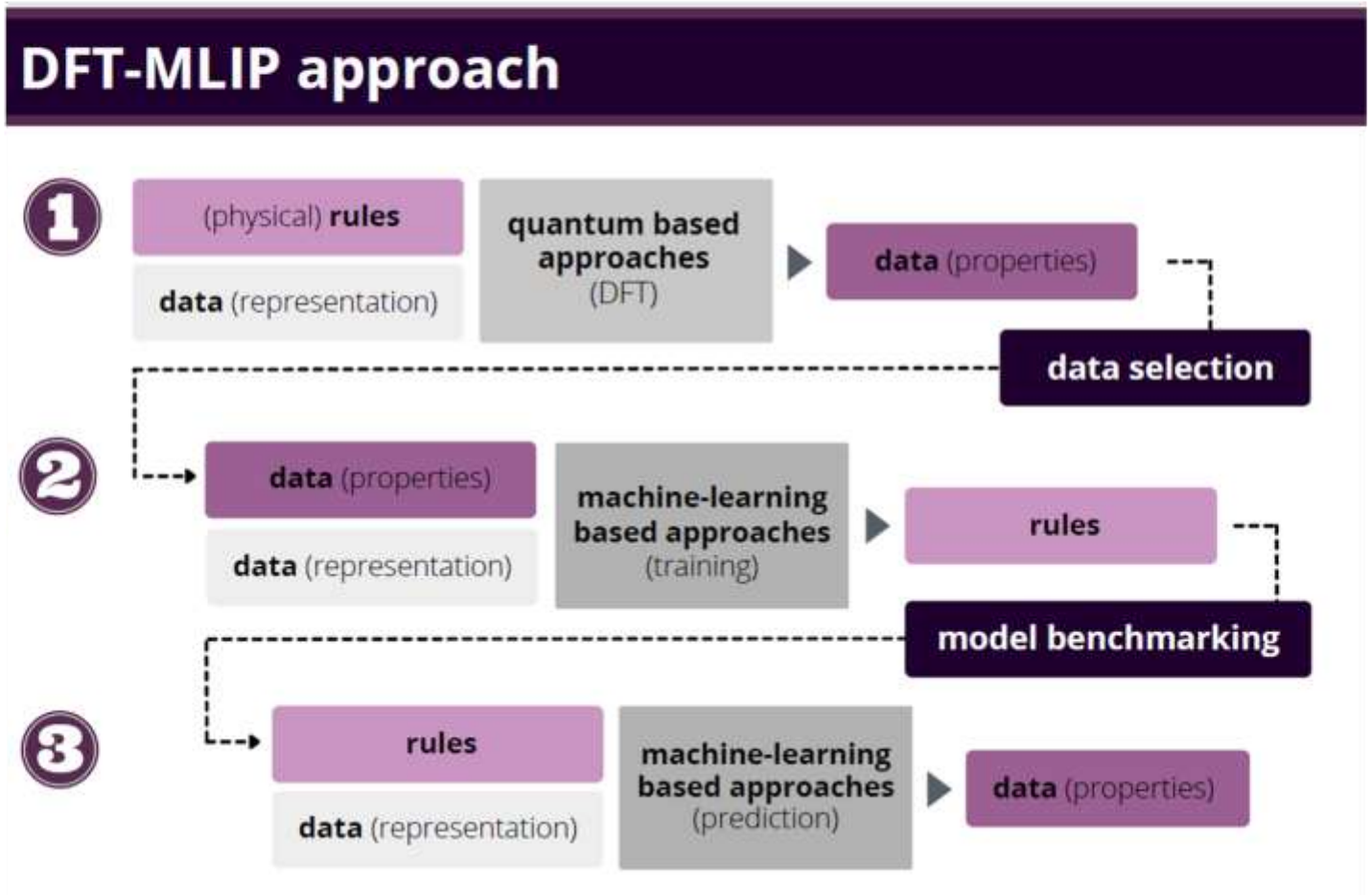


FRANCE 2030 PROGRAMME DE RECHERCHE MATÉRIAUX ÉMERGENTS





Akshay Ammothum Kandy (postdoc)

DIADEM Academy : programme de formation du PEPR DIADEM

Formation initiale

(Noël Jakse et Marco Saitta)

Création de l'Ecole Internationale DIADEM

Hackathon

Stages de Master

Formation continue

(Fabrice Rossignol)

Formations spécialisées (théorie & pratique)

Formation « sensibilisation à la découverte accélée autour des MAPs

Journée annuelle de sensibilisation à l'IA

Programme doctoral et post-doctoral international

(Frédéric Schuster)

Thèses et post-doctorats internationaux

(Co-financements DIADEM)

https://formation.pepr-diadem.fr/

Initial Training
1st edition of the DIADEM international school

August 25-29, 2025, at Sorbonne Université in Paris

80 participants

Theory courses and hands-on tutorials

Visit of the Synchrotron SOLEIL

Initial Training
Future editions of the DIADEM international school

August 31- Sept 4, 2026, in Grenoble

120 participants (open to permanent/industrials)

2027 edition within the AISSAI-IVADO « semestre thématique IA & Matériaux »

In Paris or Bordeaux Aug 30-Sept 3 2027

DIADEM pionnier pour la collaboration internationale

Singapour

- Deux réunions de travail avec la **NRF** (04/2024, 10/2024)
- **Projet ADVANCE sur la catalyse pour la production d'H2 vert** (AAP 2023) Pr. LIU Zheng, CINTRA IRL 3288 (CNRS, NTU Singapore, Thales)
- 3 thèses avec **NTU** (H2, recyclage, 3D printing de métamatériaux) et 1 thèse avec **NUS** (batteries)

Canada

- Réunions avec l'**Institut Courtois** and **Polytechnique Montréal**
- Intégration de Polytechnique Montréal dans le projet **ASTERIX** dédié aux couches minces
- 1 Post-Doc avec l'Institut Courtois (photovoltaïque)

USA

- **Projet REBORN** sur matériaux 2D pour l'électronique Ougazzaden Abdallah GT-CNRS IRL 2958 CNRS Metz, GeorgiaTech Atlanta
- 1 thèse sur 4D printing avec **Georgia Tech Atlanta** (robotic freeform direct ink writing)

Japon

- **Projet MADNESS** (synthèse de nanomatériaux en sels fondus - AAP 2023) et **projet GREENTEA** (synthèse de nouveaux alliages de sulfures thermoélectriques - AAP 2024) avec le **LINK** (NIMS Tsukuba)
- Discussion sur la coopération sur la structuration des bases de données avec le **NIMS**
- 2 thèses en discussion avec le **LINK**

Développer les outils d'interaction avec les industriels

Partenaires de DIADEM

Scientific Advisory Board

ARKEMA SYENSQO

SAFRAN THALES

EDF ArcelorMittal SAINT-GOBAIN

Constellium oerlikon

Futures actions

- ✓ Appel à Projets « Pionniers de l'IA » coordonné par le SGPI : contribution des outils DIADEM à l'accélération du design de nouveaux matériaux et à la mise en oeuvre de nouveaux procédés (ex : base de données nationale sur les polymères, Valorisation insdustrielels d'Expressif Materials...)
- ✓ AG DIADEM avec des tables rondes avec PEPR et Agences de Programmes – 24 nov à l'ENS Paris-Saclay
- ✓ Première édition de la journée « DIADEM Industrial Day » 12 décembre 2025 / Maison de la Chimie

AI for materials science in France: GDR IAMAT

- Created in 2022, to federate from « developments in AI » towards applications in materials science, interdisciplinarity
- Broad interpretation of AI & data sciences: machine learning, data mining, high throughput, dimensionality reduction, clustering etc…

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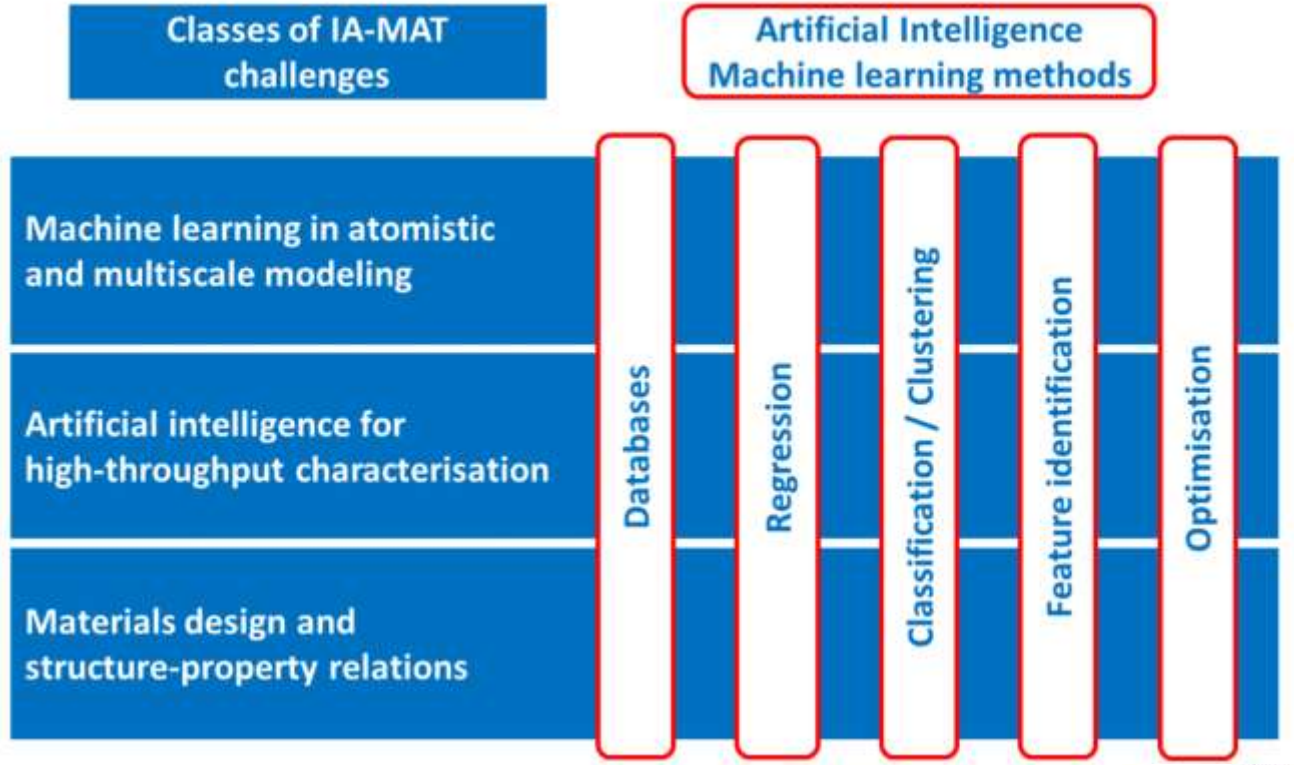
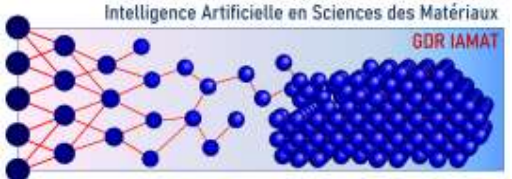
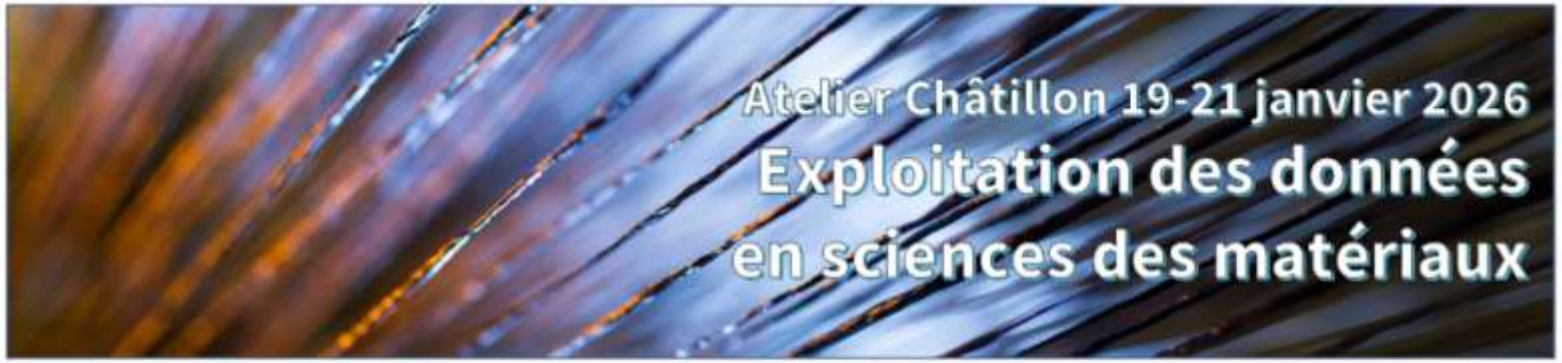




AI for materials science in France: GDR IAMAT

- **Upcoming activities 2026 : Workshop Big and Small Data**



- **Plénières 2026: 2-5 juin, ENSAM, Aix-en-Provence**

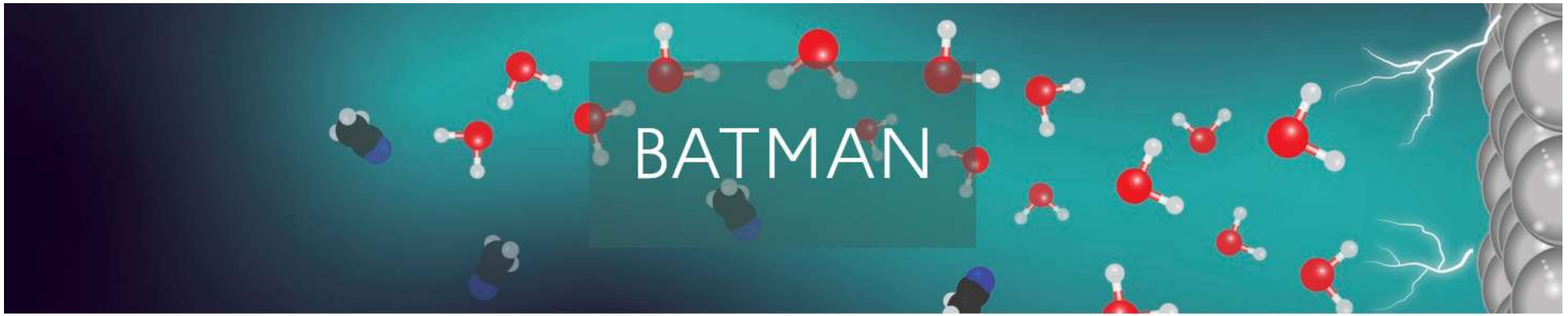
PEPR Batteries

Piloté par

Financé par

Opéré par

PEPR Batteries



Combiner l'intelligence artificielle aux modèles physiques **pour développer de nouvelles batteries**

Aperçu

Exploration de données, intelligence artificielle et jumeaux numériques pour la nouvelle génération de batteries

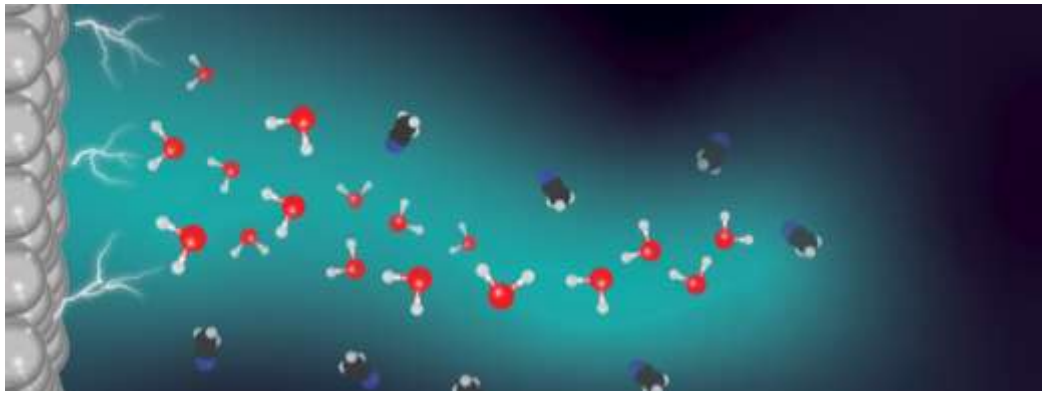
Pr. Mathieu Salanne (PHENIX, Sorbonne Université / CNRS)
Pr. Alejandro Franco (LRCS, Université de Picardie Jules Verne / CNRS)

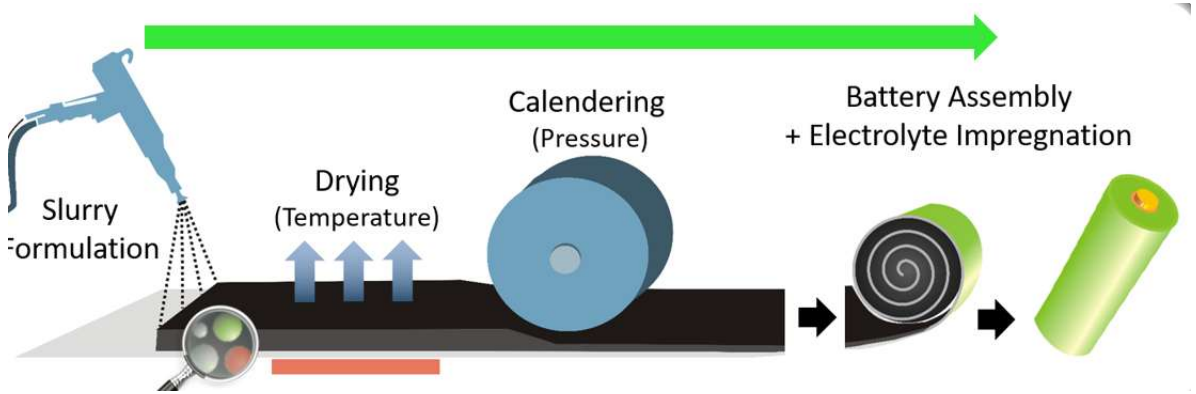
La recherche sur le stockage de l'électricité utilise de plus en plus les simulations numériques, généralement basées sur des principes physiques. BATMAN vise à développer de nouveaux modèles intégrant les approches de la science des données et de l'intelligence artificielle. Trois objectifs principaux sont visés : trouver des électrolytes et des matériaux optimisés, comprendre les réactions chimiques aux interfaces des batteries, et optimiser les processus de fabrication. Le projet vise également à créer un jumeau numérique pour prédire les performances des batteries en fonction des propriétés des électrodes fabriquées.

BATMAN BATteries: data Mining, Artificial intelligence and digital twins for the Next generation

Coordinator Mathieu Salanne (PHENIX – Sorbonne Université/CNRS)
Co-coordinator: Alejandro Franco (LRCS – UPJV/CNRS)

January 2nd, 2023 → January 1st, 2029





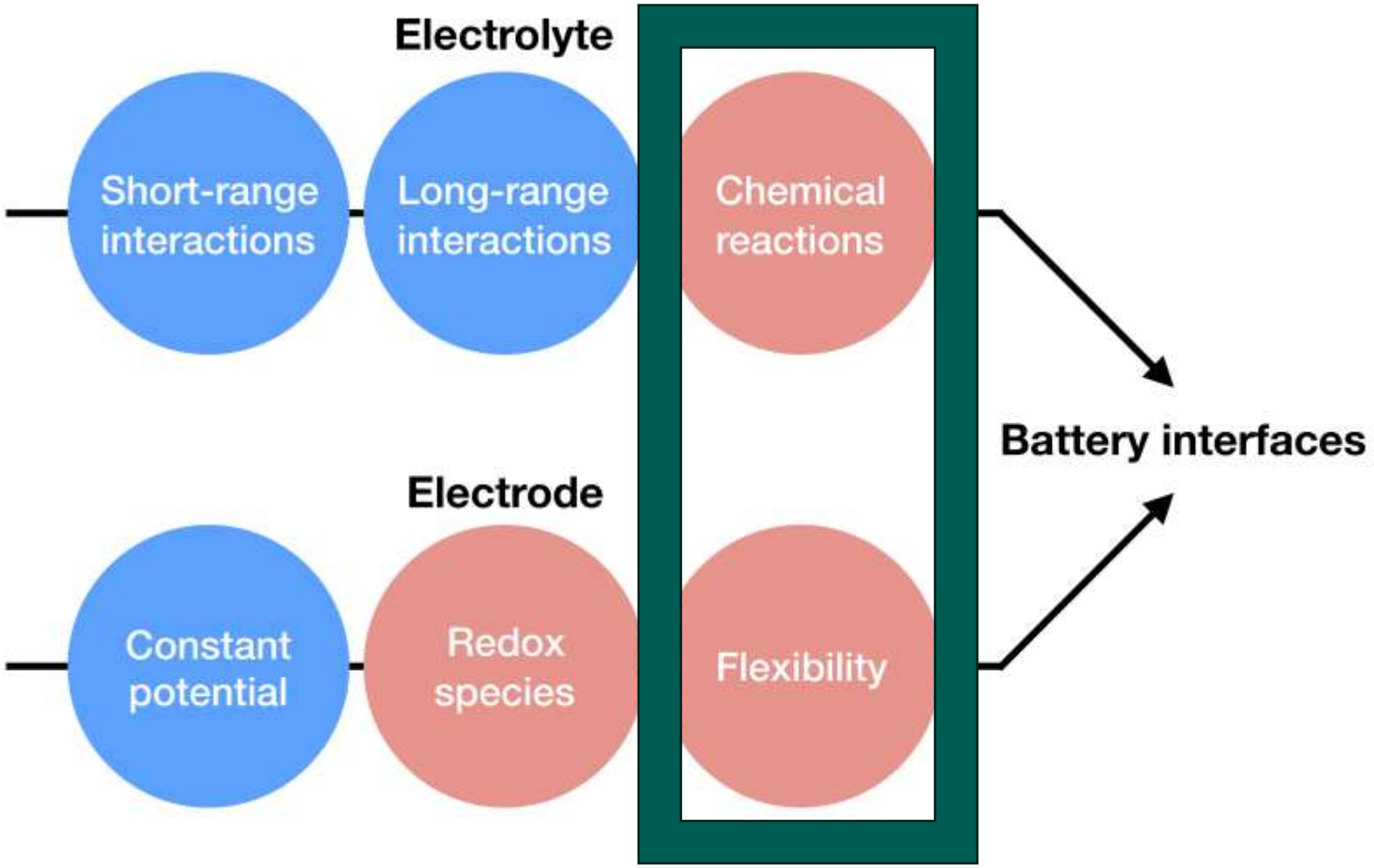
Challenges & objectives

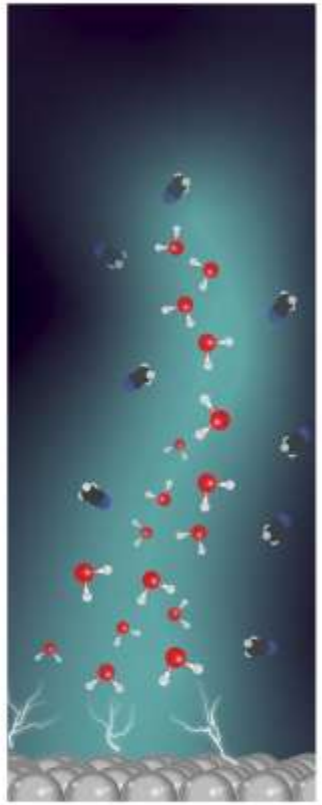
Challenges
• Stability of the lithium metal / solid electrolyte interfaces • Choice of the electrolytes/electrodes for Na-ion batteries and for high power batteries • Optimization of the fabrication processes of next-generation batteries

Objectives
i. Database of liquid electrolyte properties (in particular additives in Na-ion batteries) ii. Selection of solid state electrolytes forming mechanically and chemically stable interfaces with lithium metal iii. Selection of 2D materials with optimized stability and energy density for high power batteries iv. Codes based on physical modeling and machine learning for the optimization of the manufacturing processes

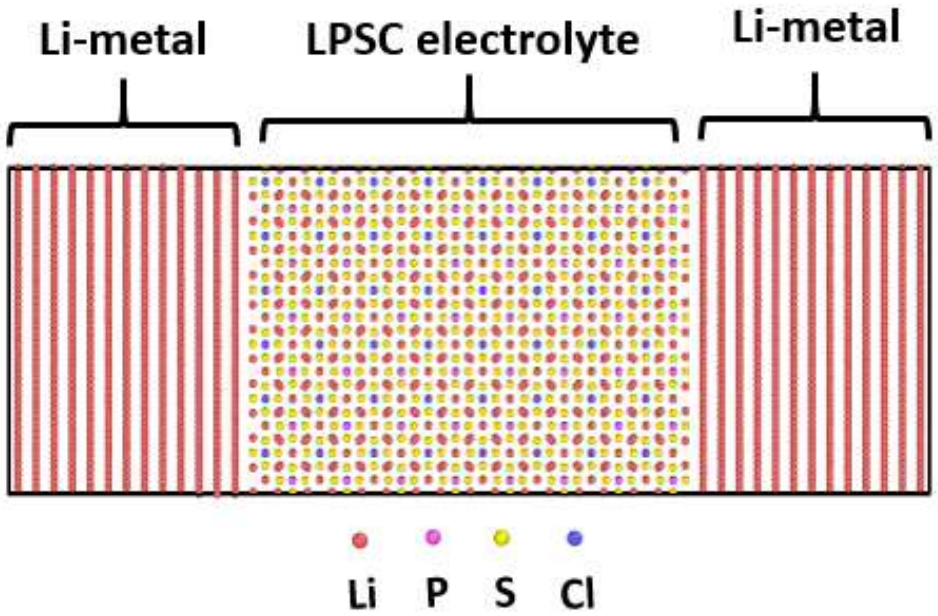
Use of machine-learning / data science approaches to improve simulations **accuracy** and **efficiency**

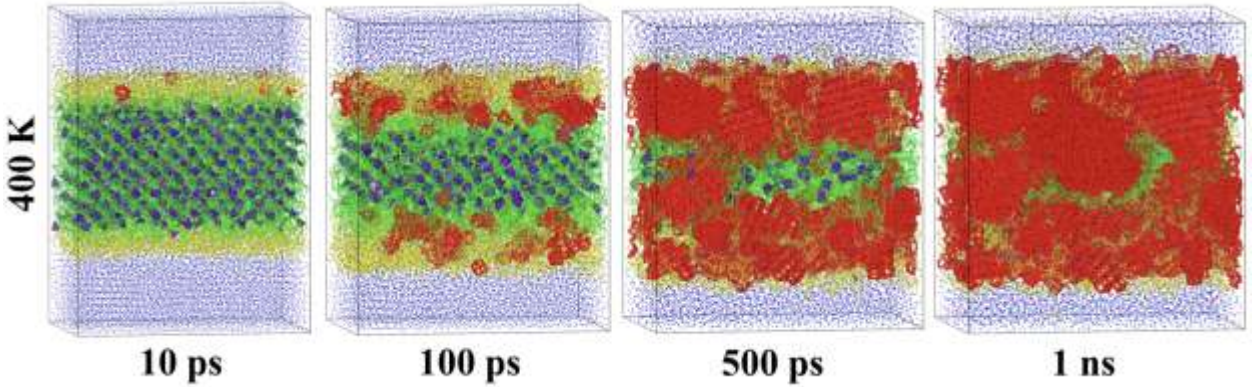
AI-based models for the study of battery interfaces





Simulating the SEI formation in all-solid-state batteries





- Argyrodite degradation reaction at the contact of the lithium anode:

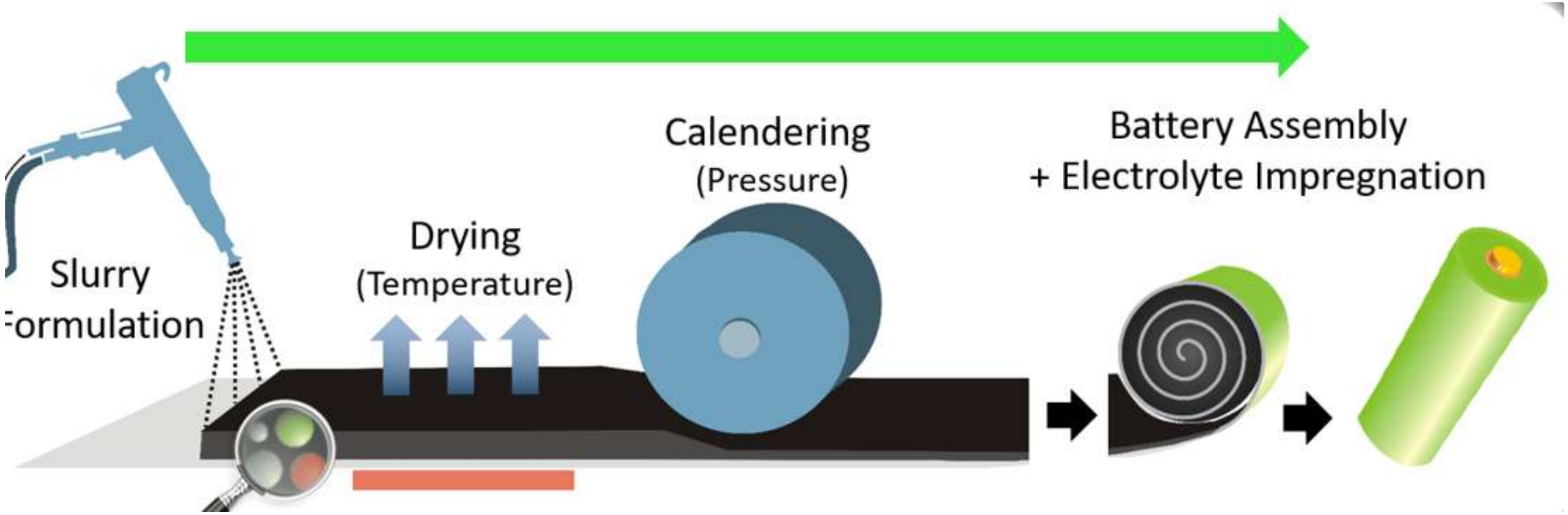
$$Li_6PS_5Cl + 8Li = 5Li_2S + LiCl + Li_3P$$

- Simulation of large interfaces using machine-learning interaction potentials

- Two-step growth process consisting of an initial electrolyte reduction followed by the gradual crystallization of the reaction product

Chaney *et al*, *ACS Appl. Mater. Interfaces* 16, 24624 (2024) doi:10.1021/acsami.4c02548.]

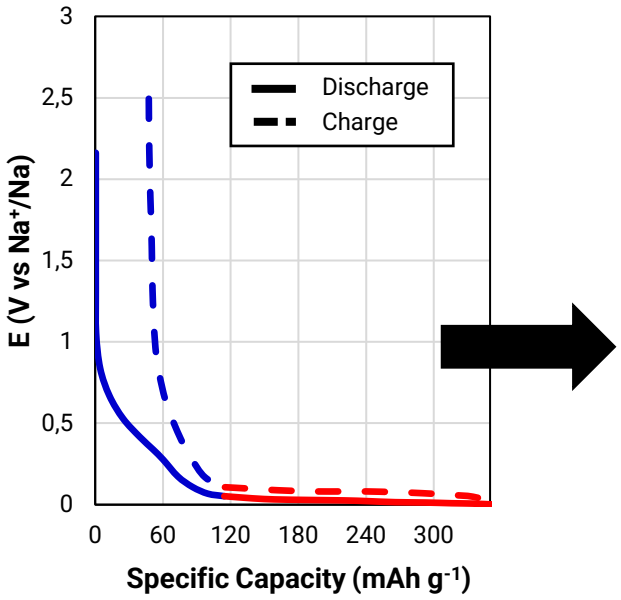
Optimization of the fabrication processes of next-generation batteries



- Fabrication process of next-generation batteries is expected to be similar to Li-ion
- Much fewer data: can we optimize quicker the process thanks to the use of artificial intelligence

3D-resolved electrochemical model of hard carbon electrodes

HC electrochemistry



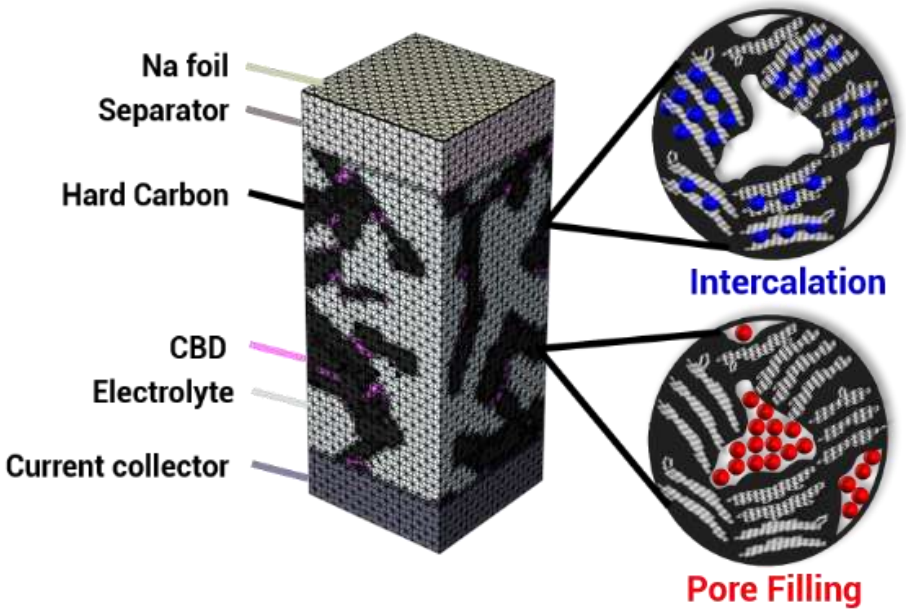
GOALS:

1. Model multiple sodiation processes of HC
2. Use the model for electrode design (for formulation and porosity)

?

CONTROVERSIAL SODIATION MECHANISM

Effective “blend” approach



Cardenas-Sierra *et al, J. Power Sources 655*, 237878 (2025)

PEPR Hydrogène

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Conclusions

- AI & ab initio for energy, hydrogen, carbon dioxide storage
- Materials for energy storage, supercapacitors
- Supercapacitors modeling: ab initio calculations, molecular dynamics
- AI and Machine Learning Interatomic Potentials
- Towards the design of efficient realistic electrodes
- French/European ecosystem for AI & Materials

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Thanks to:

- Sonia Salomoni (PhD “Phase transformations” SCAI)
- Zacharie Waysenson (PhD “Supercapacitors” PEPR Batteries)
- Loan Renaud (PhD “Hydrogen storage”)
- Akshay Ammothum Kandy (Computer engineer “MLIP databases” DIADEM)
- Stefano Ferrero (Postdoc “CO_2 sequestration”)

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ED397 Physique et Chimie des MATÉRIAUX

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