Web 2.0 Based Platform for Nano-Materials Design

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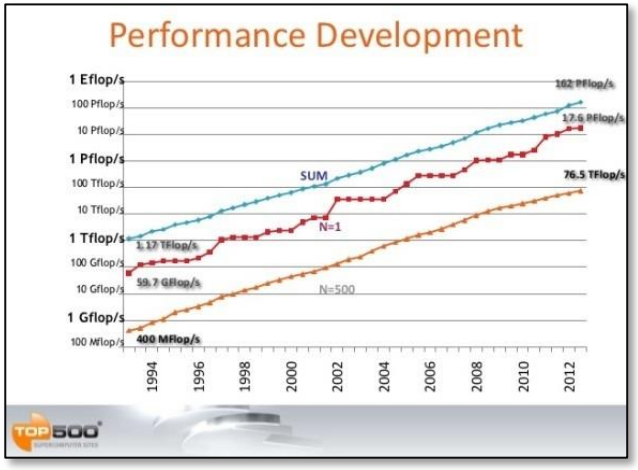
“Design of Materials”

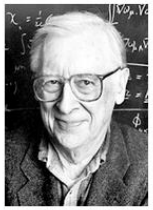
- **Increased computing power**
- **Advancement of computing method**
  (1998 Nobel Prize in Chemistry)
- **Accumulated knowledge of the interatomic modeling**
  (2013 Nobel Prize in Chemistry)
- **Increased predicting power of the materials simulation**



~10^6 times faster during last 20 years

The Nobel Prize in Chemistry 1998

Walter Kohn
Prize share: 1/2



John A. Pople
Prize share: 1/2

The Nobel Prize in Chemistry 1998 was divided equally between Walter Kohn *"for his development of the density-functional theory"* and John A. Pople *"for his development of computational methods in quantum chemistry"*.

The Nobel Prize in Chemistry 2013

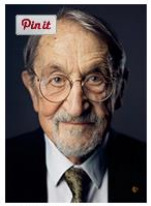


Photo: A. Mahmoud
Martin Karplus
Prize share: 1/3

Photo: A. Mahmoud
Michael Levitt
Prize share: 1/3

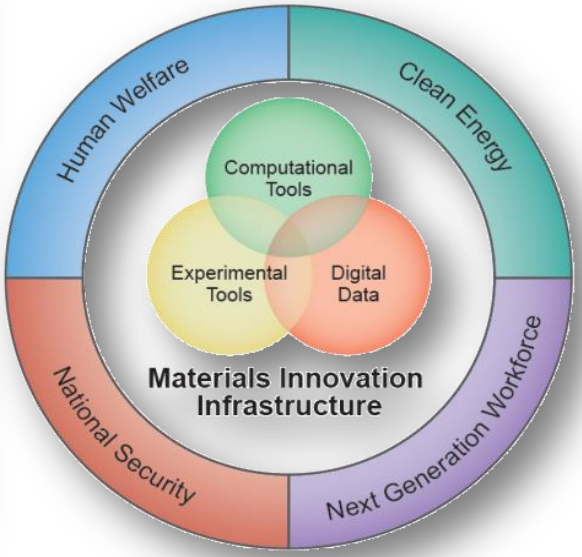
Photo: A. Mahmoud
Arieh Warshel
Prize share: 1/3

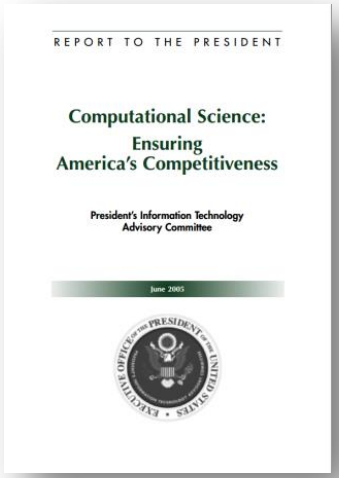
The Nobel Prize in Chemistry 2013 was awarded jointly to Martin Karplus, Michael Levitt and Arieh Warshel *"for the development of multiscale models for complex chemical systems"*.

New Paradigm of Materials Research

Source : Sci. Am. (2013.12)

Materials Genome Initiative (USA)



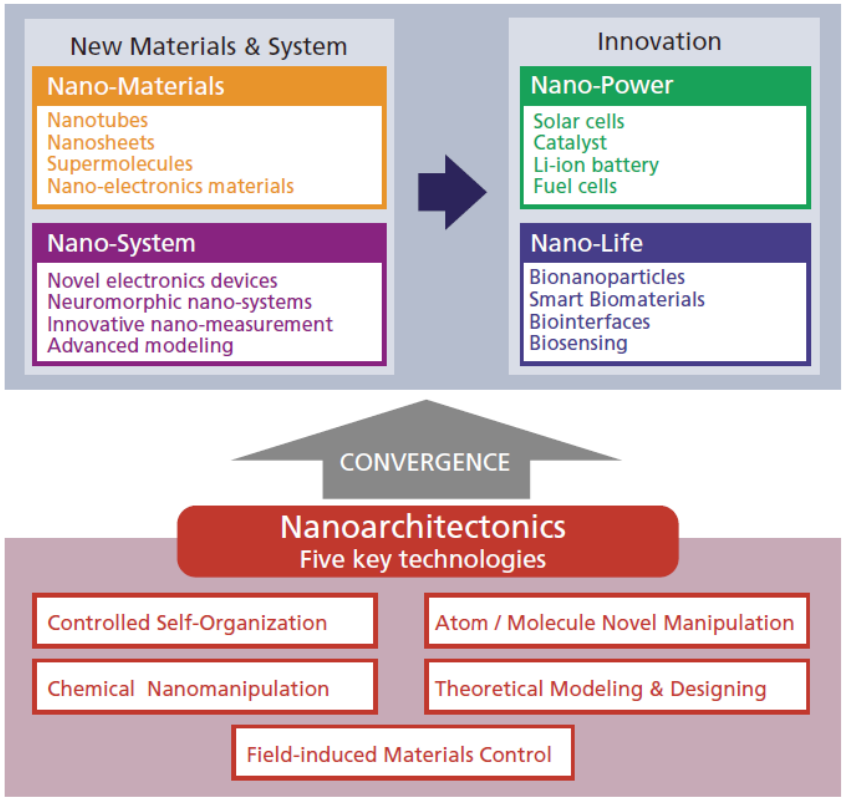


Hybrid Research Centers in Japan

wpi World Premier International Research Center Initiative

Nano Revolution for the Future

Since 2007

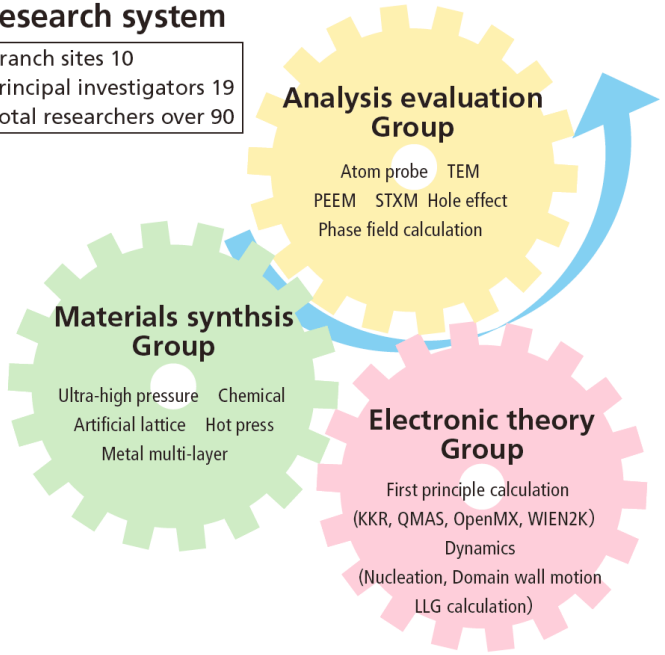


ESIC MM

Elements Strategy Initiative Center for Magnetic Materials

Research system

Branch sites 10
Principal investigators 19
Total researchers over 90

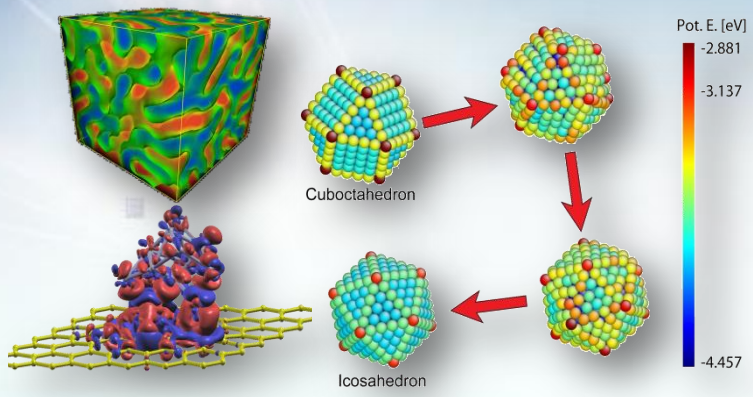


Since 2010

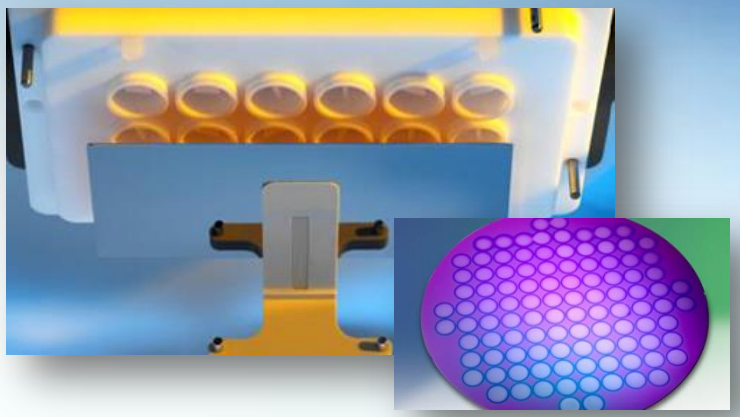
素材强國
창의소재 디스커버리 사업

미래창조과학부

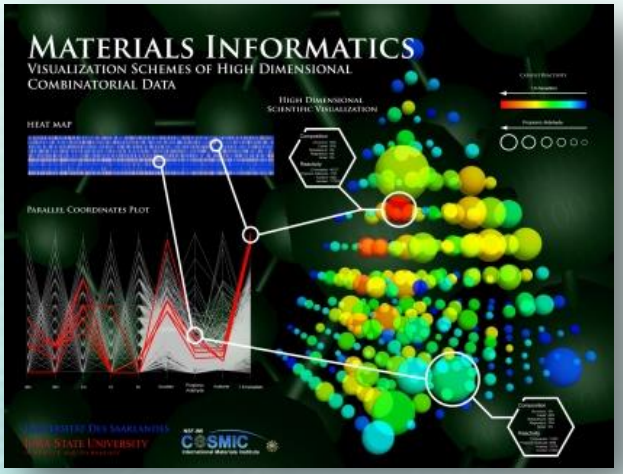
IT Based Research Methods



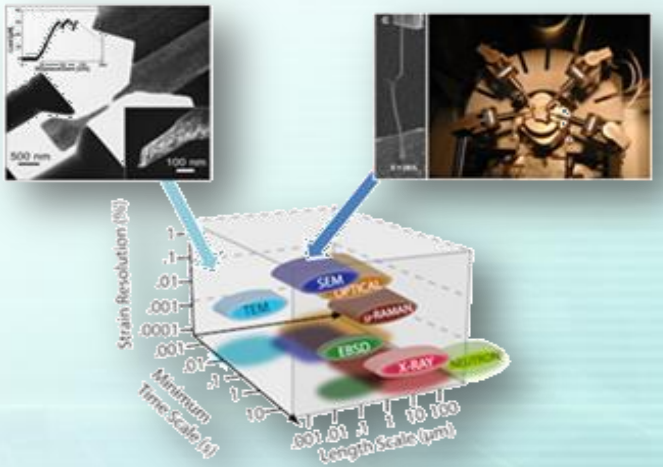
Design of Materials & Processes by Computer Simulation



Optimization of Materials Process by Combinatorial Experiment

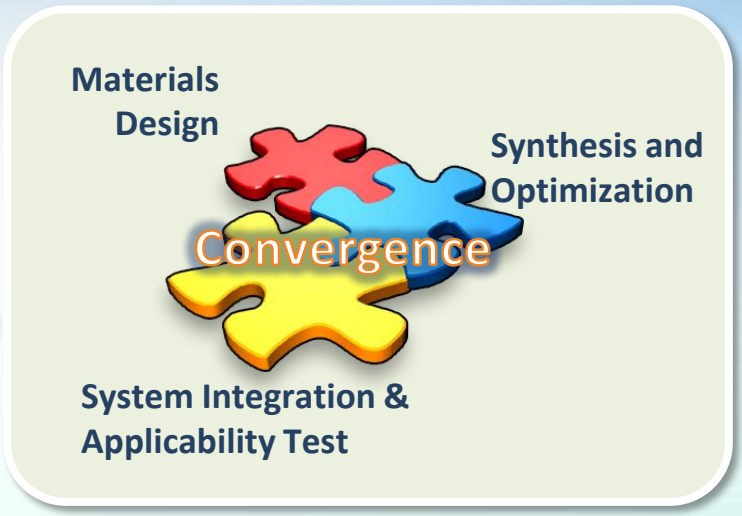


Search for Optimized Materials by Informatics



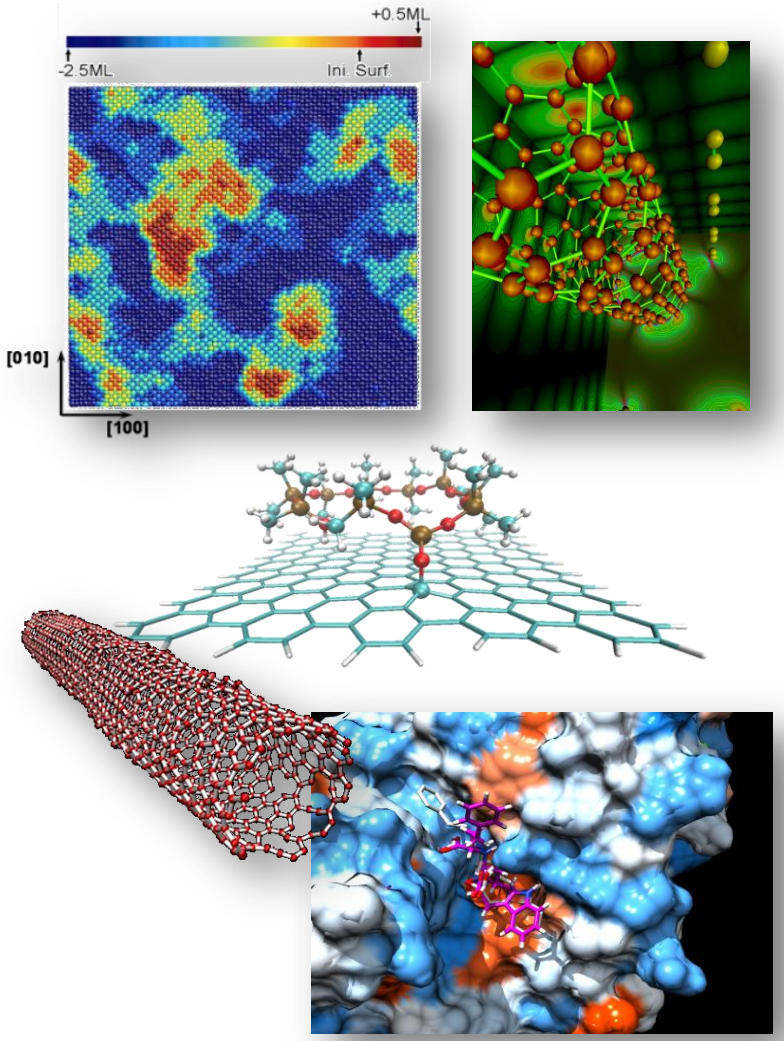
***in-situ* Multi-property Characterization**

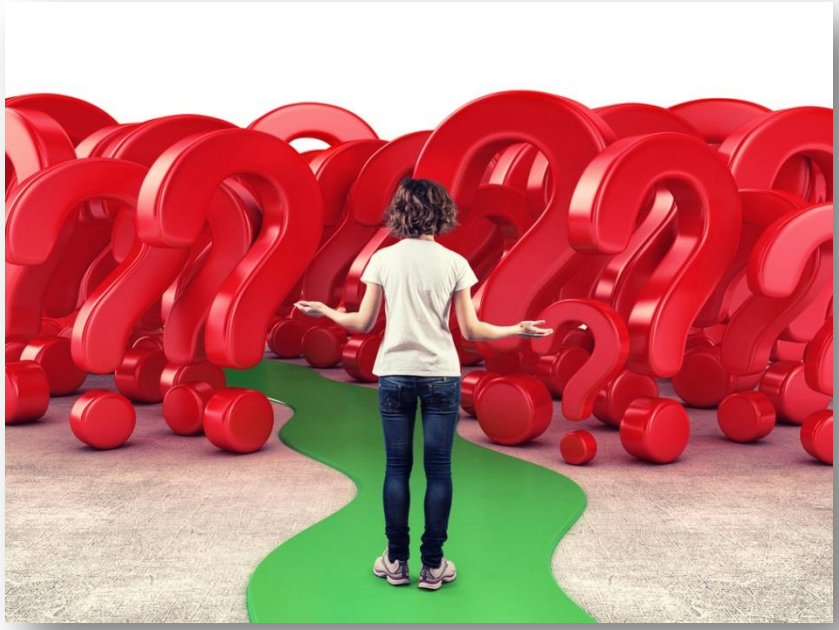
Center for Creative Materials



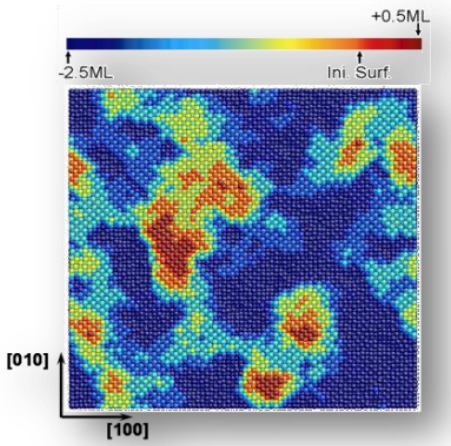
- Period : ½ Yr. (Pre) & (3+3) Yr. (Main)
- Budget : 1.5~2.0 M$/Yr.
- PI : 5~7
- Type : Convergence Research Center

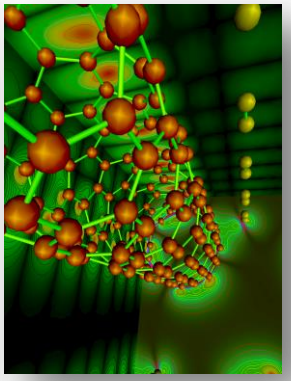
Materials Design for Everyone

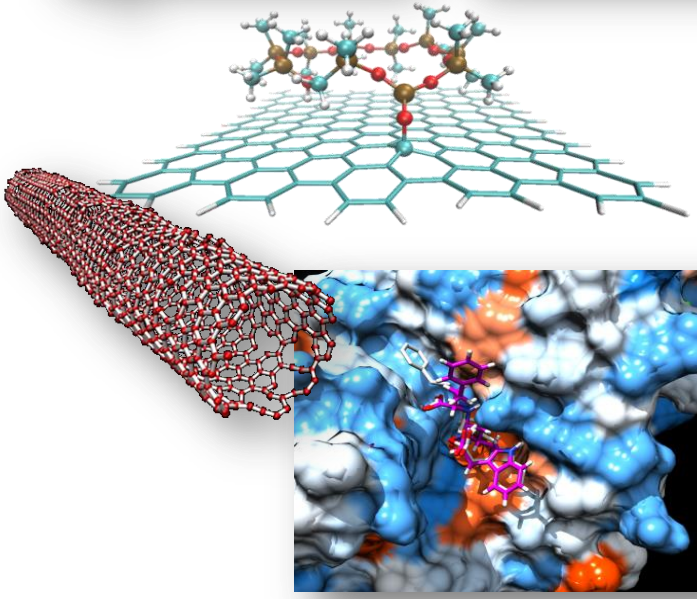




Materials Design for Everyone







Atomic Simulation Environment

The Atomic Simulation Environment (ASE) is the common part of the simulation tools developed at CAMd. ASE provides Python modules for manipulating atoms, analyzing simulations, visualization etc.

Note: The old ASE-2 webpage has moved to http://wiki.fysik.dtu.dk/ase2.

Actively maintained ase.calculators:

abinit Asap EMT Gaussian GPAW! GROMACS NWCHEM

Supported ase.calculators (we are looking for maintainers!):

CASTEP DFTB+ exciting Fleur Hb JACAPO Mopac siesta TURBOMOLE VASP

Cyberinfrastructure for Atomistic Materials Science

UF UNIVERSITY of FLORIDA
The Foundation for The Gator Nation

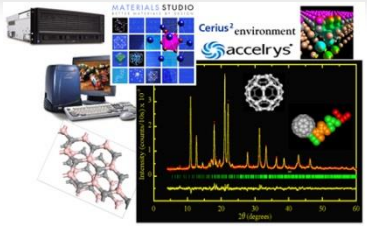
DTU COMPUTATIONAL MATERIALS REPOSITORY DTU

OpenKIM

Welcome to the Knowledgebase of Interatomic Models

nanoHUB
online simulation and more
an NCN project

Quantum Wise



Simulation Platform as a Virtual Fab

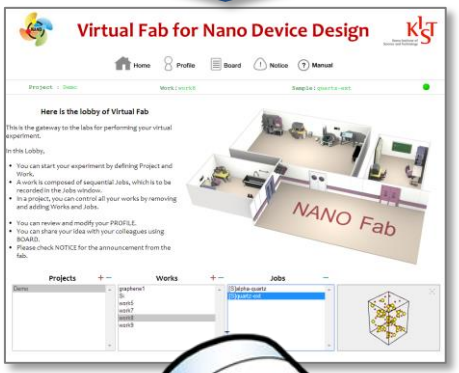
LAMMPS

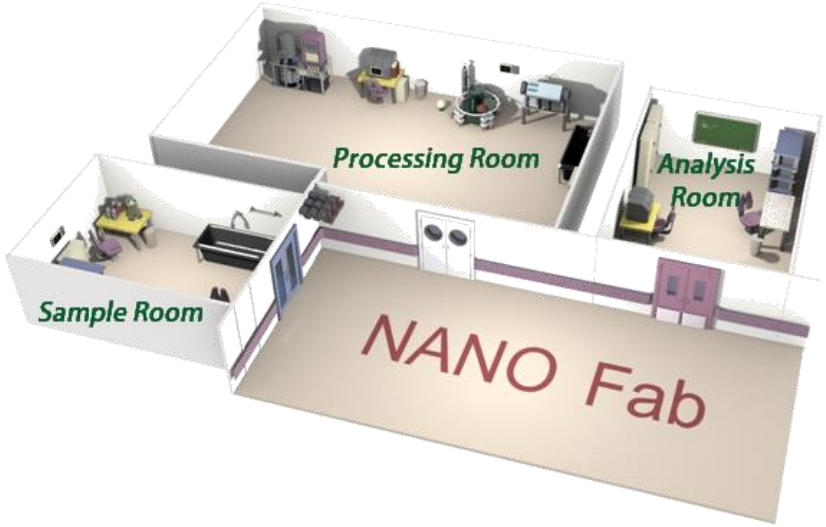
siesta

SRIM & TRIM

RxFF

Home Made Codes

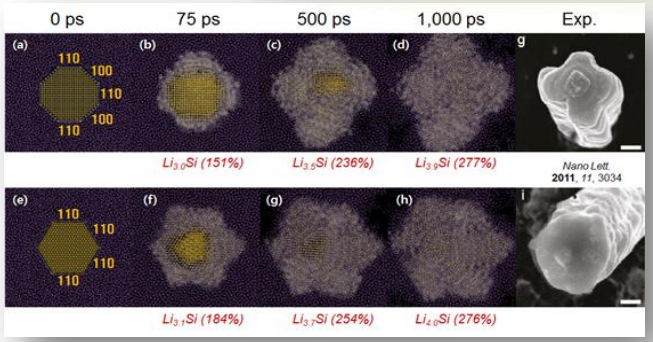


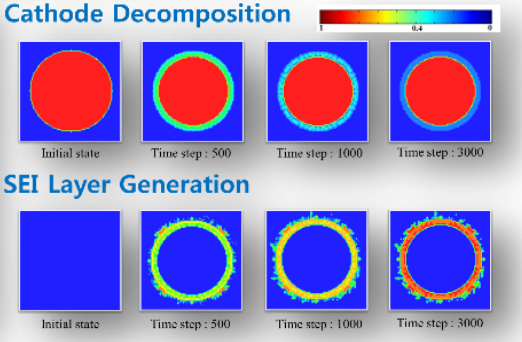


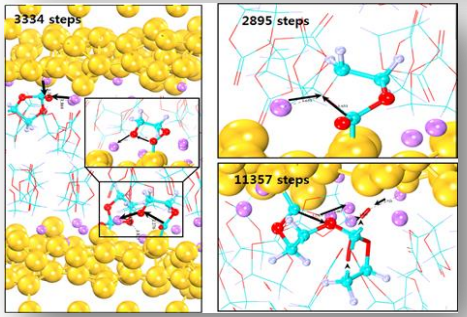
Trying to mimic the procedure of the experimental works in the FAB of real space,

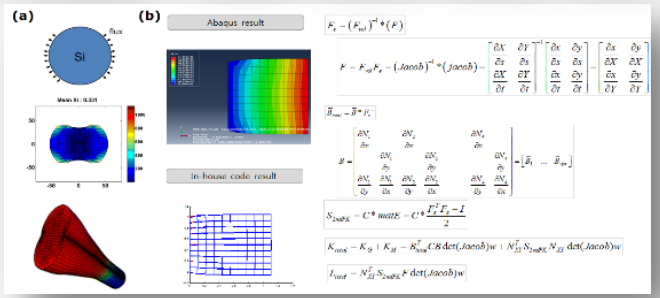
As closely as possible!

Virtual Lab for Li Ion Battery Materials







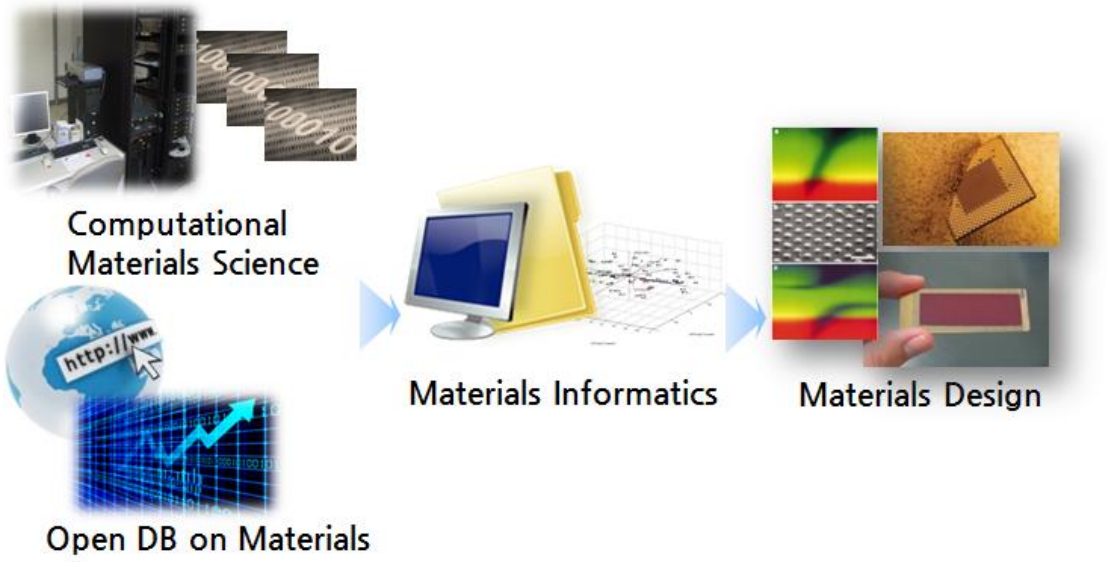


Virtual Fab for Nano Device Design

http://vlab.kist.re.kr/VLAB_NANO

Goal of KIST Nano Virtual Fab

Web-based Platform for Materials Design by Computer Simulation and Materials Informatics



- **Multiscale Simulation Environment**
  - Virtual Fab for Everyone (QM, MD, MC, Meso, FEM)
- **Material Informatics Environment**
  - Database + Data Warehouse
  - Data Analysis Algorithm

Major Bottle-neck or Issues

- Accuracy and Speed of DFT Calculation
- Lack of Calculation Method
  - Exited State / Electrochemical Reaction
- High Throughput DFT Calculation (Generalized)
- Insufficient Development of the Interatomic Potential
- Lack of Transferability of the Empirical Potential
- Limited Time Scale of MD
- Off-lattice k-MC Simulation

Dynamic Link with KIM-API

OpenKIM

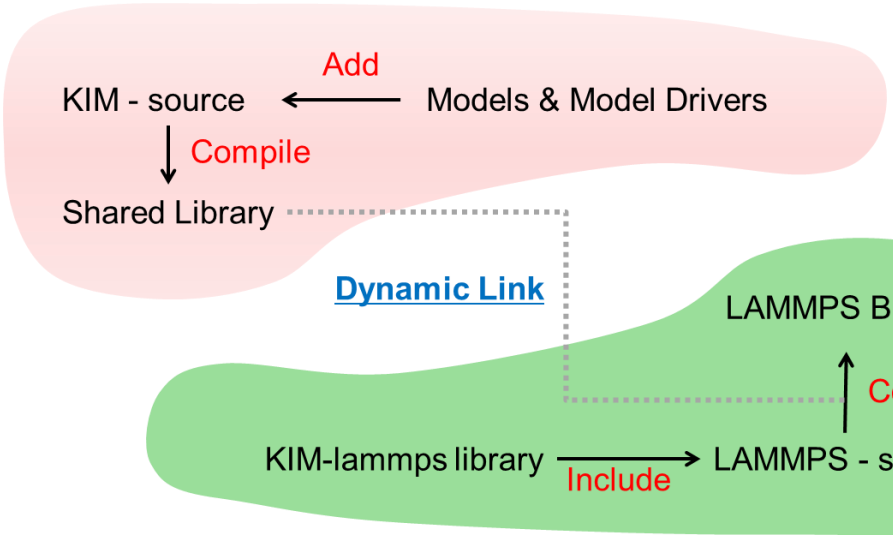
Welcome to the Knowledgebase of Interatomic Models

An online resource for standardized testing and long-term warehousing of interatomic models and data. This includes the development of *application programming interface* (API) standards for coupling atomistic simulation codes and interatomic potential subroutines.

Based on a NSF Cyber-Enabled Discovery and Innovation (CDI) Program (since 2012)
PI : Ellad Tadmor (U Minn) / James Sethna (Cornell) / Ryan Elliott (U Minn)

KIM

KIM by NSF
(2M$ for 4 years)



Virtual Fab by NRF
(2.5M$ for 5 years)

Summary

- Virtual Fab for Materials Design will become an essential tool of the (near) future materials research.
- Global collaboration is the only way to realize the tools.

KIM Workshop for Content Contributors (2014.8. Univ. Maryland)

Dear Seungchul,

It was a great pleasure to have you and Minho attend KCC Maryland this summer.

We were very impressed with the progress you made connecting Virtual Fab with KIM.

We would be pleased to continue the collaboration. Please let us know if there are any developments on the US-Korea collaboration proposal that we put together.