



## INDTECH2018

### Innovative industries for smart growth

29-31 October, 2018  
Vienna, Austria

[www.indtech2018.eu](http://www.indtech2018.eu)  
[@IndTech2018](https://twitter.com/IndTech2018)  
#IndTech2018

#### PILLAR 3

##### Session 3.1

Integrating modelling and characterization  
at Cea Minatec: rationale, ways and challenges

Yves Samson



CEA

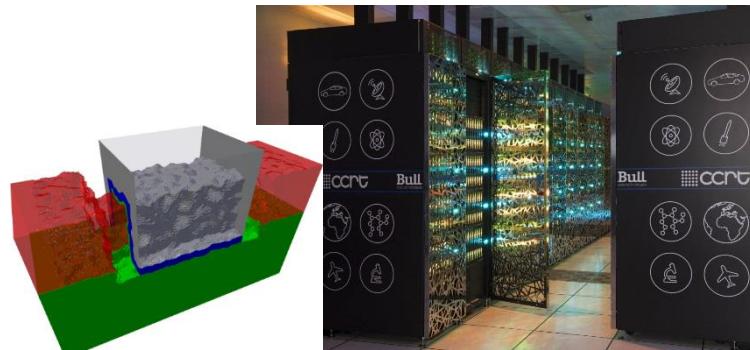
30 October 2018



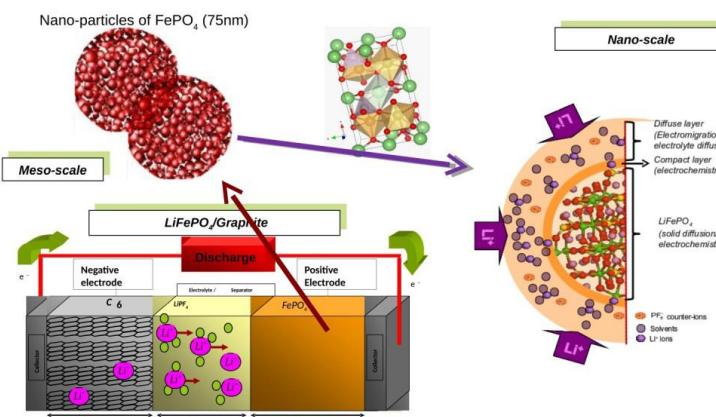
## Why a (CEA) centre for predictive simulation?

### Fully leveraging on HPC power

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



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



### Handling and exploiting huge data flow from advanced characterization



Facilities at



Minatec Nanocharacterization Centre

## What are the challenges?

- ✓ **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



> 60 full time scientists

Nanoelectronics  
and related technologies

**leti**

**INAC**  
INSTITUT NANOSCIENCES  
ET CRYOGÉNIE

Basic research  
(nanoelectronics, energy, health  
technologies)

**liten**

New  
technologies for energy

Own and national computing facilities

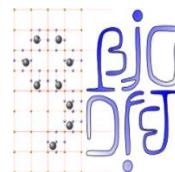


**FFG**  
Promoting Innovation.

Federal Ministry  
Republic of Austria  
Transport, Innovation  
and Technology

The Centre for Predictive Simulation

Key softwares (mainly GPL) developed in collaboration



Density Functional  
Theory



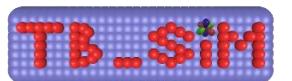
V\_Sim (visualization)  
BOAST (metaprogramming)  
MC\_Sim (kinetics)



optical spectroscopy based  
on many-body perturbation theory



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

e 2 0  
u 1 8  
- a t

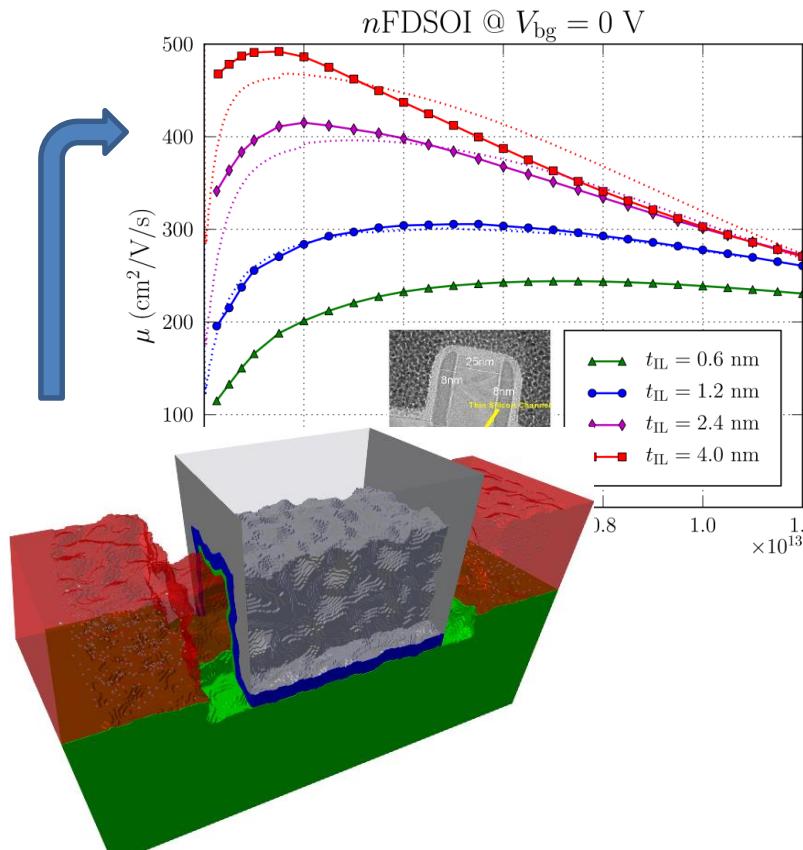


This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 767162.

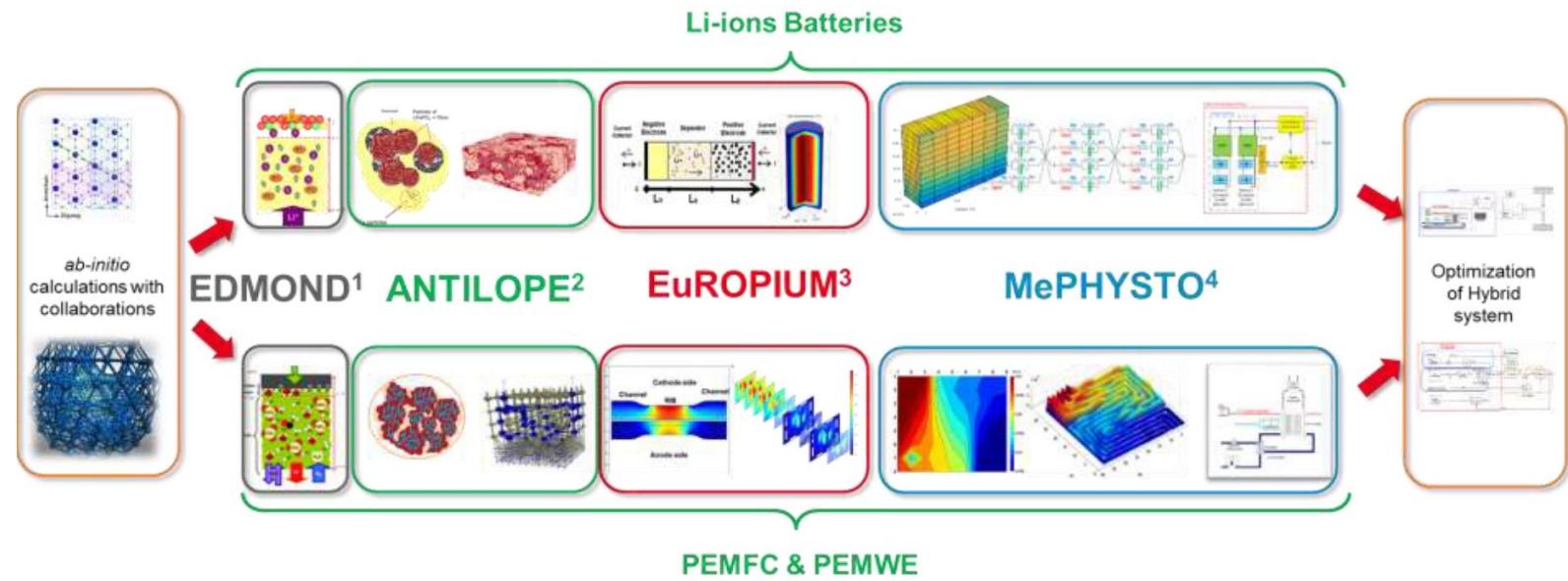


## Predictive simulation for research and industry

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



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



<sup>1</sup>Electrochemical Double layer MOdel for Nano Dynamics

<sup>2</sup>ANalysis of Transports In Layers Of Porous and active mEdia

<sup>3</sup>ElectRochemistry OPTImization Understanding Modeling framework

<sup>4</sup>MultiPHYSical Simulation TOol