

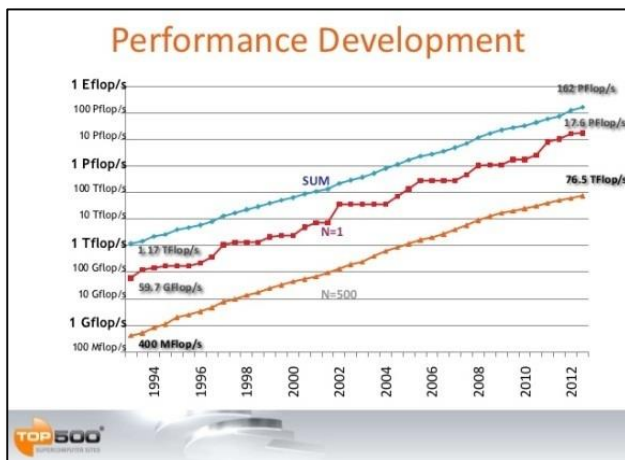
Web 2.0 Based Platform for Nano-Materials Design

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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**



~10⁶ 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

SCIENCE AMERICAN

WORLD CHANGING IDEAS

The Alchemist

How super... are transform... innovation... materials d...

Twelve global trends to 2020

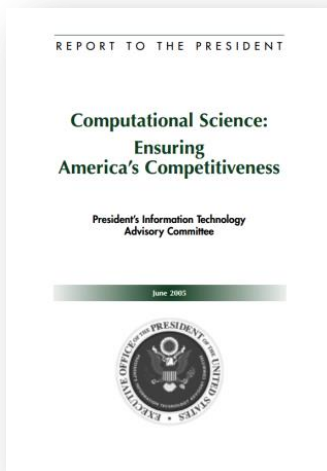
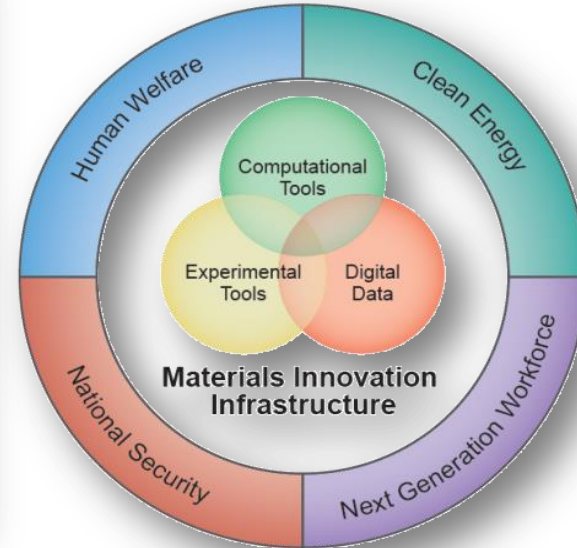
www.wtec.org/nano2/

- Theory, modeling & simulation: x1000 faster, essential design
- “Direct” measurements – x6000 brighter, accelerate R&D & use
- A shift from “passive” to “active” nanostructures/nanosystems
- Nanosystems, some self powered, self repairing, dynamic
- Penetration of nanotechnology in industry - toward mass use; catalysts, electronics; innovation- platforms, consortia
- Nano-EHS – more predictive, integrated with nanobio & env.
- Personalized nanomedicine - from monitoring to treatment
- Photonics, electronics, magnetics – new capabilities, integrated
- Energy photosynthesis, storage use – solar economic by 2015
- Enabling and integrating with new areas – bio, info, cognition
- Earlier preparing nanotechnology workers – system integration
- Governance of nano for societal benefit - institutionalization

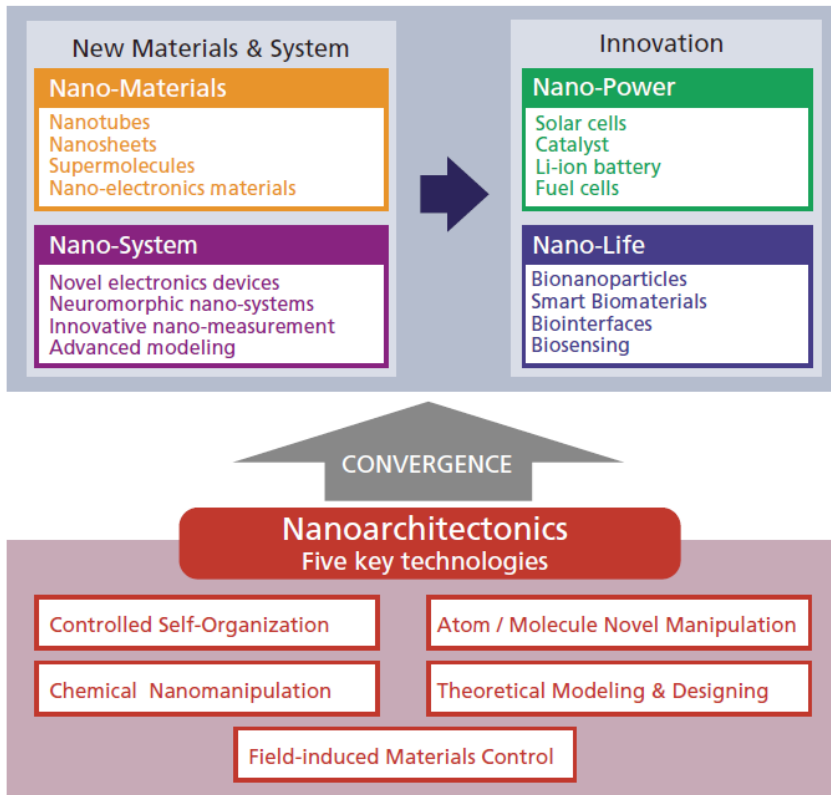
ScientificAmerican.com 1 of 4 DECEMBER 2013

Source : Sci. Am. (2013.12)

Materials Genome Initiative (USA)

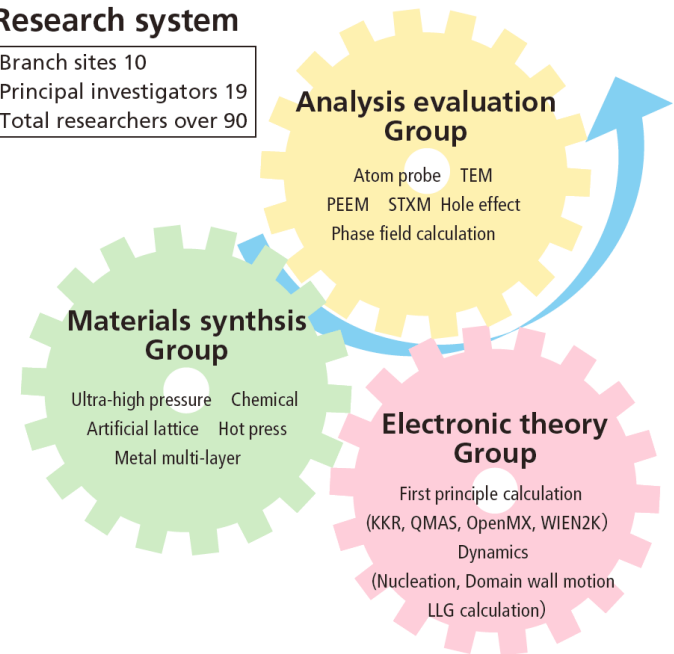


Hybrid Research Centers in Japan



Research system

Branch sites 10
Principal investigators 19
Total researchers over 90

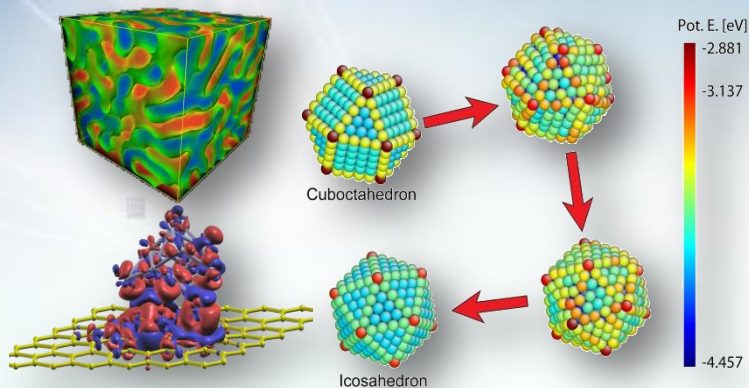


Since 2010

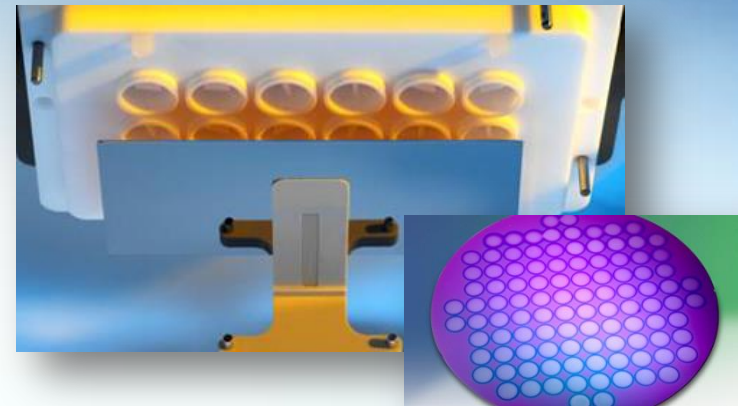
A vibrant blue-themed graphic for 'Creative Materials Discovery'. The background features a large globe with a grid pattern, partially obscured by a bright sun and white clouds. A green leaf with two leaves is positioned above the globe. The title 'Creative Materials Discovery' is written in a bold, yellow, sans-serif font with a blue outline. Several circular inset images are scattered around: a DNA double helix, a glowing fiber optic cable, and a stylized atomic model. The overall design is futuristic and scientific.

Creative Materials Discovery

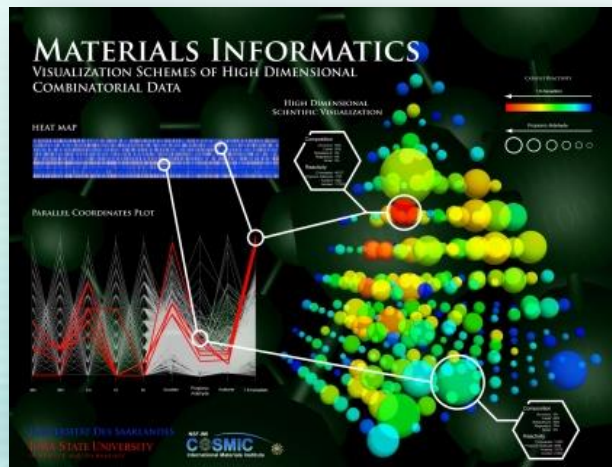
IT Based Research Methods



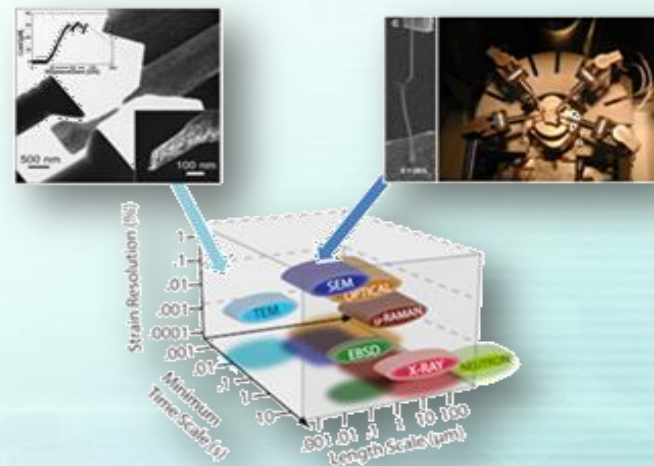
**Design of Materials & Processes
by Computer Simulation**



**Optimization of Materials Process
by Combinatorial Experiment**



**Search for Optimized Materials
by Informatics**



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

Center for Creative Materials



Materials Design

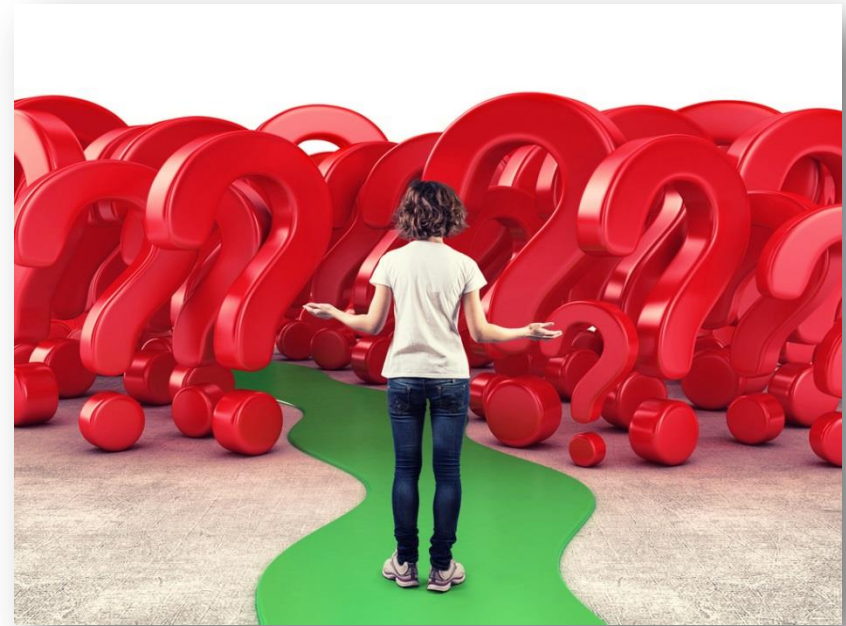
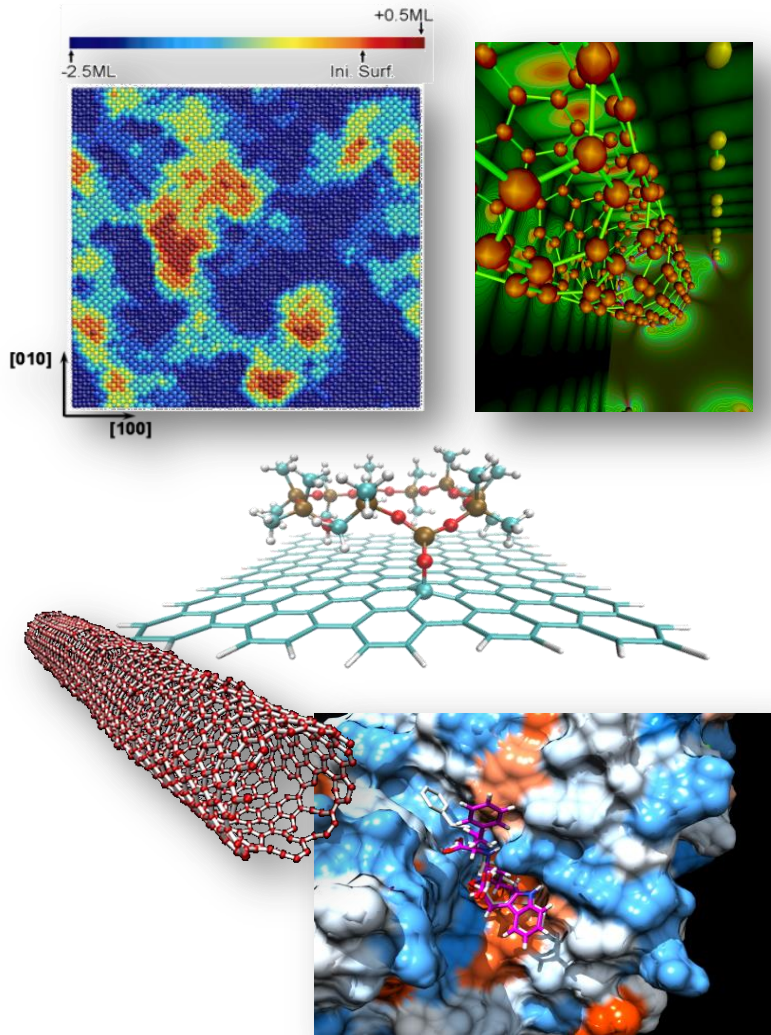
Synthesis and Optimization

Convergence

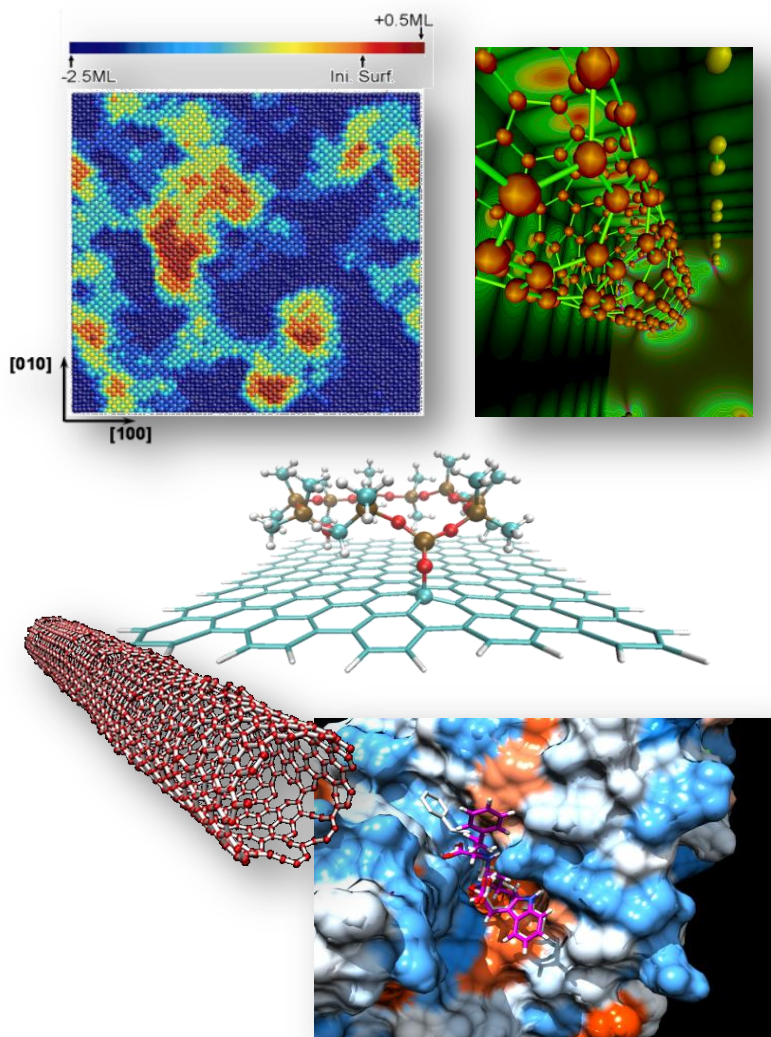
System Integration & Applicability Test

- 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 CAMK. 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:

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

Cyberinfrastructure for Atomistic Materials Science

**COMPUTATIONAL
MATERIALS
REPOSITORY**

OpenKIM

Welcome to the Knowledgebase of Interatomic Models

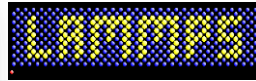
nanoHUB

an NCN project

online simulation and more

Quantum
Wise

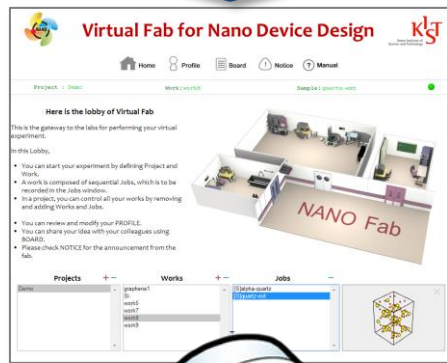
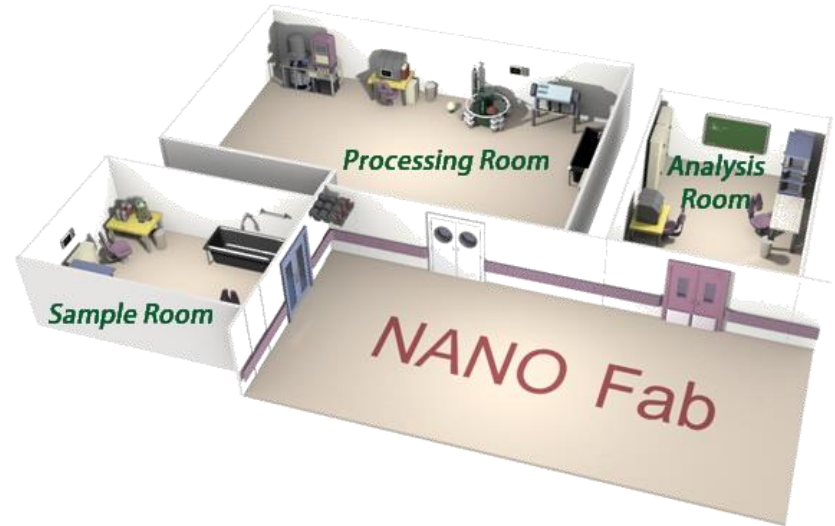
Simulation Platform as a Virtual Fab



SRIM & TRIM



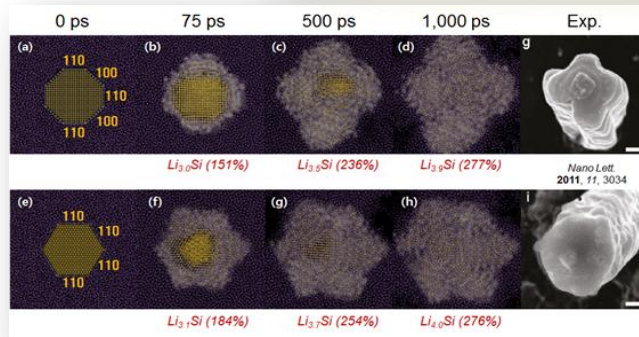
Home Made Codes



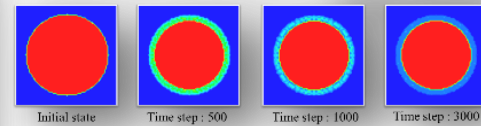
Trying to mimic the procedure of the experimental works in the FAB of real space,

As closely as possible!

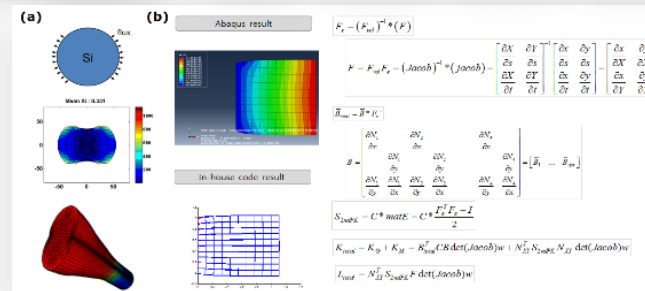
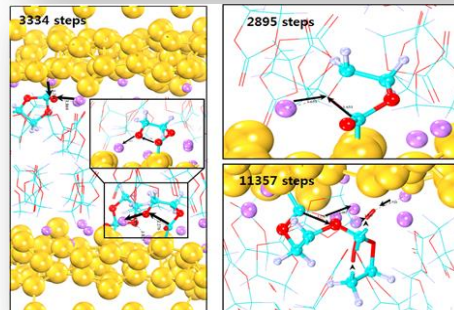
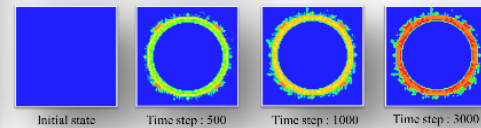
Virtual Lab for Li Ion Battery Materials



Cathode Decomposition



SEI Layer Generation



Virtual Fab for Nano Device Design



Virtual Fab for Nano Device Design

Projects

Team

Credits

TCAD

Manual

Log out

Welcome to the Virtual Fab for Nano Device Design at KIST!

As the devices scaled down to nanometer regime, conventional TCAD technology based on the continuum media hypothesis frequently fails. In order to overcome the limit, we are developing a multiscale simulation platform for nano device simulation based on the atomistic simulation technology.

The computation methods integrated in this platform span from the first principles calculation based on the density functional theory, quantum transport calculation, (reactive) molecular dynamics simulations to the Monte Carlo simulation. In addition, various analysis tools are also being integrated.

This website is to provide the simulation environment under a similar environment of the experimental nano fab facility. This Virtual Fab consists of three laboratories : Sample Preparation Room, Process Laboratory and Analysis Laboratory. We try to provide a flexible working environment where the users can design and perform their own process and analysis workflows.

This Virtual Fab resulted from a project funded by the Converging Research Center Program of Korea. For more details, please refer to the [Project page](#)

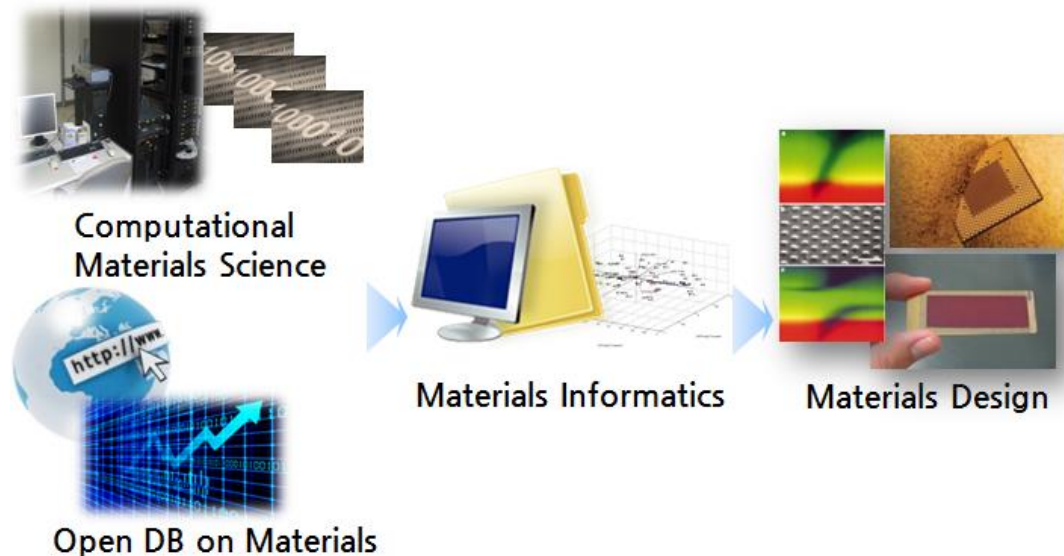
CURRENT USER 이광철 (KIST)



Last update : 2014/5/20

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

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



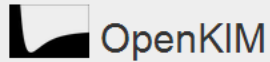
- **Multiscale Simulation Environment**
 - Virtual Fab for Everyone (QM, MD, MC, Meso, FEM)
- **Material Informatics Environment**
 - Database + Data Warehouse
 - Data Analysis Algorithm

Major Bottle-neck or Issues

- Accuracy and Speed of DFT Calculation
- Lack of Calculation Method
 - Excited 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



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.

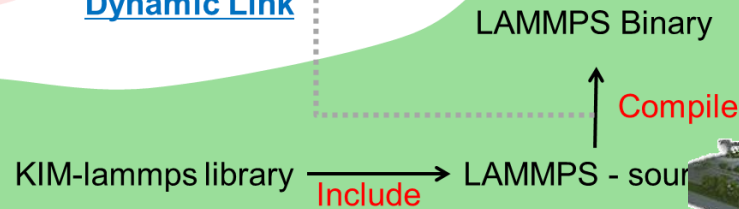
*Based on a NSF Cyber-Enabled Discovery and Innovation (CDI) Program (since 2012)
PI : Ellad Tadmor (U Minn) / James Sethna (Cornell) / Ryan Elliott (U Minn)*



KIM by NSF
(2M\$ for 4 years)



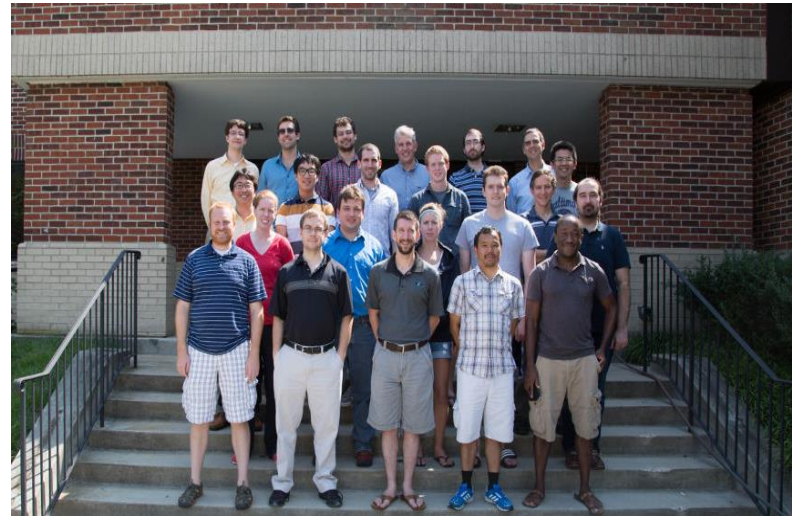
Dynamic Link



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.

