Industrial Innovation
by Combinatorial Computational Chemistry
Miyamoto Laboratory

Multi-Level Combinatorial Computational Chemistry for Industrial Innovation

Practical Computational Chemistry New Methodology for Industrial Innovation

Prof. Akira Miyamoto
NICHe, Tohoku University

1967-1989
Suzuka Tech. Coll. ～Tohoku Univ.
～Nagoya Univ.～Kyoto Univ.
・Experimental study on solid catalysis etc.

1987-
Kyoto Univ.～Tohoku Univ.
・Computer-aided design of molecules and materials
(Toward the establishment of novel chemistry-based method for industrial innovation)

Synergetic Interaction of Industry/Academia (Miyamoto Lab. Model, NICHe, Tohoku Univ.)

Solution of Industrially Most Important Issues
-Development of original computational method for practial problems
-Commercialization of developed software:
private fund from software company and creation of software industry
-Realization of sustainable laboratory administration by private funds

Economic Value
Academic Value
Promotion of Industry/Academia collaboration
Social & Cultural Value

Academic Frontier Young Top Researchers
-Top research environment
-Academic breakthrough
-Next generation educator
-Competitive fundings

Contribution to Society
-Creation of local employment
-International exchange through inviting foreign researchers
-Training industrial researchers
-Recurrent education

Research Environment for Strong Industry/Academia Collaboration

Leader : Akira Miyamoto
Core Members : Hiromitsu Takaba, Akira Endou
Nozomu Hatakeyama, Hideyuki Tsuboi, Ai Suzuki, Ryuji Miura, Ryo Nagumo

-Many Collaborators in Miyamoto Lab.
Visiting Professors: 15
Advisor: 3
Collaborative Researchers: 10
Technical Assistants: 28
Secretaries: 5
Students: 28
Ph.D.: 13
Master: 9
Undergraduate: 5
Research Student:1
Part time-Programmer:45
Total 142 (2010.8.1)


Endowed Chair,Combinatorial Computational Chemistry


Department of Chemical Engineering


New Industry Creation Hatchery Center

Proposal of "Combinatorial Computational Chemistry" by Project Leader

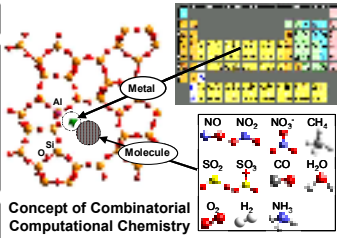
Combinatorial Chemistry

This method can synthesize hundreds of new samples systematically with one time experiment. It **significantly accelerates** the development of new materials.

Combinatorial Computational Chemistry

Introduction of combi-chem concept to computational chemistry

Computational chemistry is employed as a high-throughput screening method for designing and developing new materials.



Concept of Combinatorial Computational Chemistry

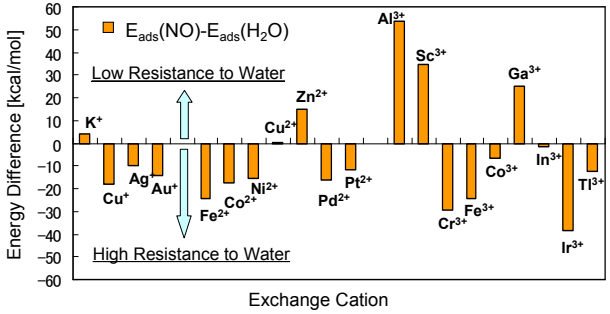
High-Throughput Screening

We developed huge number of original programs for theoretical high-throughput screening.

This new methodology is recognized as **an essential technique** for **industrial innovation**.

IrZSM-5 – New Catalyst Designed by Combinatorial Computational Chemistry

Strong NO adsorption indicates high H_2O resistance.



High resistance to water in Pd, Fe, and CoZSM-5 agrees well with previous experiments. High resistivity of IrZSM-5 catalyst was experimentally confirmed by Waseda Univ., after our proposal.

Education of Practical Computational Chemists in Strategic Industries

Strategic Industrial Fields	Industrial Researchers
Electronics Semiconductors	Experimental Researchers in Industries
Catalysts Batteries	Semiconductor Co.
Environments Energies	Electric Co.
Ceramics Bio-Molecules	Chemical Co.
Tribology Machinery	Automobile Co.
	Machine Co.
	Heavy Industry Co.
	Oil Co.
	Electric Power Co.
	Gas Co.
	Pharmaceutical Co.
	Software Co.
	etc.

Coursework Carriculum
Systematic learning system for fundamental knowledge through lectures and exercise programs.

On the Job Training
Application of combinatorial computational chemistry method to individual topic in each company.

Effective Utilization of Internet
State of the art programs are accessible from each company.

Large Impact
Project researchers transfer acquired knowledge to other researchers in the company.

Leading Power of Industry
Creation of new market & industry by Japanese initiative.

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Multi-Level Combinatorial Computational Chemistry for Industrial Innovation: Originally Developed Computational Chemistry Software

Molecular Dynamics
1. Integrated Molecular Dynamics System (NEW-RYUDO)
2. Tribology Simulator (TRIBOSIM)
3. Molecular Dynamics with Chemical Reaction Extention (NEW-RYUDO-CR)
4. Crystal Growth Simulator (MOMODY)
5. Grand Canonical Molecular Dynamics
6. Non-Equilibrium Molecular Dynamics (DEMD)

Quantum Chemical Molecular Dynamics
1. Accelerated Quantum Chemical Molecular Dynamics (QCMD) (Colors)
2. QCMD with Excited State Extention
3. Hybrid QCMD with Dynamic Hybridization Scheme
4. Partial Diagonalization QCMD
5. Chemical Mechanical Polishing Process Simulator
6. Plasma Process Simulator
7. Etching Process Simulator

Programs are sold by
PEGASUS Software Inc.
http://www.psinc.co.jp/
Ryoka Systems Inc.
http://www.rsi.co.jp/

Physical Properties Prediction Simulator
1. Electrical Conductivity Simulator (Colors-Cond)
2. Phonon-based Thermal Conductivity Simulator (THERMOSIM)
3. Conduction Electron-based Thermal Conductivity Simulator (THERMO-Colors)
4. Viscousity Simulator
5. IR Simulator

Combinatorial Computational Chemistry Systems Developed in Miyamoto Laboratory

Monte Carlo
1. Grand Canonical Monte Carlo Considering Chemical Reactions (MONTA)
2. Non-Equilibrium Monte Carlo (DEMC)
3. Kinetic Monte Carlo Considering Chemical Reactions
4. Particle Growth & Thin Film Growth Kinetic Monte Carlo Simulator

Graphic User Interface (GUI)
1. Integrated 3D Graphic Platform with Virtual Reality (NEW-RYUGA)
2. Integrated Molecular Modelling Program (NEW-RYUKI)
3. 3D Graphic User Interface for Windows (WRYUGA)

Practical Multi-Scale Simulator
1. Porous Structure Simulator
2. EL Device Simulator
3. Sintering Simulator
4. Macroscopic Pharmaco-kinetics Simulator

Design of Electronics Materials
1. Ion Implantation
2. Chemical Mechanical Polishing
3. Etching, Oxidation, Nitridation
4. Blue Phosphors
5. Organic Electroluminescence Device
6. Plasma Display
7. Crystal Growth

Design of Catalysts
1. deNOx Catalysts for Automobile
2. Desulfurization Catalysts
3. Combustion Catalysts
4. Polyolefin Synthesis Catalysts
5. Fischer-Tropsh Synthesis
6. Photocatalysts
7. Methanol and DME Synthesis
8. Sensor Devise Electrode Catalyst

Dynamics of Catalysts and Adsorbates
1. Adsorption and Diffusion of Molecules in Zeolites
2. Proton Diffusion Dynamics in Heteropolyacids
3. Sintering of Supported Precious Metal Catalysts
4. Periodic Microporous Catalyst

Design of Ceramics Materials
1. Crystal Growth of Oxides
2. Mesoporous Ceramics
3. Hetero-Interface Junction
4. Design of Buffer Layer
5. Ferroelectrics
6. Transparent Conductors
7. Ion Conductors
8. Ferromagnetics, Spintronics

Various Applications of Combinatorial Computational Chemistry in Miyamoto Laboratory

Design of Membrane and Adsorbent
1. Pd Hydrogen Permeation Membrane
2. Hydrogen Absorption Metal Alloys
3. Carbon Nanotube
4. Zeolite Membrane
5. Dialysis Polymer Membrane

Design of Battery and Fuel Cell Materials
1. Carbon-supported Pt Catalyst
2. Proton Exchange Membrane
3. Li Ion Battery Cathode
4. Li Ion Battery Electrolyte

Design of Mechanical Engineering Materials and Tribology Materials
1. Nano-Fabrication, Nano-Tribology
2. Traction Oil, Engine Oil
3. Solid Lubrication (ZnDTP, MoDTC, DLC)
4. Lubricants for Hard Disk

Miscellaneous
1. Electrical Breakdown
2. Thermoelectric Conversion
3. Biocatalysts
4. Dye sensitizer
5. Self-Organization

Pamphlet for Developed Software Sold by PEGASUS Software and Ryoka Systems

Computational Chemistry Software for Industrial Innovation

Theoretical High-Throughput Screening of Electronics Materials, Ceramics, Catalysts...

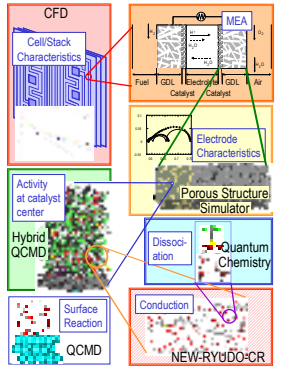
【Combinatorial Computational Chemistry Engines】

- ○ Accelerated Quantum Chemical Molecular Dynamics (QCMD) Program "Colors"
- ○ Hybrid QCMD Program "Hybrid-Colors"
- ○ Accelerated QCMD Program with Rare-earth Extention "Colors-Rare Earth"
- ○ Accelerated QCMD Program with Excited State Extention "Colors-Excite"
- ○ Electrical Conductivity Simulator "Colors-Cond"
- ○ Macroscopic Electrical Conductivity Simulator "Macro-Cond"
- ○ Molecular Dynamics Program "NEW-RYUDO"
- ○ Molecular Dynamics with Chemical Reaction Extention "NEW-RYUDO-CR"
- ○ Monte Carlo Program "MONTA"
- ○ Tribology Simulator "TRIBOSIM"
- ○ Porous Structure Simulator

【Combinatorial Computational Chemistry Graphic Engines】

- ○ Graphic User Interface "NEW-RYUGA"
- ○ Modeling Program "NEW-RYUKI"

Multi-Level Combinatorial Computational Chemistry Realized by Original Software



Application

Chemistry, Physics, Machinery, Bio-system…

-Ceramics	-Tribology
-Semiconductors	-Adsorbent
-Membranes	-Lubricants
-Electronics	-Batteries & Fuel cells
-Catalysts	-Luminescence material
-Absorption	-Medicine etc.

Hardware Environment

- ○ Workstation by Silicon Graphics, Inc., Hewlett- Pakkard Co., Sun Microsystems, IBM
- ○ Linux OS on personal computer
- ○ Windows OS on personal computer

Software Developer : Miyamoto Laboratory, New Industry Creation Hatchery Center, Tohoku University
6-6-10 Aoba, Aramaki, Aoba-ku, Sendai 980-8579, Japan
TEL: +81-22-795-7233, FAX:+81-22-795-7235, e-mail: miyamoto@aki.che.tohoku.ac.jp
Software Distributor: PEGASUS Software, Inc.
4-5-2 Hatchobori, Kyodo Bldg., Chuo-ku, Tokyo 104-0032, Japan
TEL: +81-3-3553-7211, FAX:+81-3-3553-7212
Software Distributor : Ryoka Systems, Inc.
Tokyo Daiya Bldg., 1-28-38, Shinkawa, Chuo-ku, Tokyo 104-0033, Japan
TEL: +81-3-3553-9206, FAX: +81-3-3553-9207

Industrial Innovation
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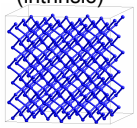
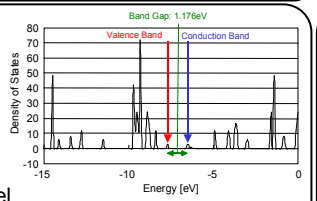
Multi-Level Combinatorial Computational Chemistry for Industrial Innovation: Accelerated Quantum Chemical Molecular Dynamics Simulations

Precise Band Calculation (Si)

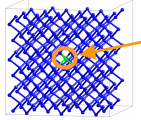
Realistic large-size model of Si system

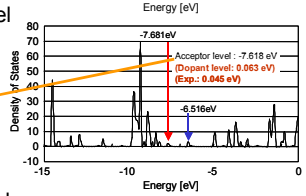
(1) Si_{216} Model (intrinsic)



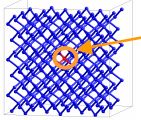


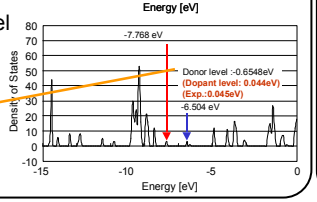
(2) $Si_{215}B_1$ Model (p-type Si)





(3) $Si_{215}P_1$ Model (n-type Si)

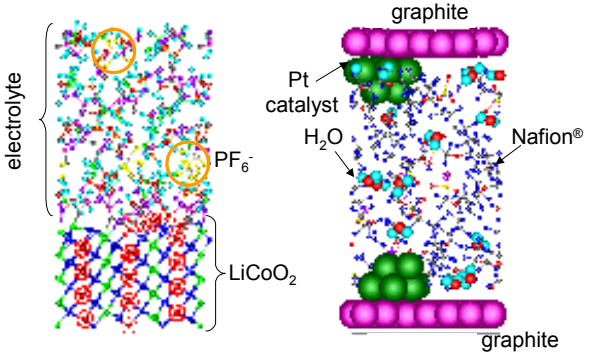




Good agreement with experimental band structure

Total System Simulator

Dynamics of Complicated System



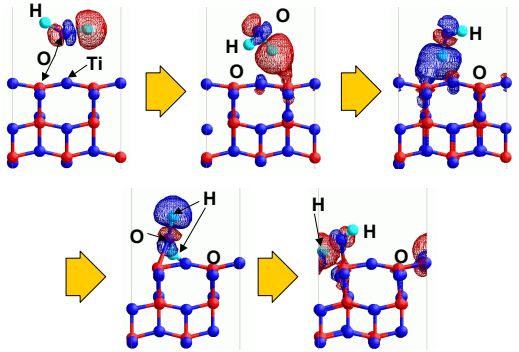
Li ion Secondary Battery Model

Polymer Electrolyte Fuel Cell Model

Successful Application: **Chemical reaction dynamics of multi-component and complicated large-scale system** e.g. batteries and fuel cells

Photo-Dynamics Simulator

Photolysis Dynamics of Water Over Anatase TiO_2 Catalyst

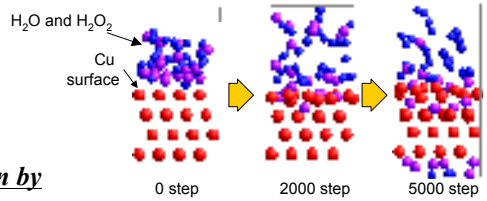


First Realization by Our New Simulator

Photoexcitation dynamics of complicated large system

CMP Process Simulator

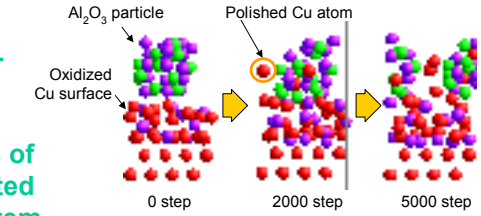
Chemical Mechanical Polishing (CMP) Process in Si Technology



Oxidation process of Cu surface

First Realization by Our New Simulator:

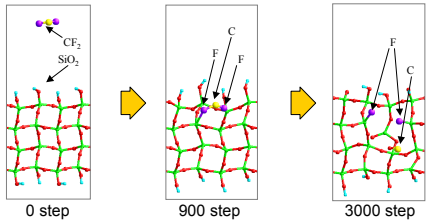
Mechano-chemical reaction dynamics of complicated large system



CMP process of oxidized Cu surface

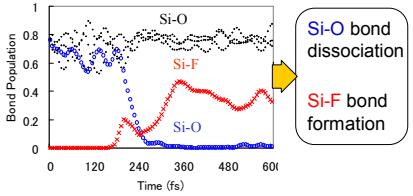
Plasma Process Simulator

Plasma Etching Process in Si Technology



First Realization by Our New Simulator:

Surface chemical reaction dynamics in plasma etching process



Plasma etching process of SiO_2 layer

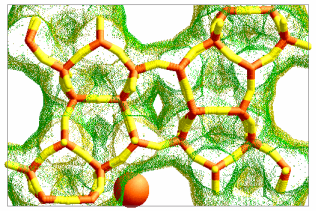
Electronic States Dynamics

First Realization by Our New Simulator:

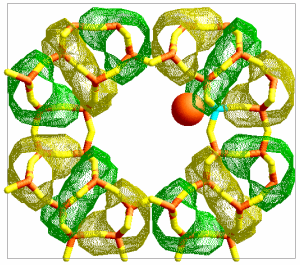
Electronic states dynamics and molecular orbital dynamics on complicated large system

Visualizer:

Our original three dimensional graphics user interface "NEW-RYUGA"



Molecular orbital of Cu-ZSM5



Molecular orbital of Cu-Mordenite

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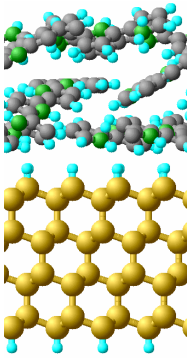
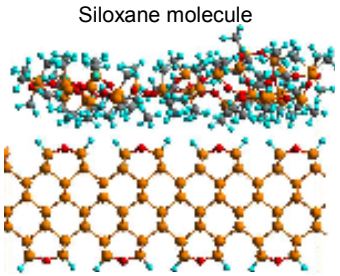
Multi-Level Combinatorial Computational Chemistry for Industrial Innovation: Leading of New Technology and Creation of New Industry

Monte Carlo Simulator MONTA

Conductive Polymer on Si Surface



Chemical Contamination on Si Surface

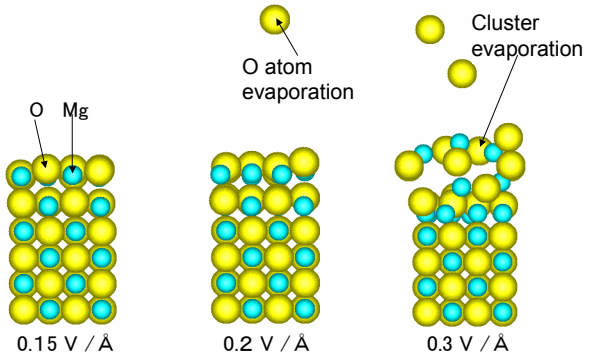


First Realization by Our New Simulator

Rapid and accurate Monte Carlo simulation of complicated large system

Electric Field Simulator

Destruction Process of MgO Protecting Layer of Plasma Display under Electric Field

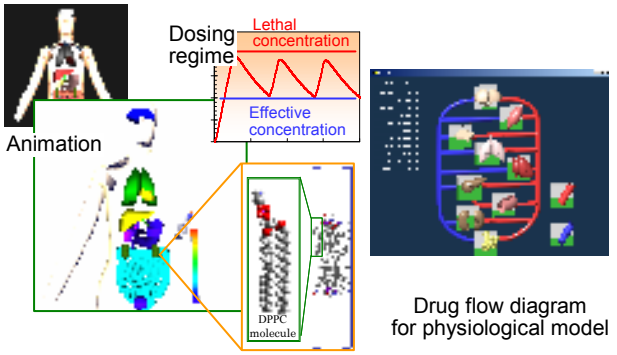


First Realization by Our New Simulator

Quantum chemical molecular dynamics under electric field

Pharmacokinetics Simulator

Simulation and Visualization of Drug Distribution in Human Body

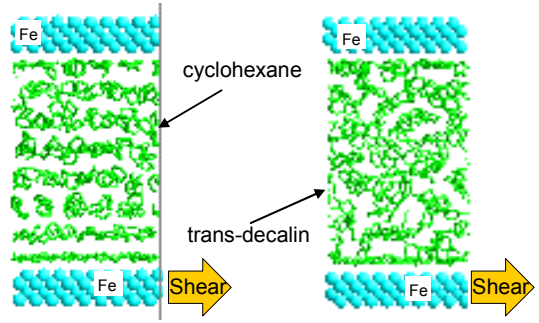


First Realization by Our New Simulator

Multi-scale graphical human interface for tailored medical services

Tribology Simulator TRIBOSIM

Friction Dynamics

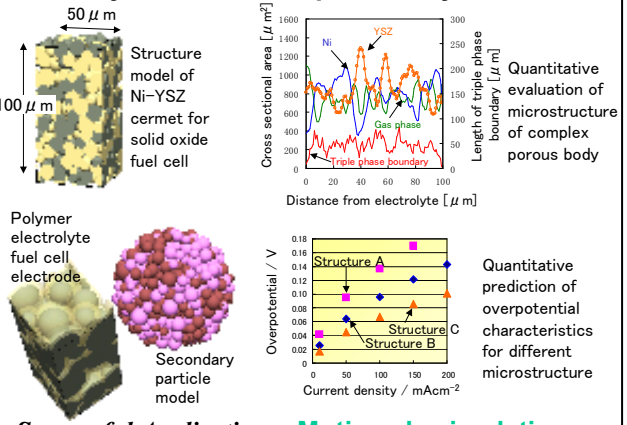


First Realization by Our New Simulator

Friction dynamics of complicated large system

Practical Multi-Scale Simulation

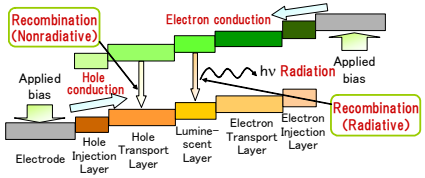
Dynamics of Complicated System



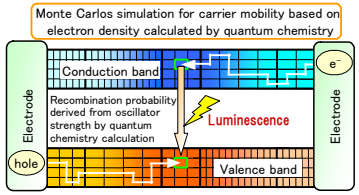
Successful Application: **Muti-scale simulation bridging microscopic properties and macroscopic characteristics**

Organic EL Device Simulator

Device Simulation based on Quantum Chemistry



Band structure of organic electroluminescent device



Schematic of organic electroluminescence device simulator

First Realization by Our New Simulator

Prediction of device characteristics based on quantum chemistry