Thematic Materials Design Platforms as a Multiscale Simulation Environment

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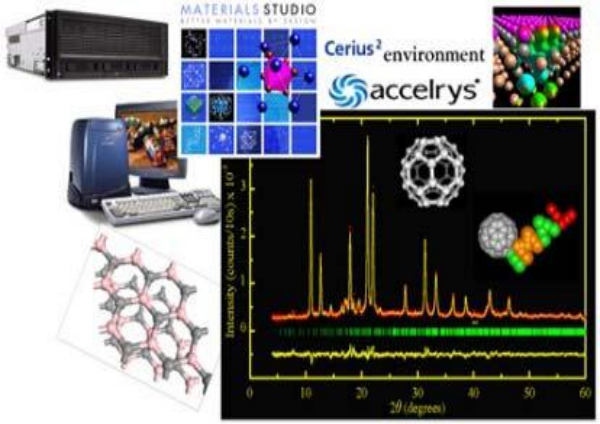
Computational Environments



Quantum Wise

ATK

Atomistix ToolKit with Virtual NanoLab

SCM Scientific Computing & Modelling

nanoHUB
online simulation and more
an NCN project

Cyberinfrastructure for Atomistic Materials Science

UF UNIVERSITY of FLORIDA
The Foundation for The Gator Nation

„5+1“

ICMEg — Integrated Computational Materials Engineering expert group
www.icmeg.eu/

Deepen — From atom-to-Device Explicit simulation Environment for Photonics and Electronics Nanostructures http://www.nmp-deepen.eu/

MMP — Multiscale Modelling Platform: Smart design of nano-enabled products in green technologies http://www.mmp-project.eu/

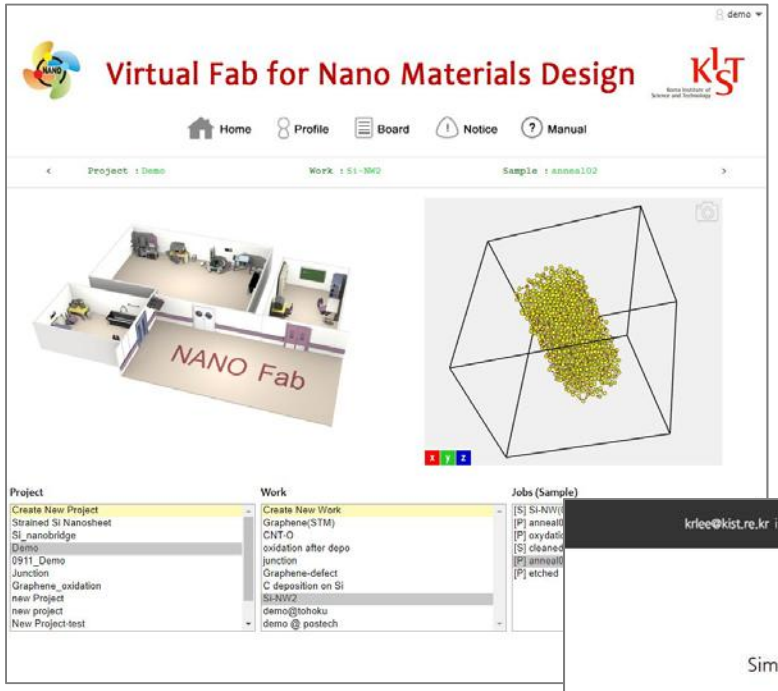
MoDeNa — Modelling of morphology Development of micro- and Nanostructures
http://modena.units.it/

NanoSim — A Multi-scale Simulation-Based Design Platform for Cost-Effective CO2 Capture Processes using Nano-Structured Materials http://www.sintef.no/Projectweb/NanoSim/

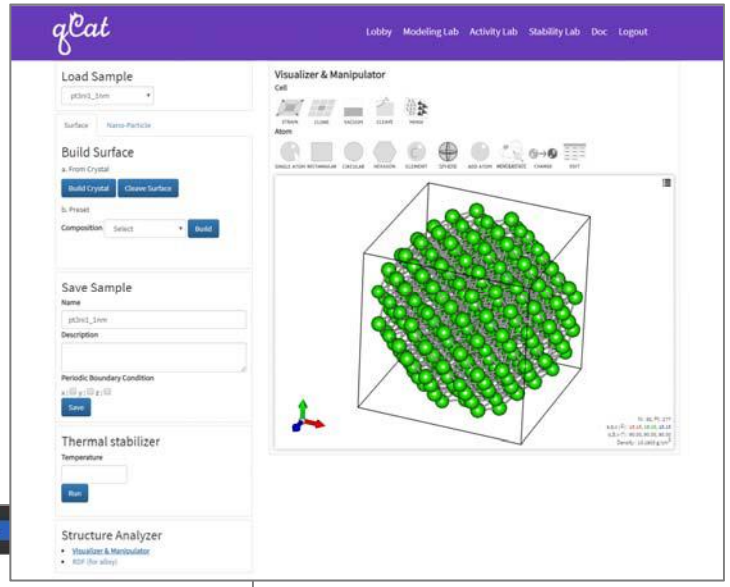
SimPhoNy — Simulation framework for multi-scale phenomena in micro- and nanosystems
http://www.simphony-project.eu/

Vfab.org

Materials Design Platforms @ KIST



nano.vfab.org : virtual nano fab



qcat.vfab.org : catalyst design platform

battery.vfab.org : battery materials design platform

Spin-off Start-up (2016)

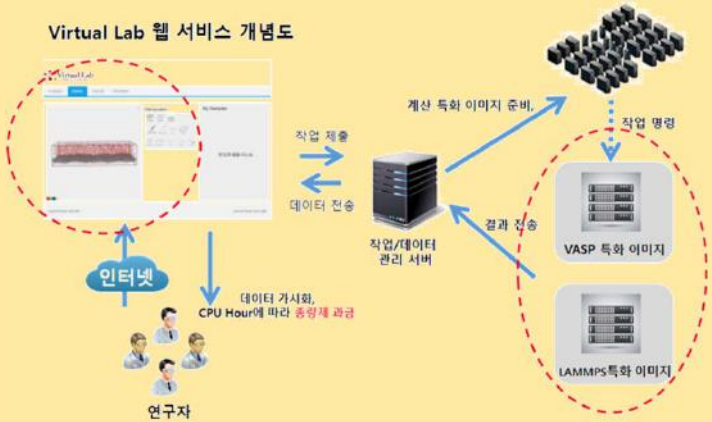
Virtual Lab
Make your own simulation

http://simulation.re.kr

Min-Ho Lee

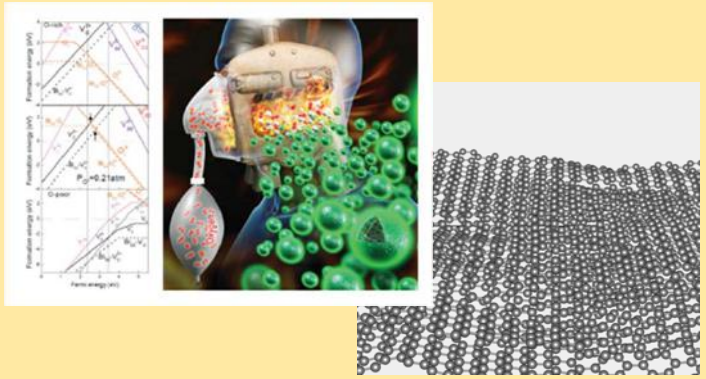
Hee Chae Choi

Han-Eol Cho



Web-based Service : Simulation on Demand

Simulation environment with lower entrance barrier

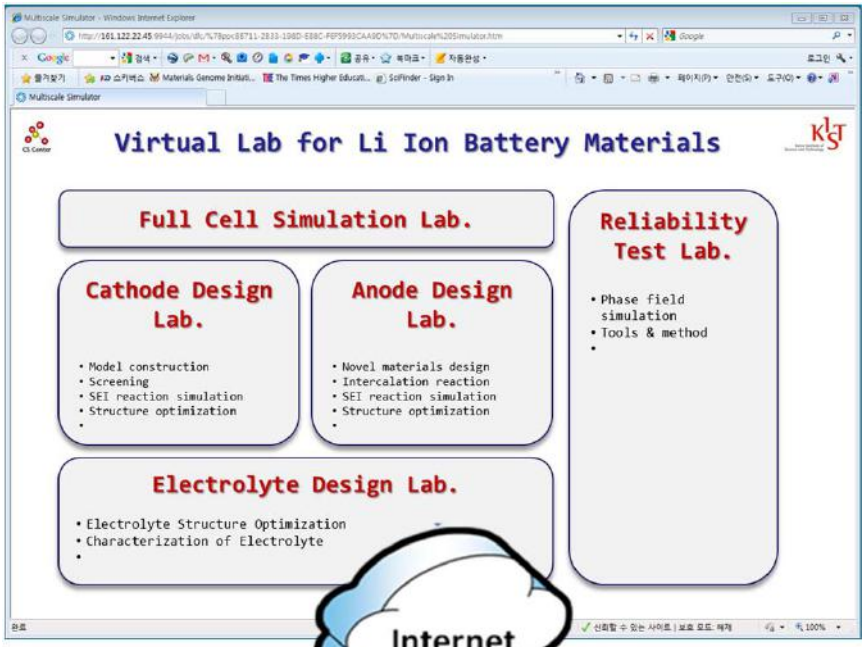


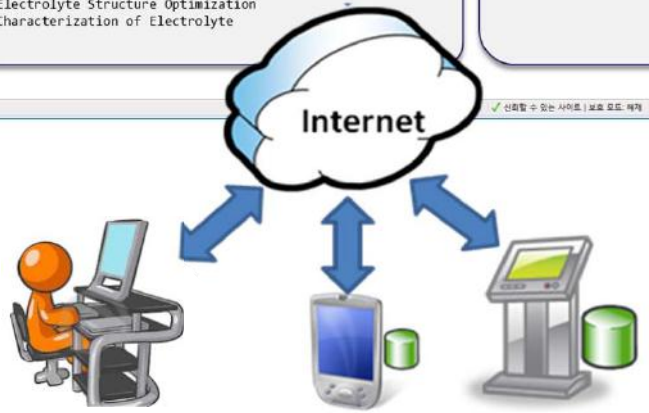
Knowledge-based Service : Simulation Consulting

Multiscale simulation for materials design

Korea Pat. Pending 10-2016-0054511 (2016.5.3)

Basic Concept of KIST Platform



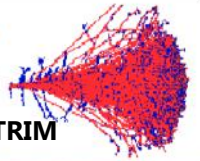


Home Made Codes

LAMMPS

siesta

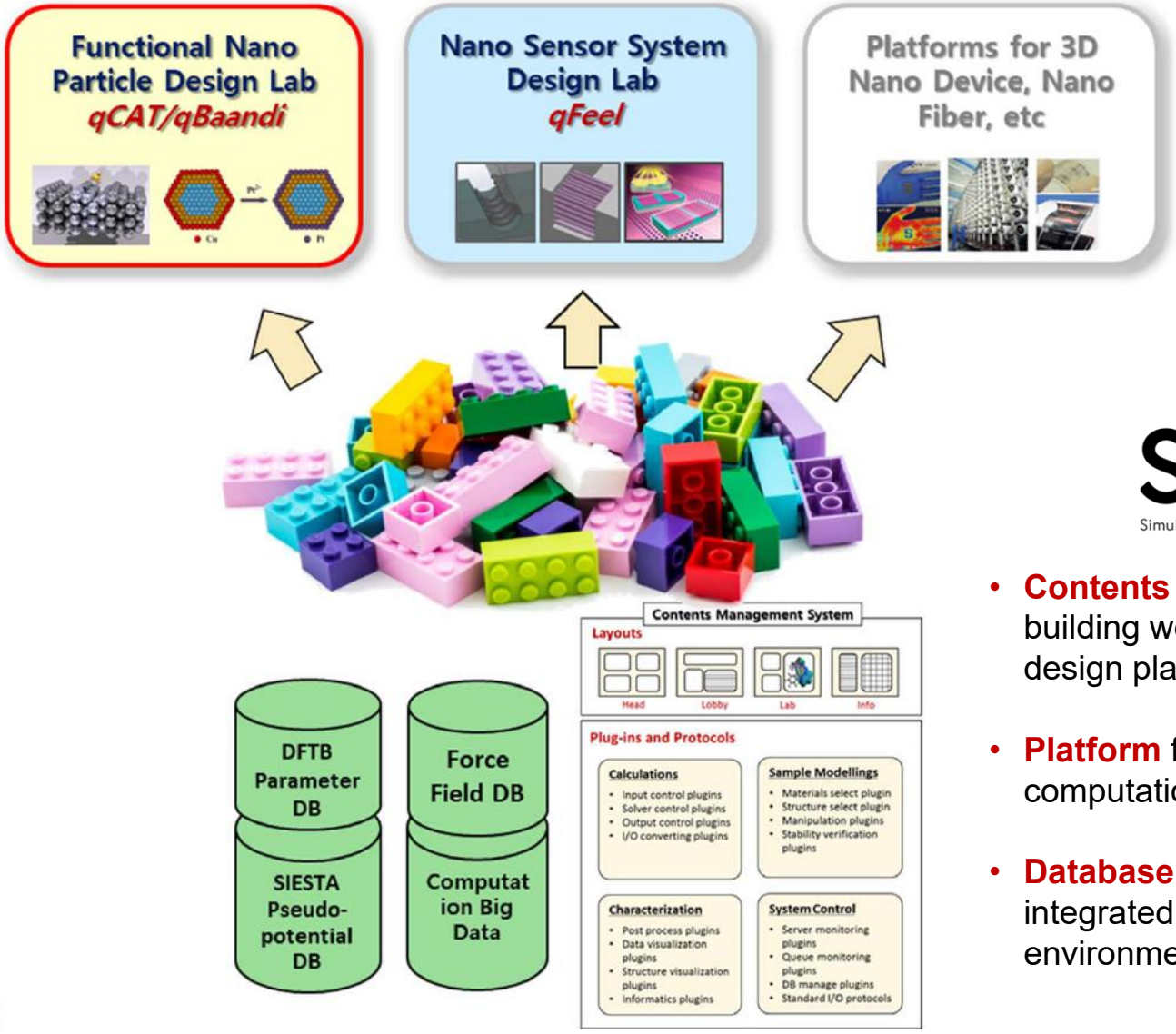
RxFF



SRIM & TRIM

Anyone can Compute Anywhere Anytime!

Simulation Platform Creator : *SimPL*

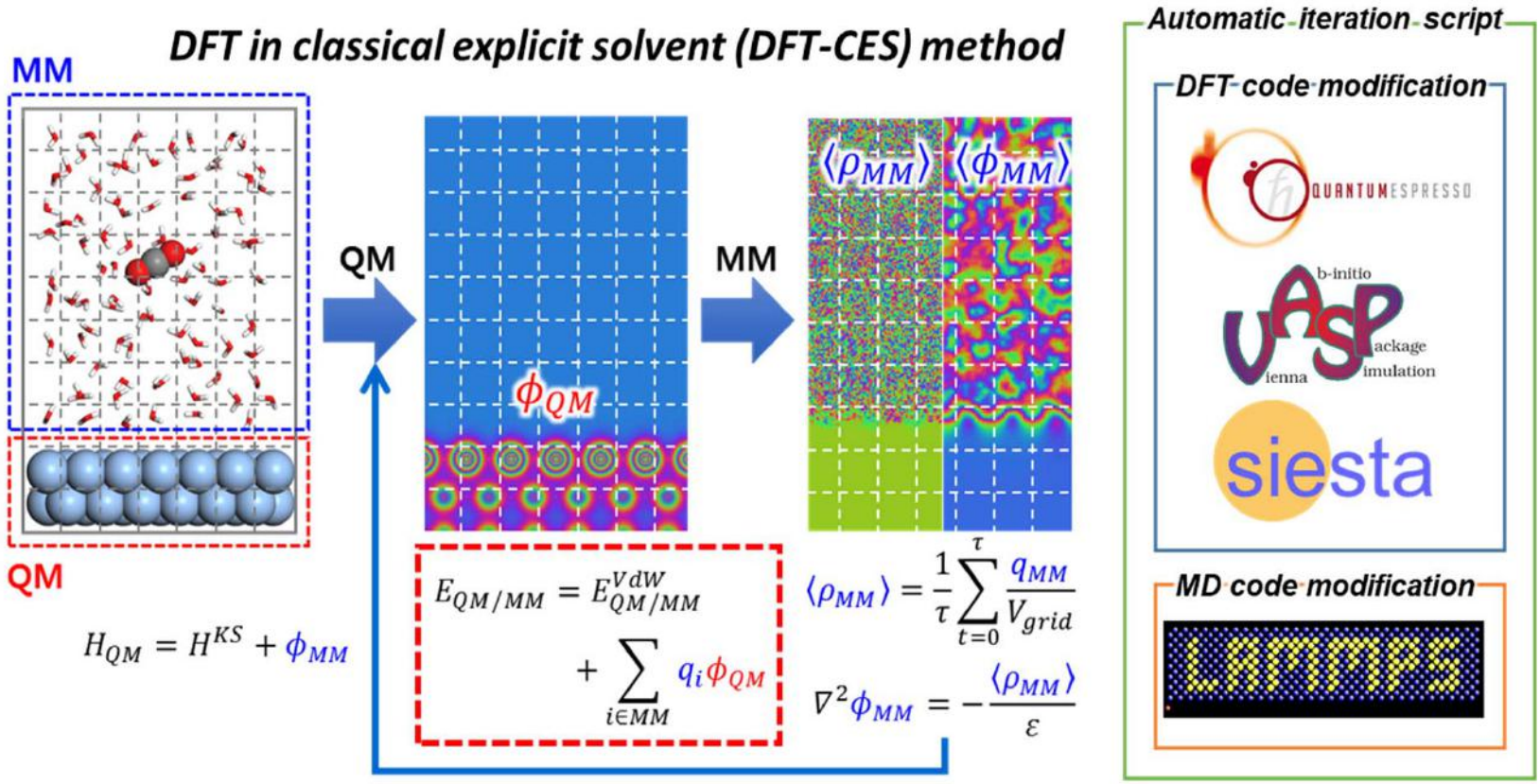


SimPL
Simulation Platform Creator a2.1

- **Contents Management System** for building web-based materials design platforms with great ease
- **Platform** for deploying developed computation codes
- **Database** of essential parameters integrated with computation environment

http://simpl.vfab.org

Interaction at Solid/Liquid Interface



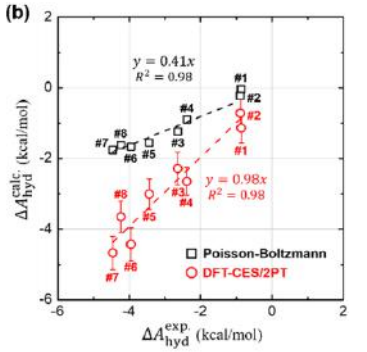
Electrostatic interaction between QM and MM is seamlessly coupled.
Mutual polarization is included by iterative self-consistent reaction field scheme.
VASP/SIESTA/Quantum-Espresso + LAMMPS + in-house automation script

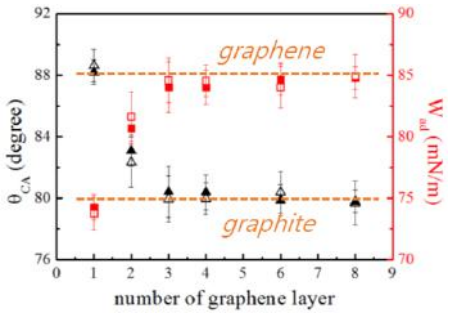
Lim et al., J. Chem. Theory Comput., 2016, *12*, 5088

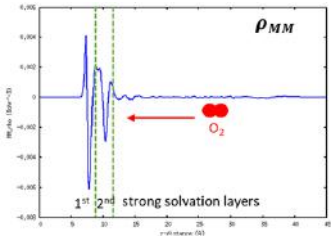
Interaction at Solid/Liquid Interface

DFT-CES Applications

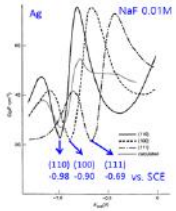
- Basic understandings of solid-water interface interaction
- ORR thermodynamics under realistic acid/base conditions
- CO oxidation on Pt within hydrophilic nano-channel



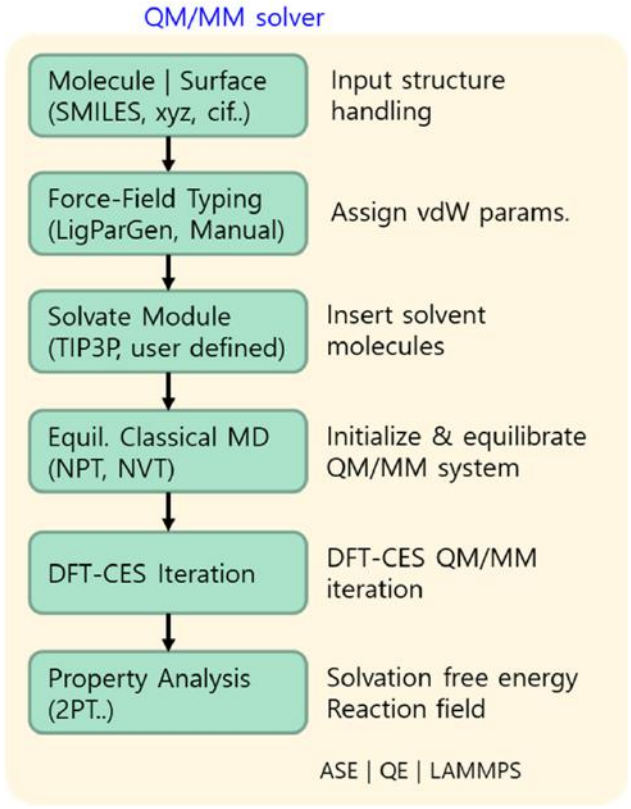




• Potential of Zero Charge

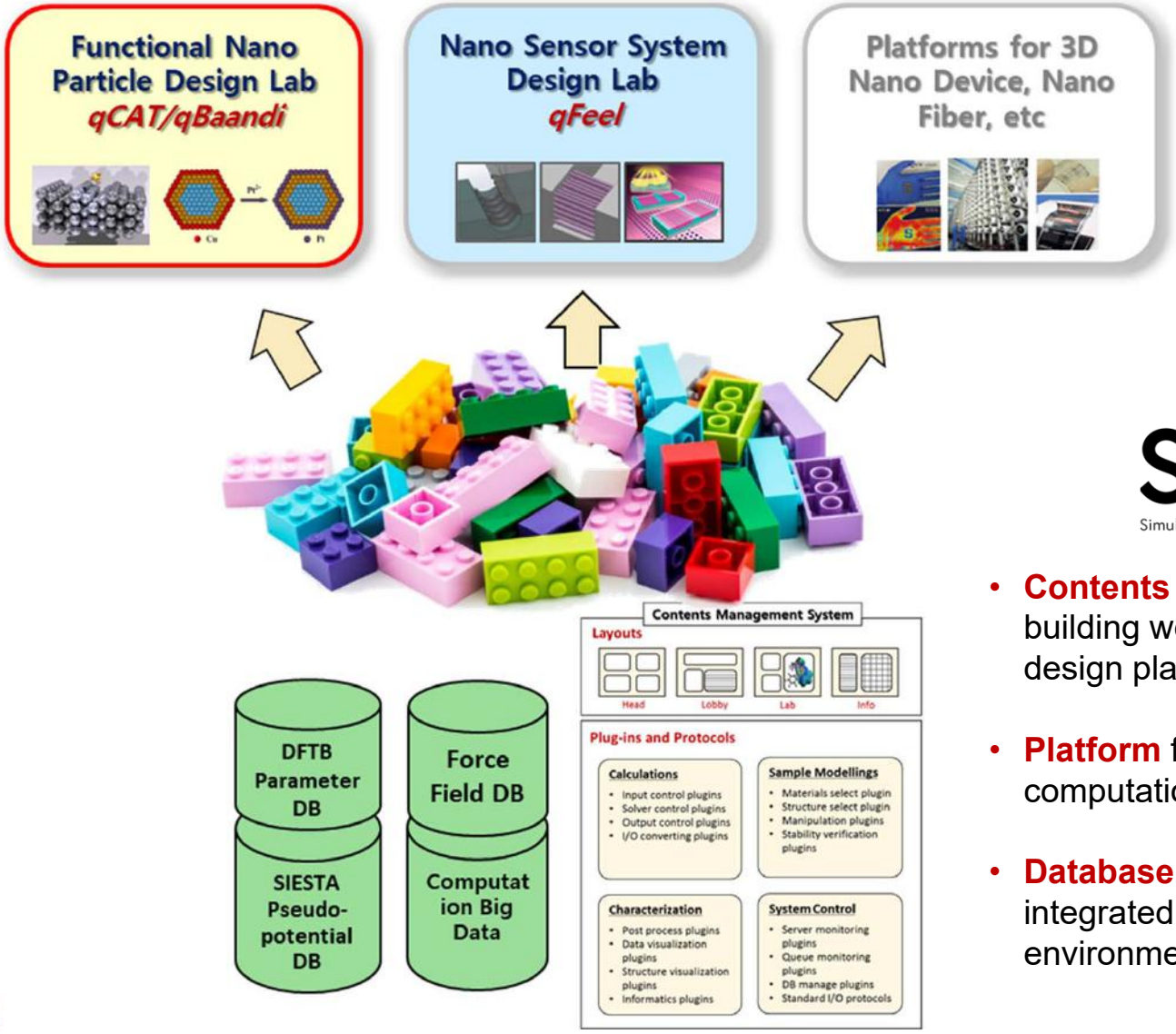


Ag	Exp.	DFT-CES
(100)	-0.66	-0.63
(110)	-0.74	-0.80
(111)	-0.45	-0.26



DFT-CES plugins on SimPL

Simulation Platform Creator : *SimPL*



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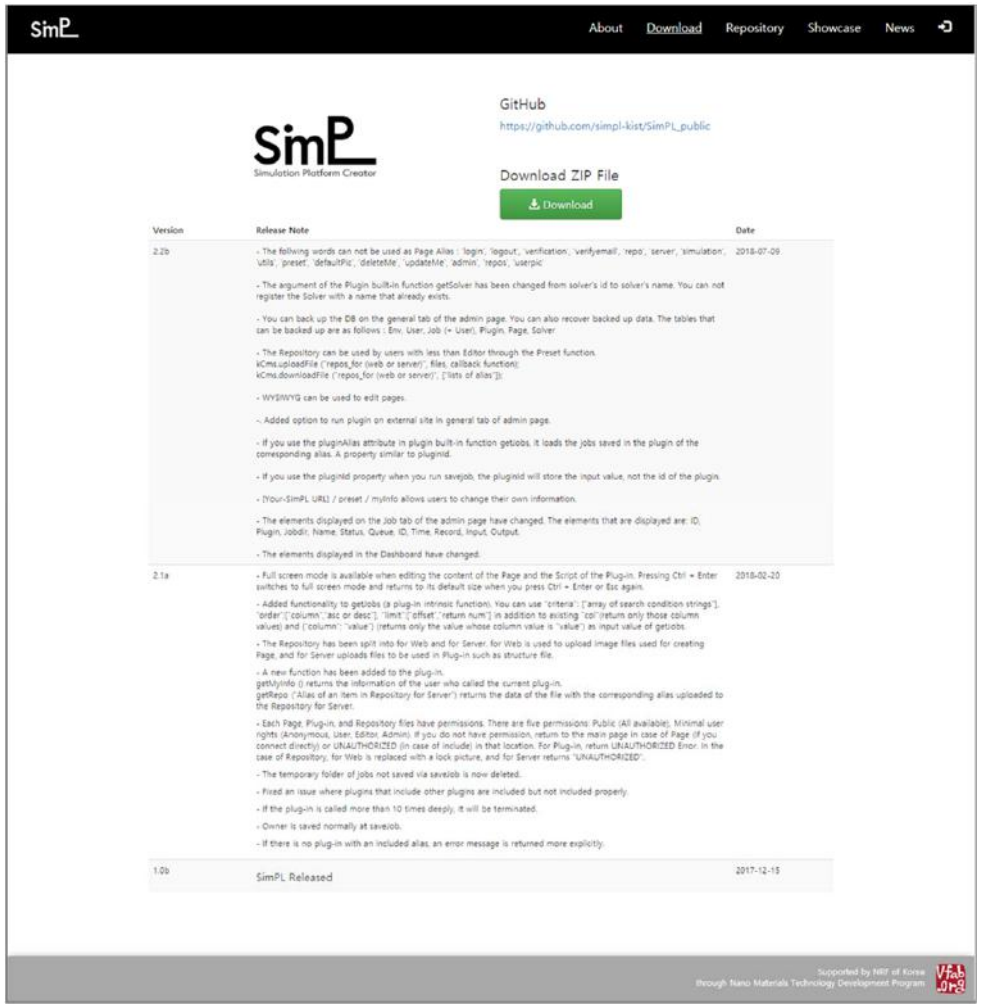
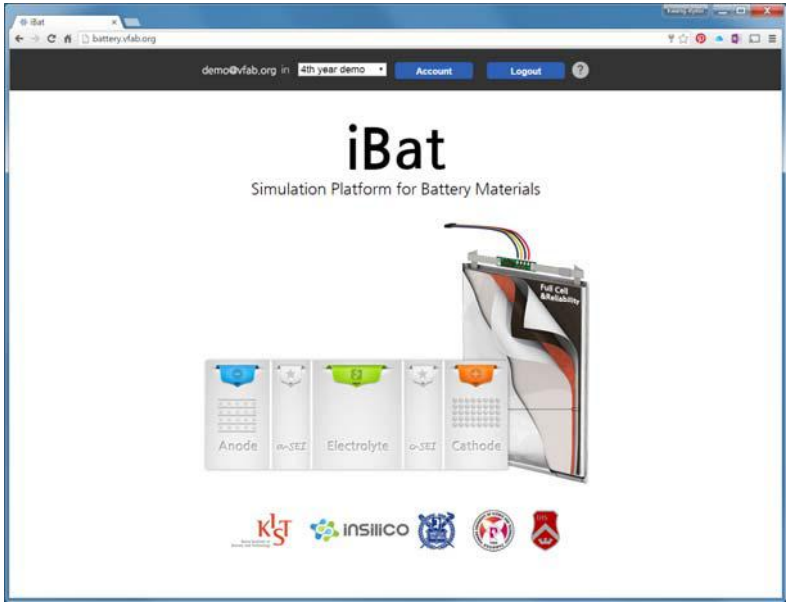
vfab.org

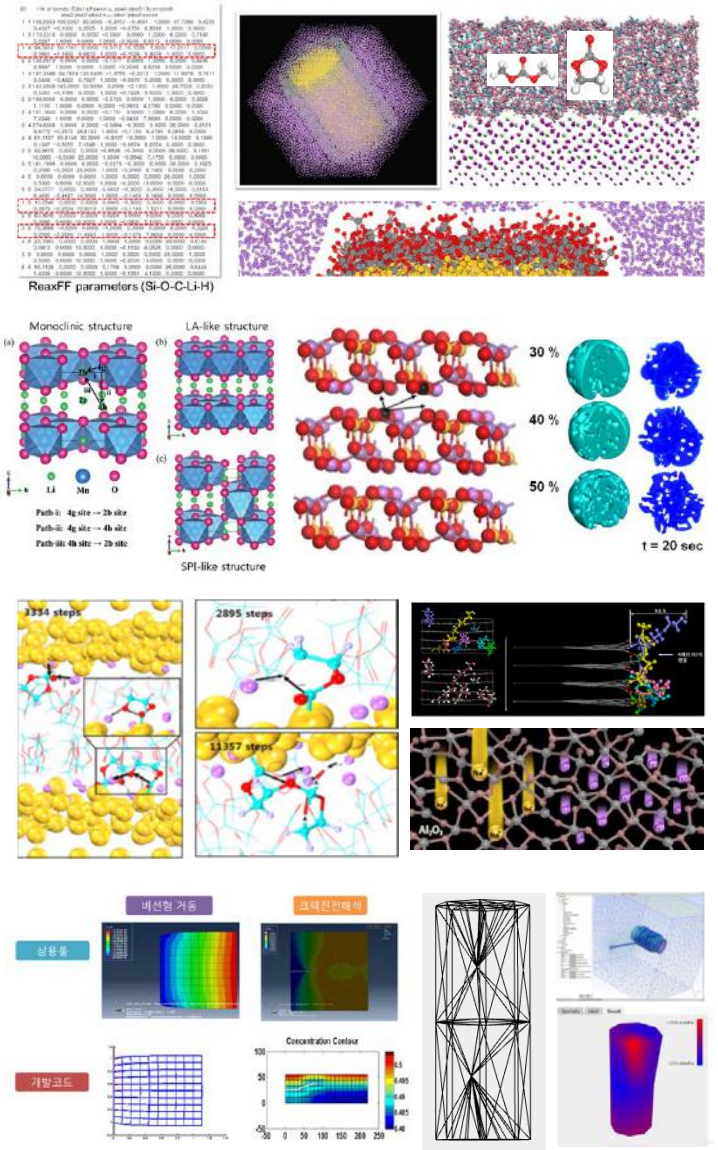


Supported by NRF of Korea
through Nano Materials Technology Development Program

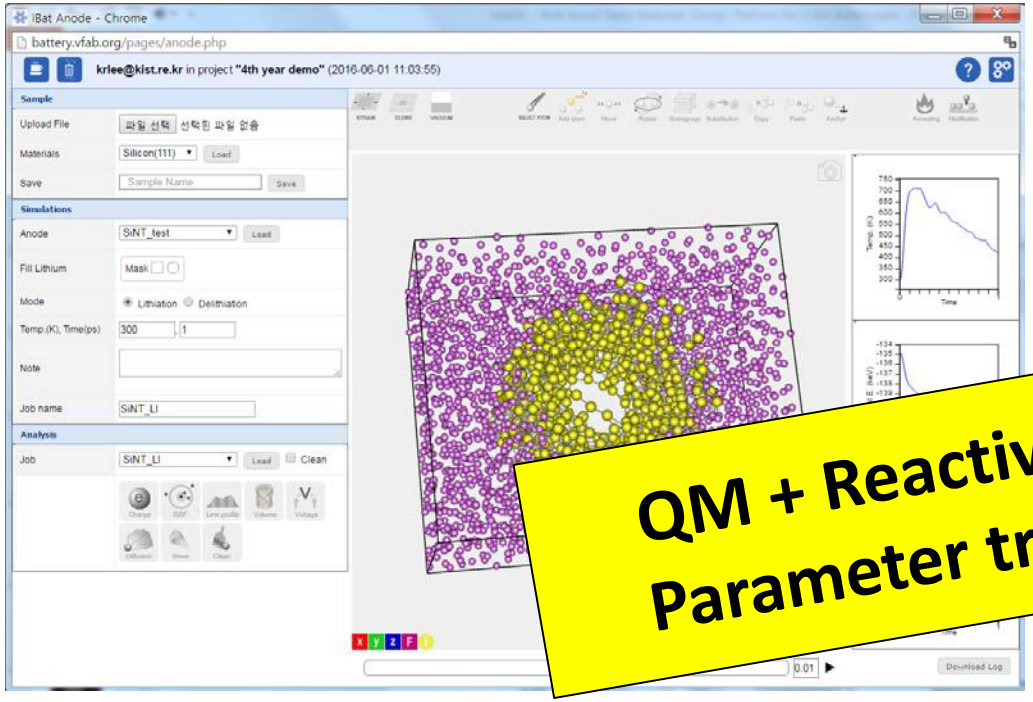
Battery Materials Design Platform



http://battery.vfab.org



Anode Design Module

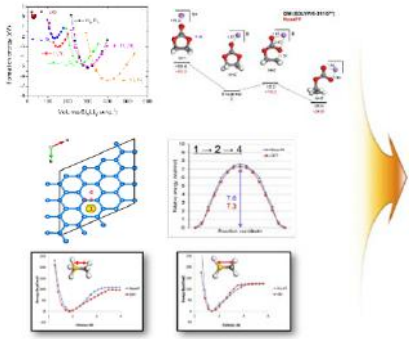


QM + Reactive MD Parameter transfer

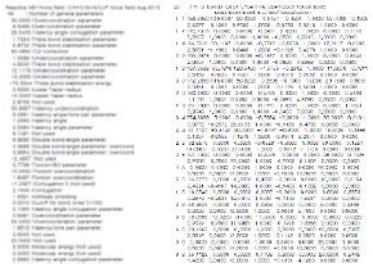
Anode Modeler

Reactive MD of Lithiation & Delithiation

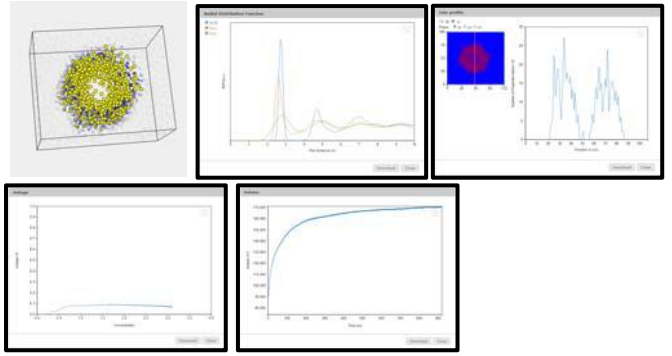
Analysis Tools



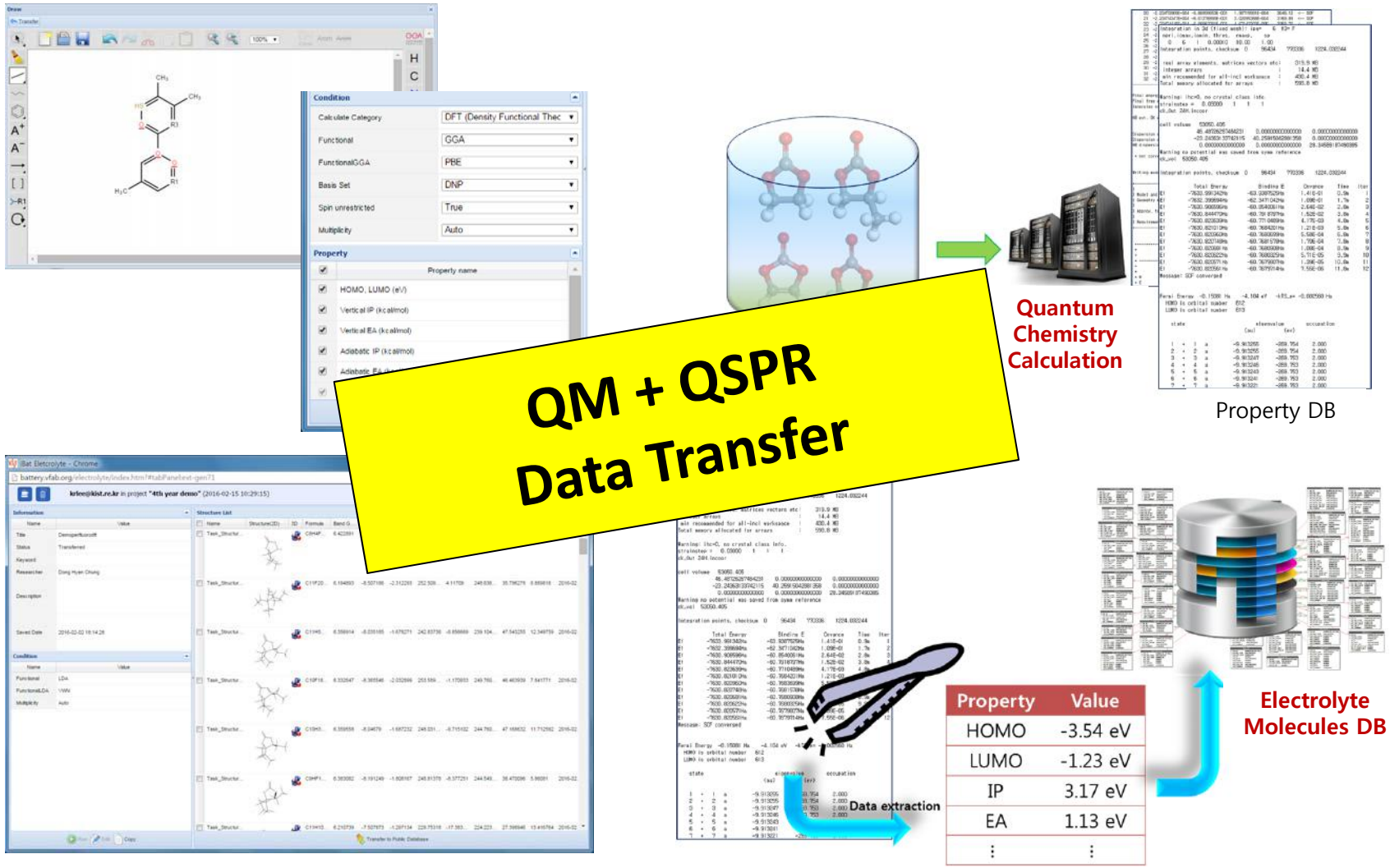
First-principles Calculations



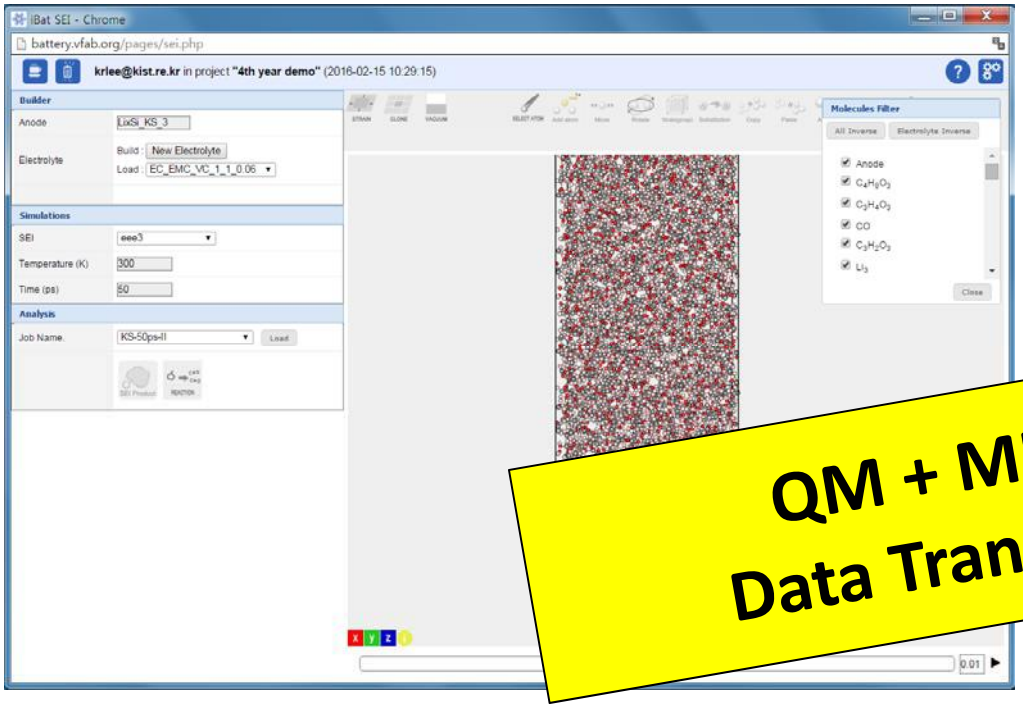
ReaxFF parameters
(C-Si-Li-O-H-P-F)



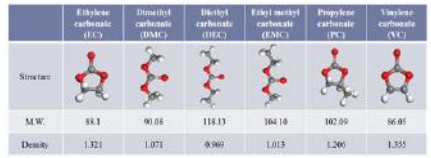
Electrolyte Design Module



SEI Simulation Module



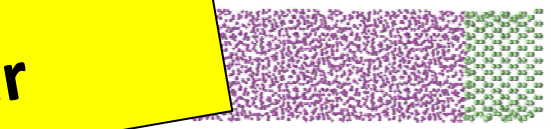
Electrolyte Molecule DB

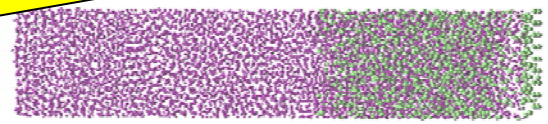


Anode DB

Electrolyte Modeler

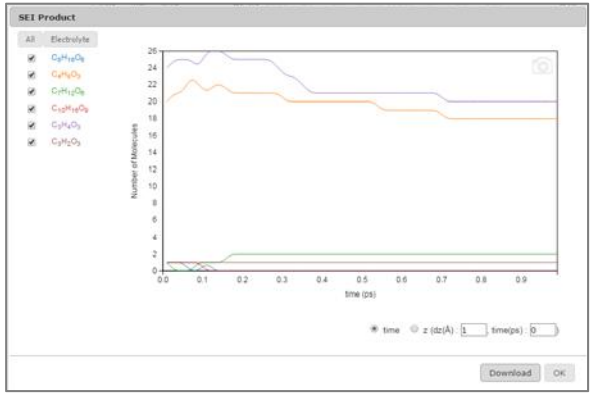
nterface Builder

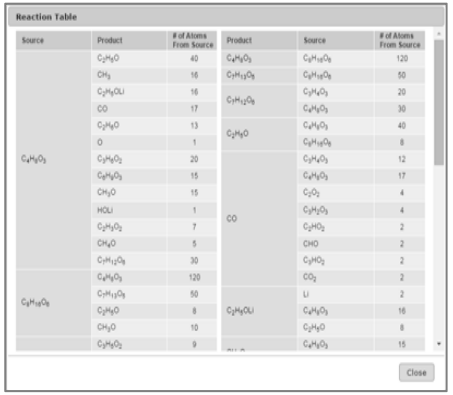




Reactive MD Simulation

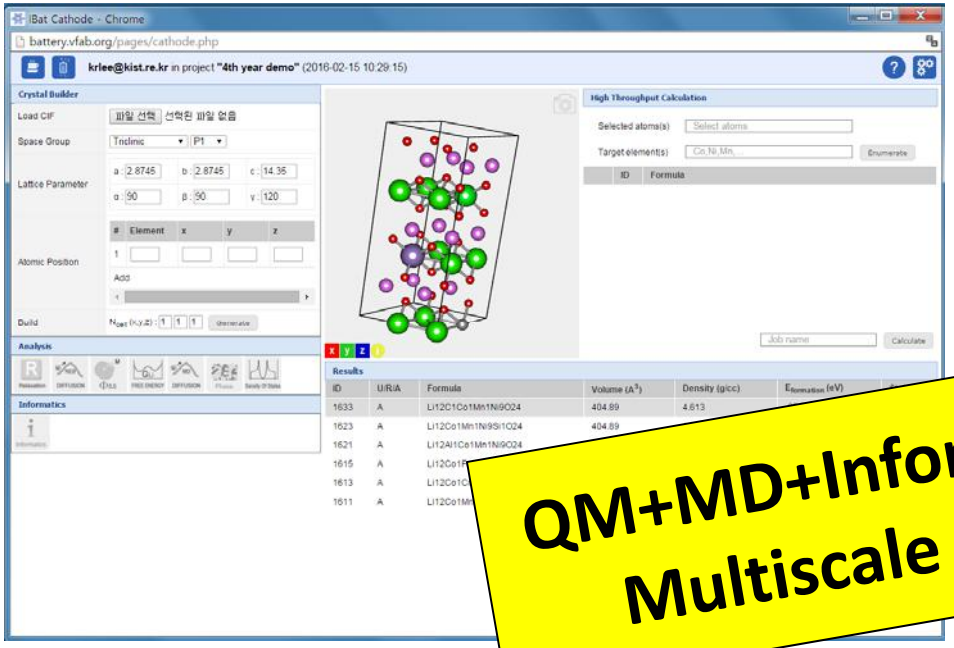
QM + MD Data Transfer



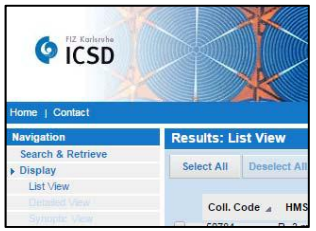


Analysis of Products

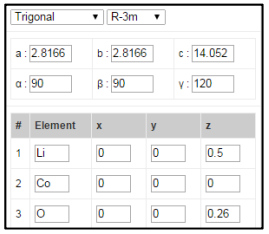
Cathode Design Module



Crystal Structure DB

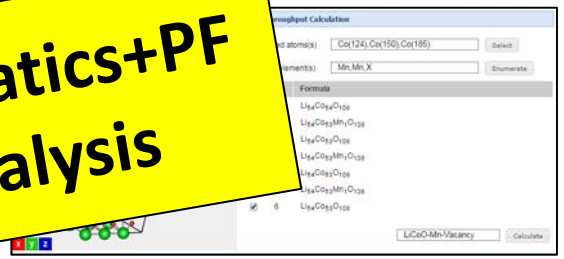


Crystal Builder



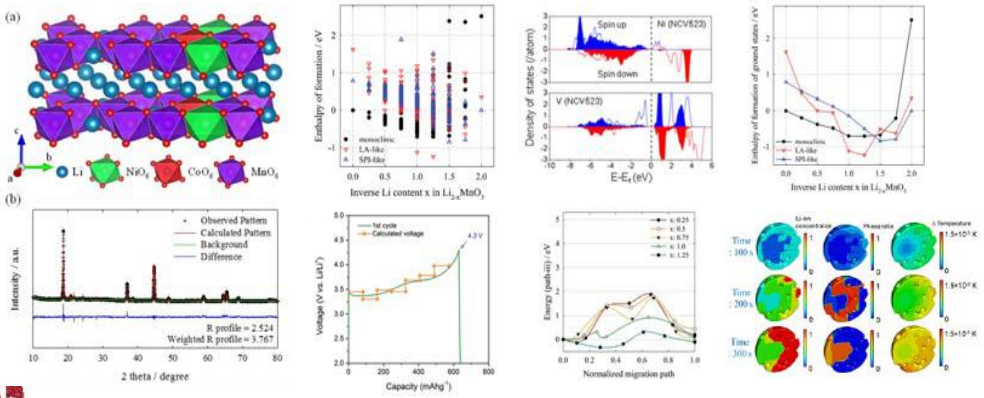
QM+MD+Informatics+PF Multiscale Analysis

Enumerate
Defective & Doped Crystals

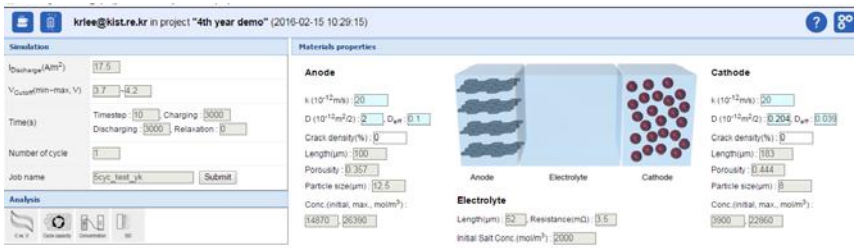


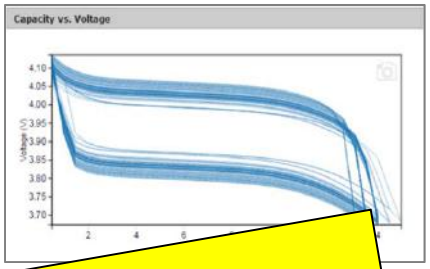
Ab initio High
Throughput Calculations

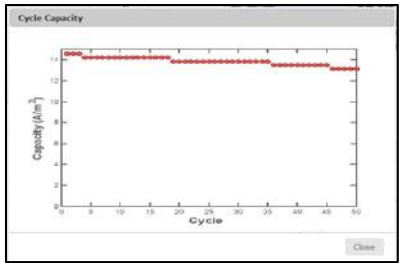
Analysis and Informatics



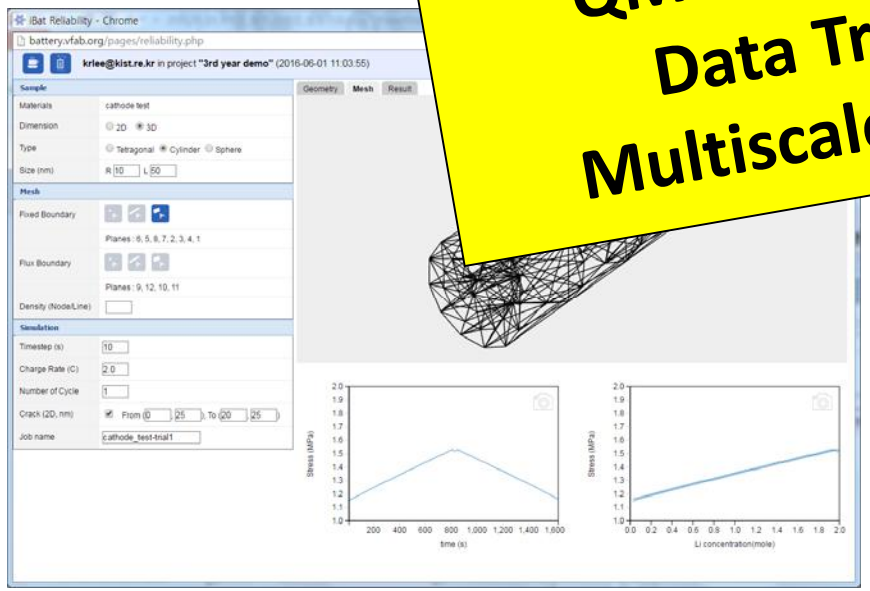
Full Cell and Reliability Test Module

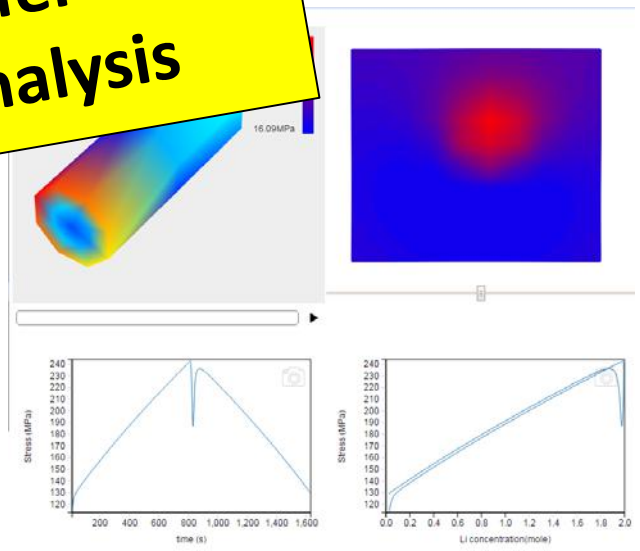




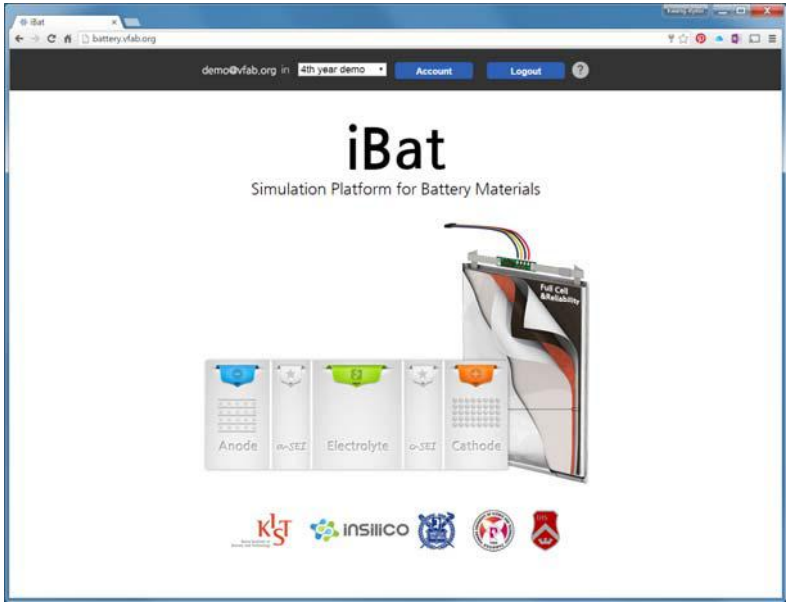


QM+MD+PF+FEM
Data Transfer
Multiscale Analysis

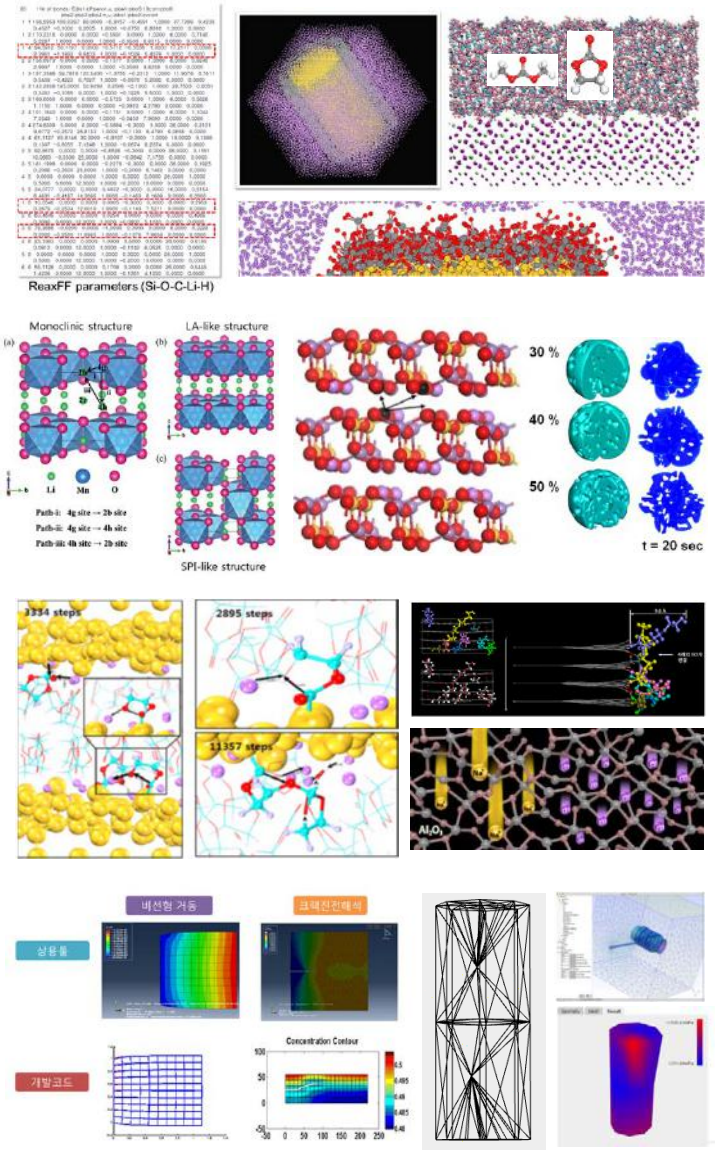




Battery Materials Design Platform



http://battery.vfab.org



Further Issues

- **Present computation method is not enough for industrial (seriously practical) applications of multiscale simulation.**
  - Kinetics matters more than energetics
  - Need long time scale simulation
  - Need much much more transferable parameters
  - Need more efficient calculation
  - Need robust visualization technique : Simulo-scope
- **Anyone can build platforms for their own purpose with great ease.**
  - Build every basic component into module of common interface
  - SimPL on Cloud would be a solution.