

INDTECH2018

Innovative industries for smart growth

29-31 October, 2018
Vienna, Austria

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PILLAR 3

Session 3.1

**Integrating modelling and characterization
at Cea Minathec: rationale, ways and challenges**

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CEA



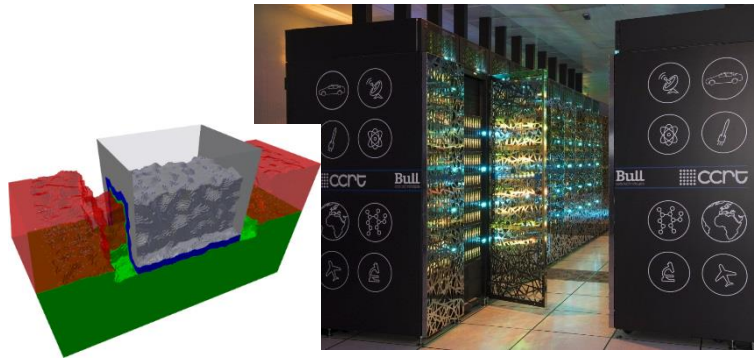
30 October 2018

Why a (CEA) centre for predictive simulation?

What are the challenges?

Fully leveraging on HPC power

e.g. 1st complete simulation of all-around gate transistor

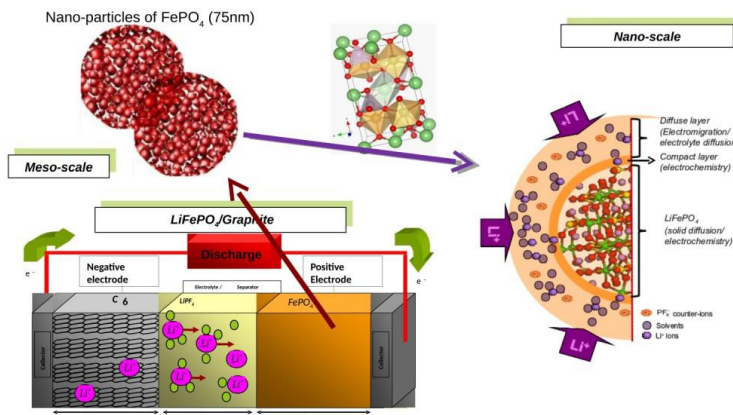


Handling and exploiting huge data flow from advanced characterization

e.g. TEM images (films), 3D FIB-SEM image reconstruction...



Tackling complexity and multidisciplinary challenges
e.g. simulation for batteries



Need of

- ✓ **Critical mass** to cover needed skills (codes, HPC, algorithms) physics, data management...
develop and use a complementary set of codes
- ✓ **Opening and partnerships** to serve CEA and partners programs, industry incl. SMEs to assemble critical competencies and gain momentum



The Centre for Predictive Simulation

> 60 full time scientists

Key softwares (mainly GPL) developed in collaboration

Nanoelectronics
and related technologies

leti

INdC
INSTITUT NANOSCIENCES
ET CRYOGÉNIE

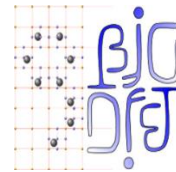
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Basic research

(nanoelectronics, energy, health
technologies)

New
technologies for energy

Own and national computing facilities



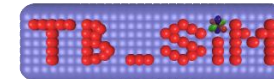
Density Functional
Theory

optical spectroscopy based
on many-body perturbation theory



V_Sim (visualization)
BOAST (metaprogramming)
MC_Sim (kinetics)

almaBTE
THERMAL SIMULATION
heat management
for novel materials



electronic transport for
transistors, qubits

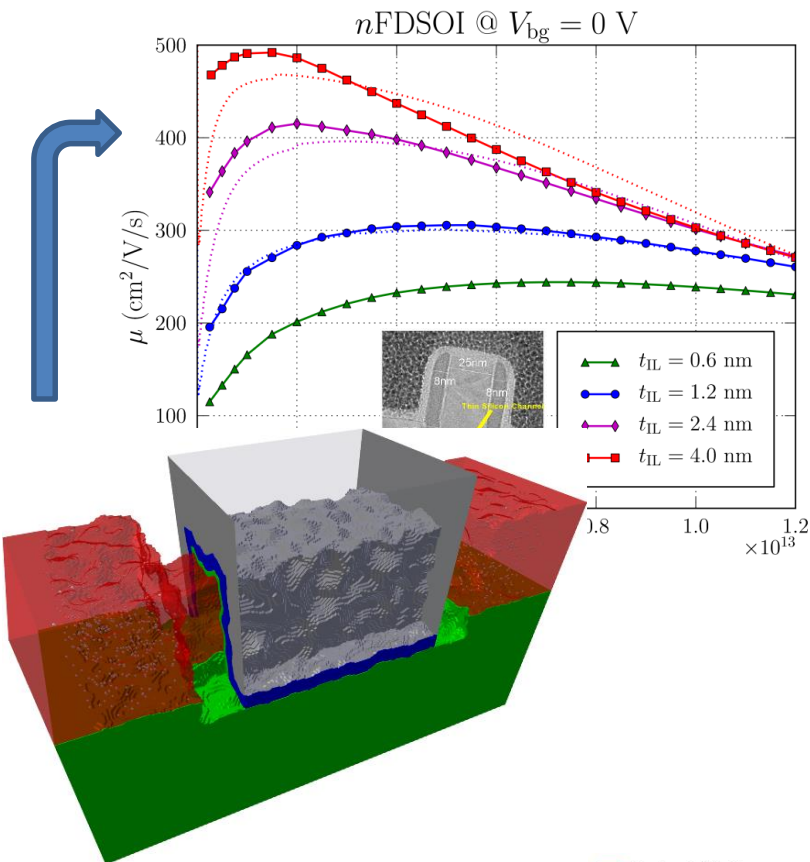


Multi-scale multi-physics simulation for
PEMFC, PEMWE and Li-ions batteries

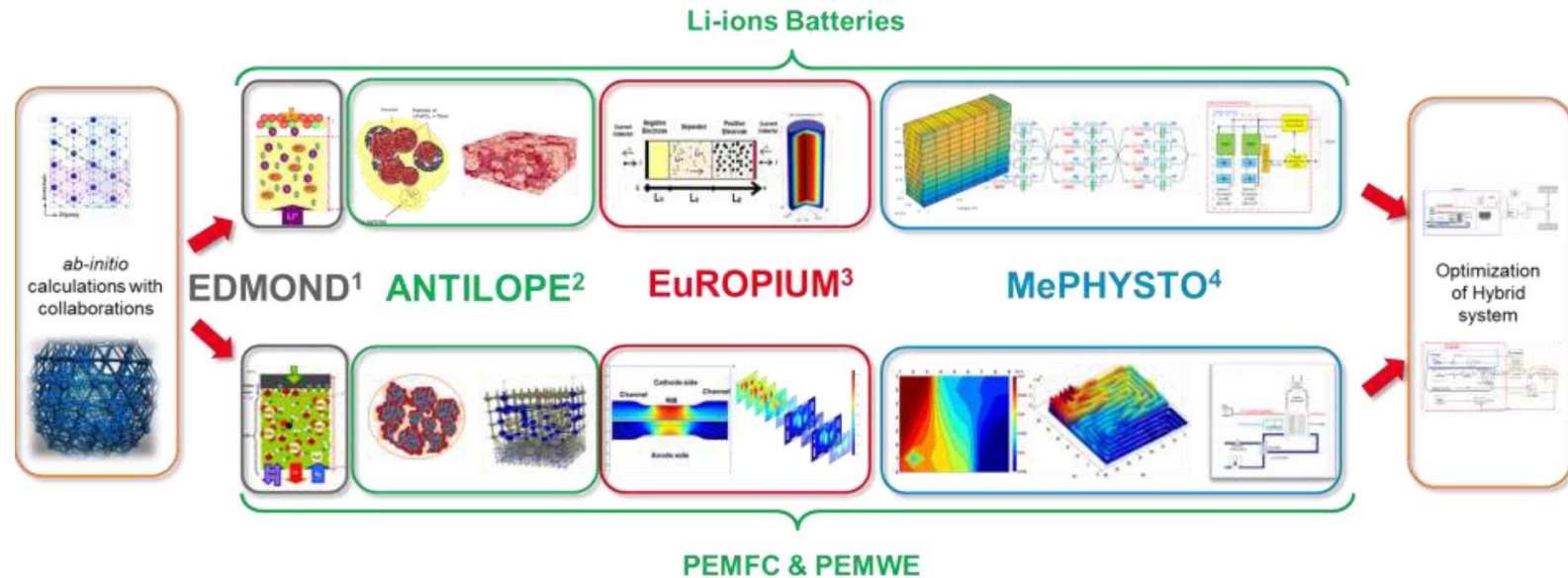
Close link to Minatec nanocharacterization facility

Predictive simulation for research and industry

Simulate the response of a real device
(gate-all-around transistor)



Supporting design and experimental data analysis
(batteries, fuel cells)



¹Electrochemical Double layer **MO**del for **N**ano **D**ynamics

²**A**nalysis of **T**ransports In **L**ayers **O**f **P**orous and active **m**edia

³**E**lect**R**ochemistry **O**pt**I**mization **U**nderstanding **M**odeling framework

⁴**M**ulti**P**hysical **S**imulation **T**ool