Multiscale, Multiphysics Modeling/Simulation for Next Generation Automobiles: Catalysts, Tribology, and Batteries

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The Nobel Prize in Chemistry 2013 - Martin Karplus, Michael Levitt, Arieh Warshel

"for the development of multiscale models for complex chemical systems"

Multiscale, Multiphysics Computational Chemistry Methods for Industrial Innovations

1. Electronic Theory: Quantum Chemistry (QC), Quantum Mechanics (QM)

2. Atomistic Theory: Molecular Dynamics (MD), Molecular Mechanics (MM), and Monte Carlo (MC) Method

3. Quantum Molecular Dynamics Theory: *ab initio* MD, First-principles MD (Car-Parinello Method), UA-QCMD

4. Informatics: Artificial Intelligence (AI), Neural Networks (NN), and Database (DB)

5. Mesoscopic and Macroscopic Theory: Kinetic Monte Carlo(kMC), Computational Fluid Dynamics(CFD), Finite Element Method(FEM)

6. Human Interface: Computer Graphics (CG) ,Virtual Reality (VR)

7. Experiments(Measurents) Integrated Computational Chemistry

Industrial Innovation
by Combinatorial Computational Chemistry
Miyamoto Laboratory

Multiscale, Multiphysics Simulators for a Variety of Industrial Collaborations: 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 Pharmacokinetics 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...

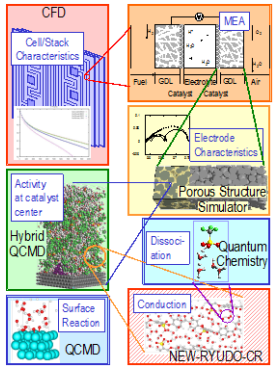
【Combinatorial Computational Chemistry Engines】

- 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

The Objective of our group in the Next Generation Automobiles/Miyagi Area Program

To contribute to Regional Innovation on the basis of successful collaborations with global companies through the following schemes:

1. **Direct collaborations with local companies**
2. **Collaborations with many partners(academic, governmental, financial, and industrial) including local companies,**

With multiscale, multiphysics modeling/ simulation methods developed in our group.

Present collaborators

Prof. A. Miyamoto
Assoc. Prof. N. Hatakeyama
Assist. Prof. A. Suzuki
Assist. Prof.. R. Miura
Sen. Res. Fellow T. Yotsuyanagi
Sen. Res. Fellow T. Inoue
Sen. Res. Fellow H. Koinuma
Visit. Prof. H. Fukui
Visit. Prof. K. Nishijima
Visit. Prof. O. Okada
Visit. Prof. M. Ippommatsu
Visit. Prof. M. C. Williams
Visit. Prof. J. Amano
Visit. Prof. M. Hisatake
Visit. Prof. M. Kohno
Visit. Prof.. P. Selvam
Adjunct Prof. A. Uehara
Res. Fellow. S. Kozawa
Visit. Assoc. Prof. N. Aoki
Visit. Assoc. Prof. M. Shibata
Visit. Assoc. Prof. H. Sato
Visit. Assoc. Prof. K. Itaka

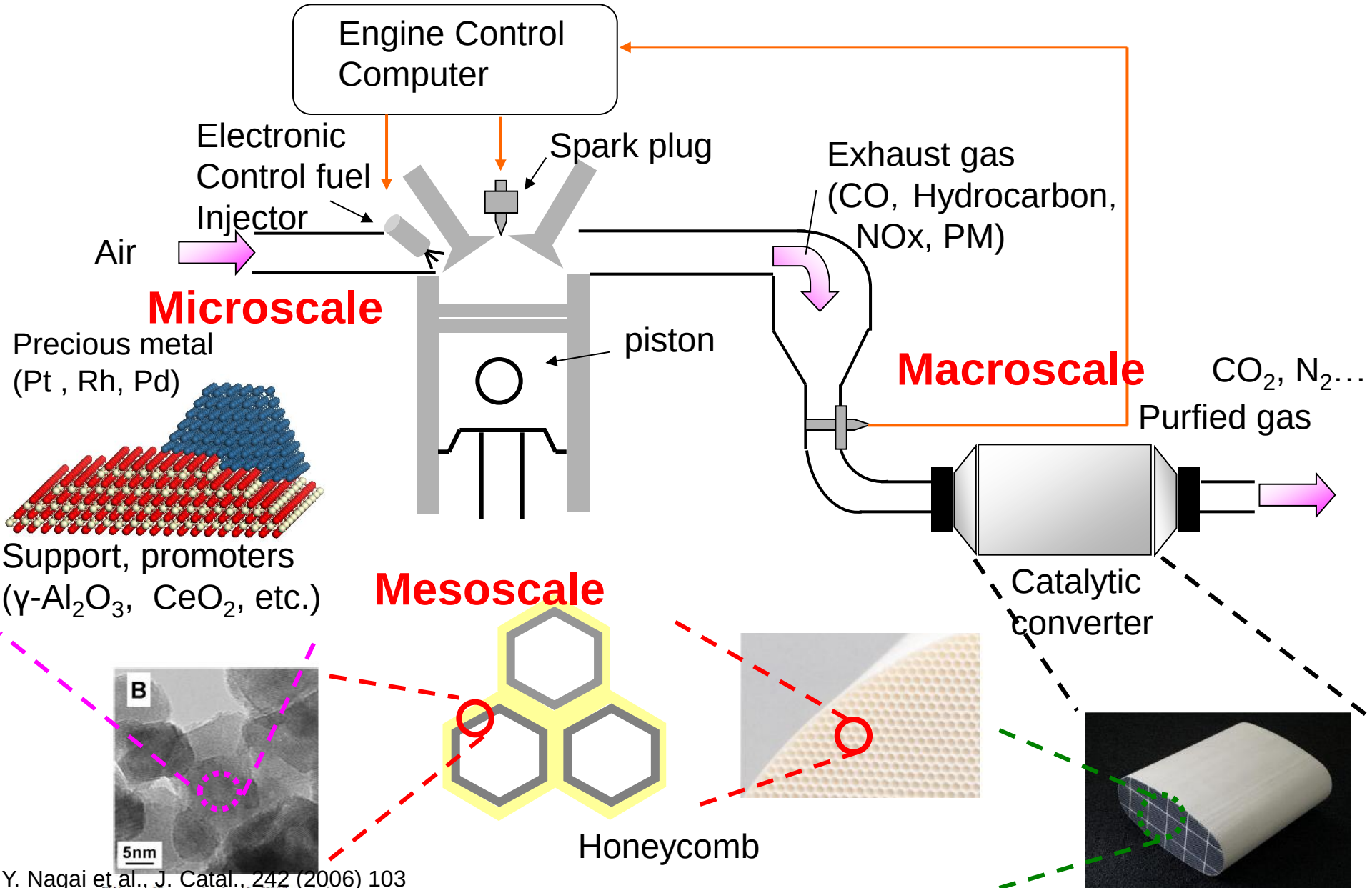
Collaborators
Prof. M. Kubo, Assoc. Prof. T. Tokumasu

Researcher	10
Techn. Staff	20
Secretaries	8
Part-time Programmer :	20

Total 82 members

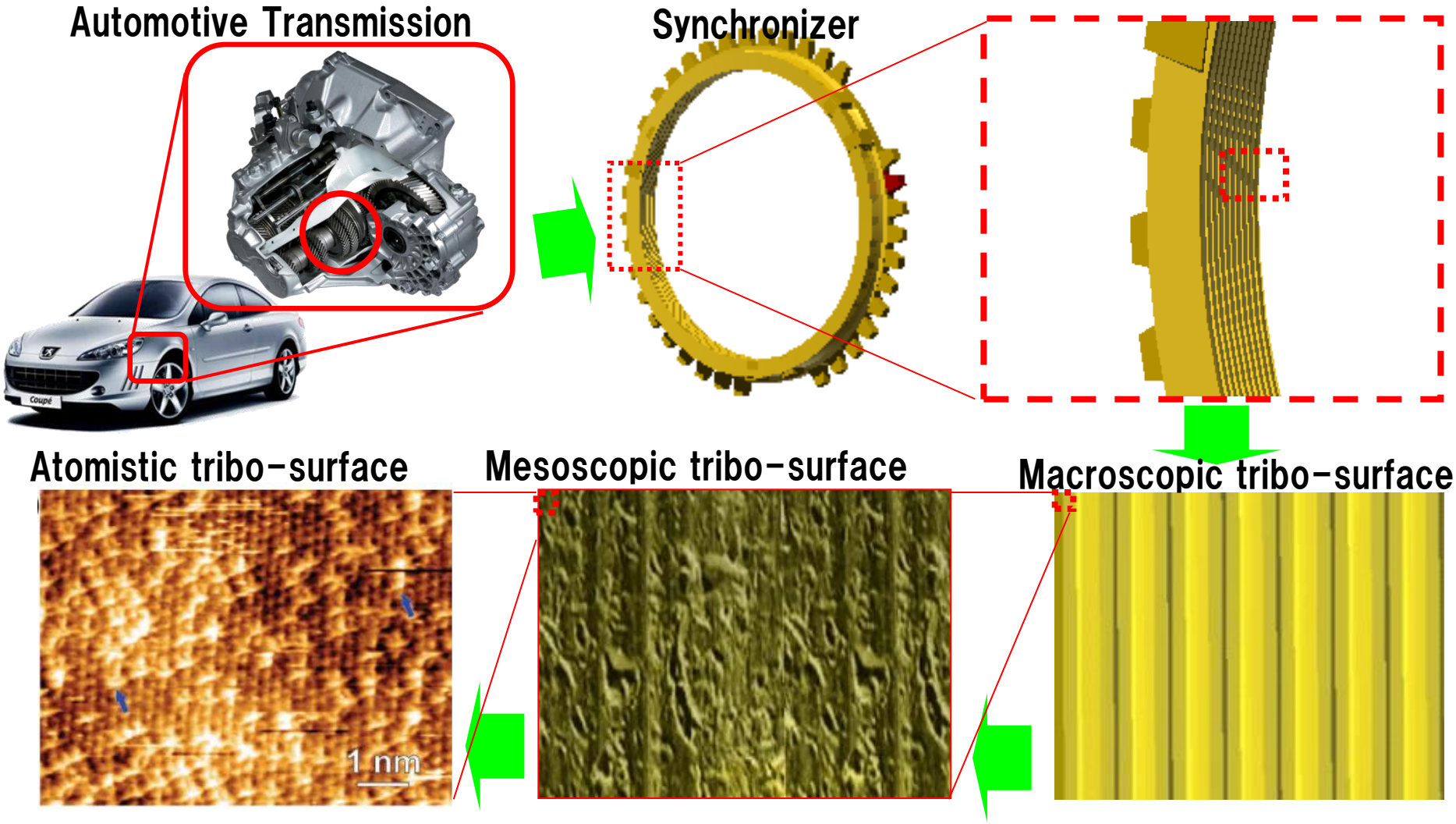
New Industry Creation Hatchery Center

Multiscale, Multiphysics Modeling/Simulation for Practical Automotive Catalysts



Y. Nagai et al., J. Catal., 242 (2006) 103

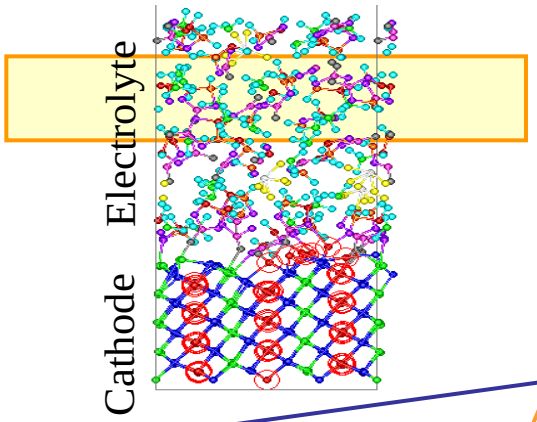
Multiscale/Multiphysics Simulators of Tribological Systems



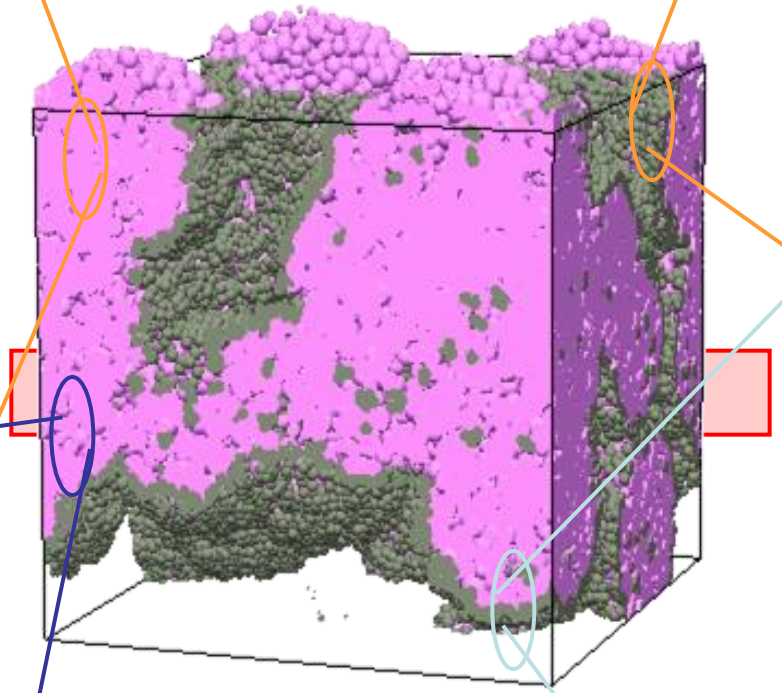
Seamless Modeling/Simulation of Practical Tribological System

Applications to Li Ion Batteries

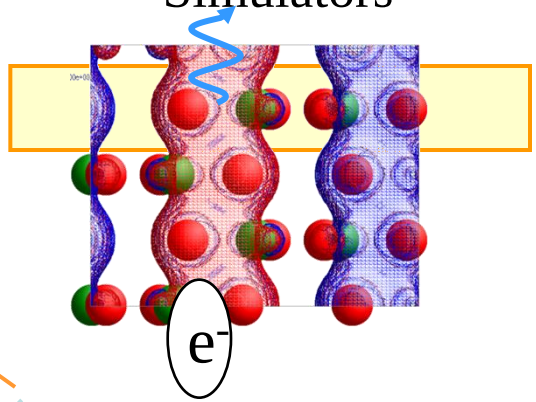
Large scale
Quantum Chemical
Molecular Dynamics



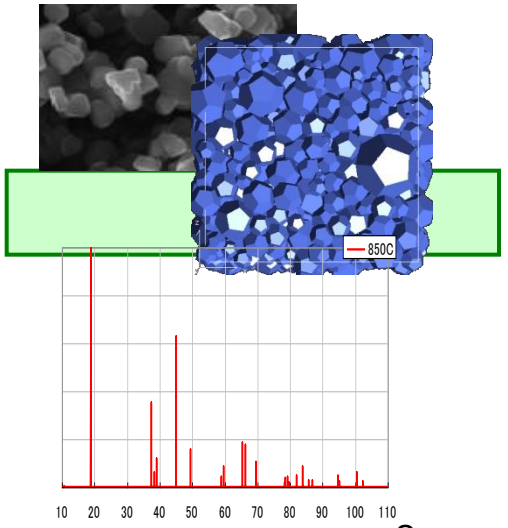
Modeling Tool of
Meso-scaled Structure



Electrical conductivity/
Thermal conductivity
Simulators

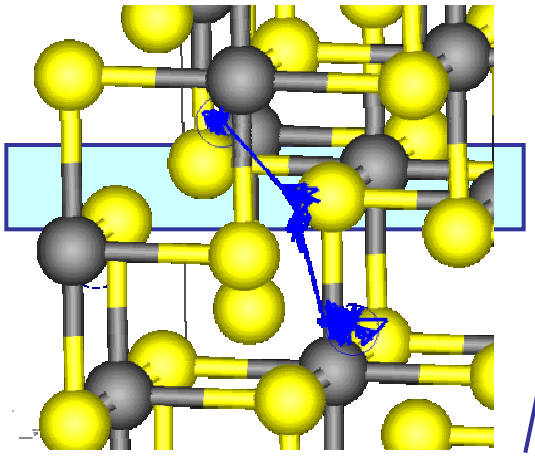


Measurement
Simulators

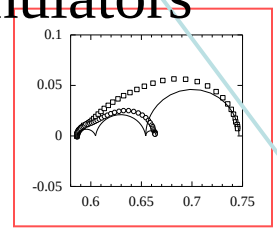


XRD ($LiCoO_2$)

Diffusion

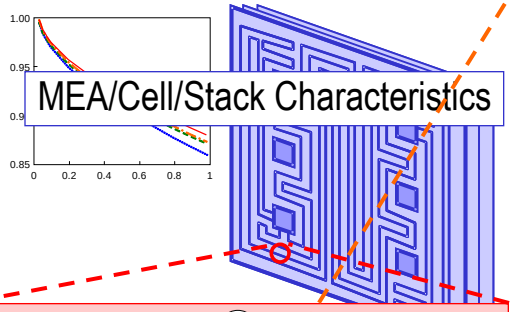


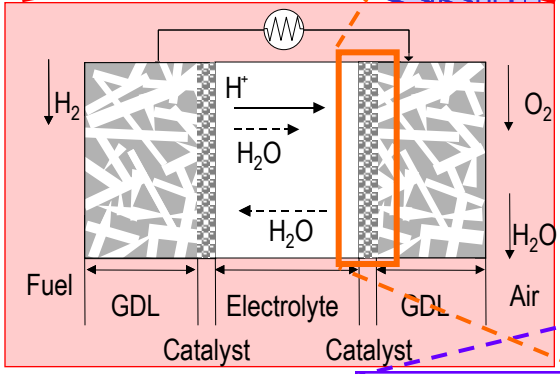
Combination with Macro
Numerical Simulators

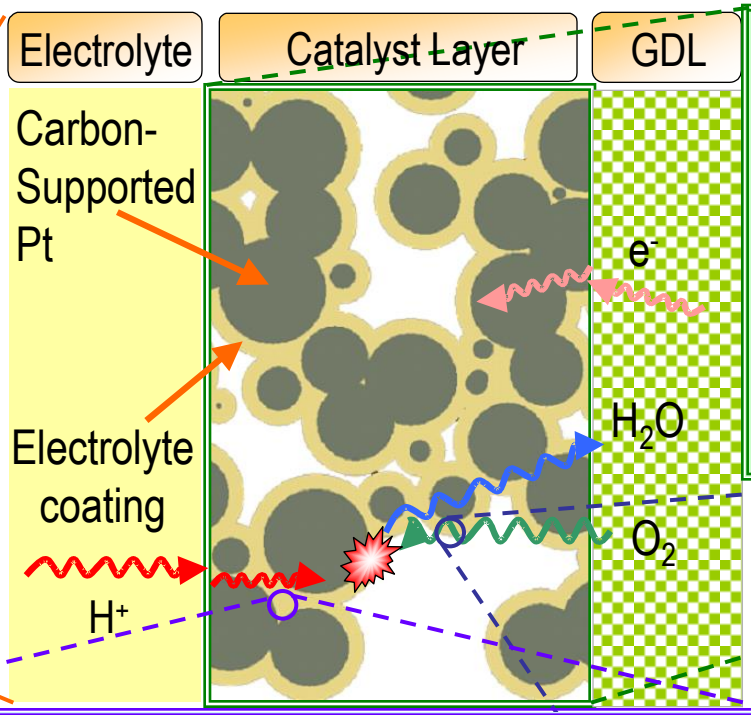


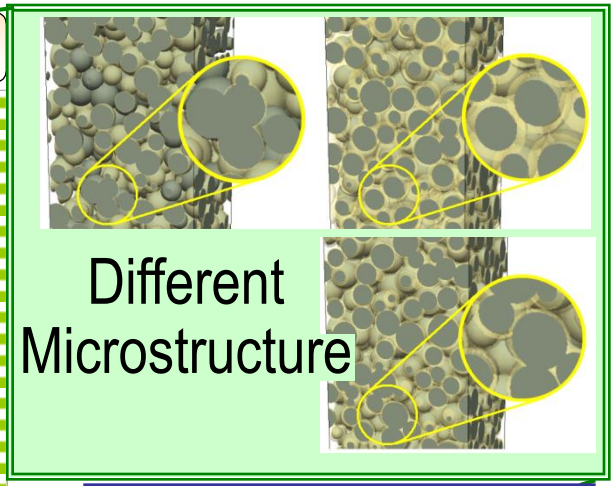
Polarization curve

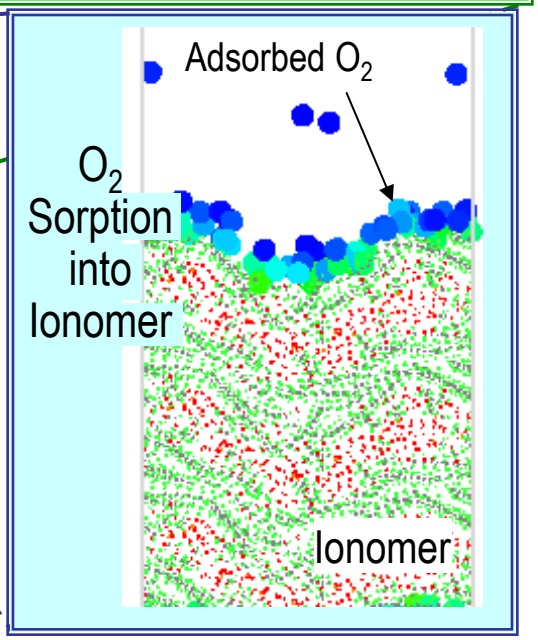
Applications to Fuel Cell Technologies

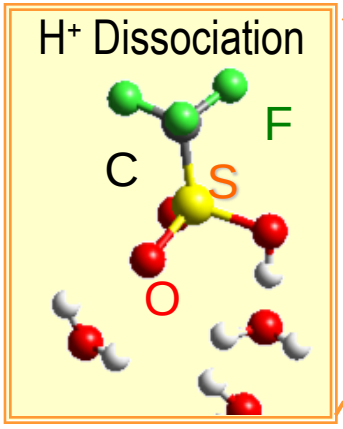


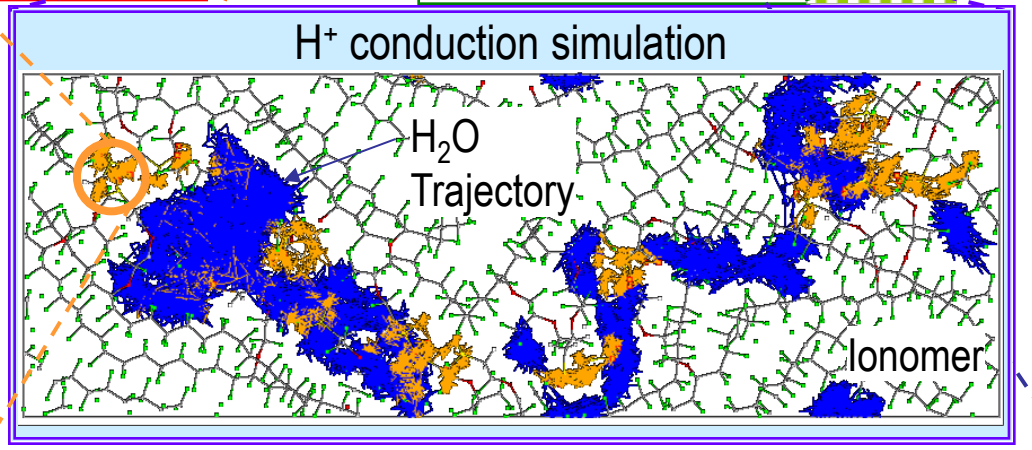












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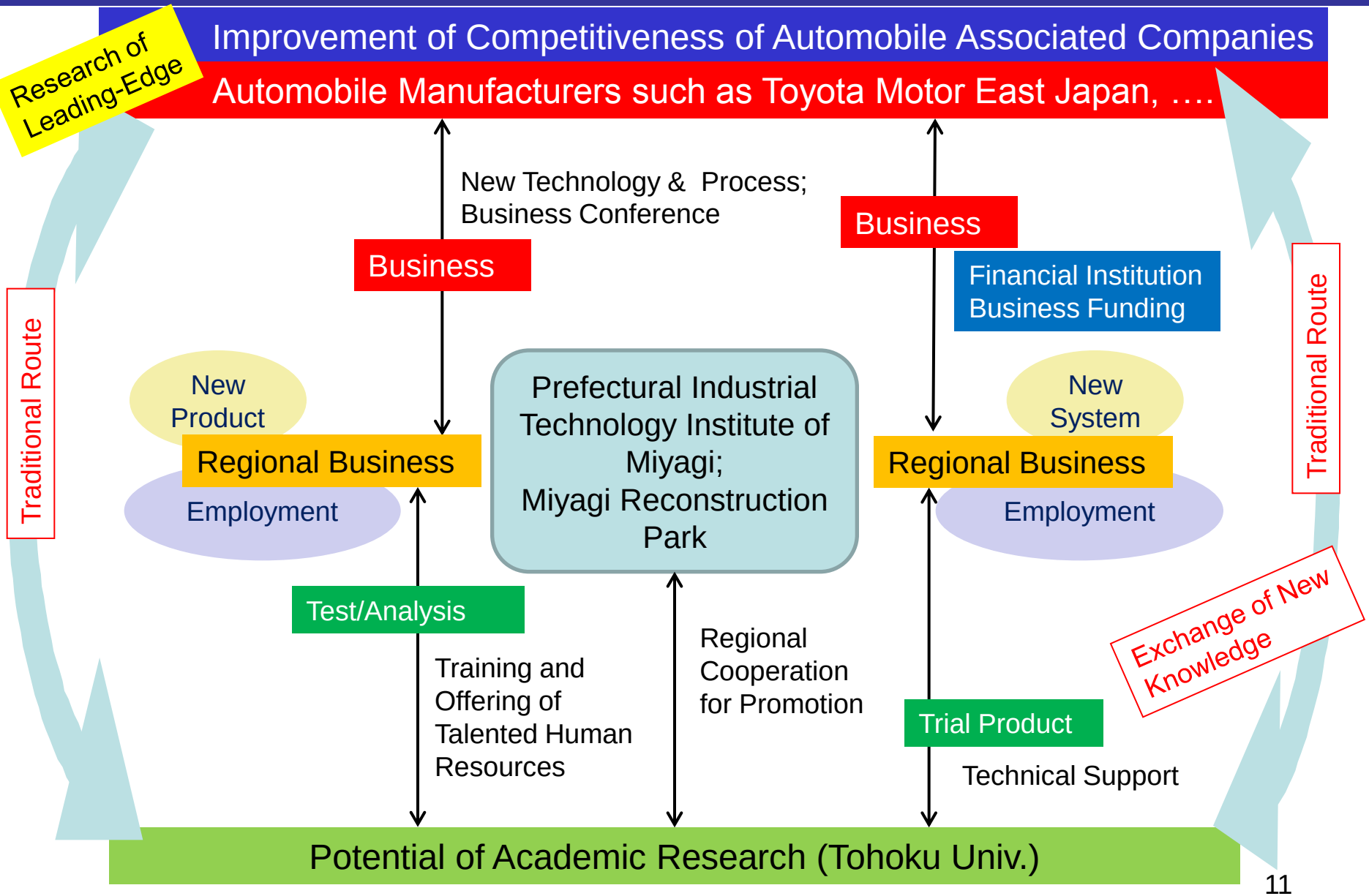
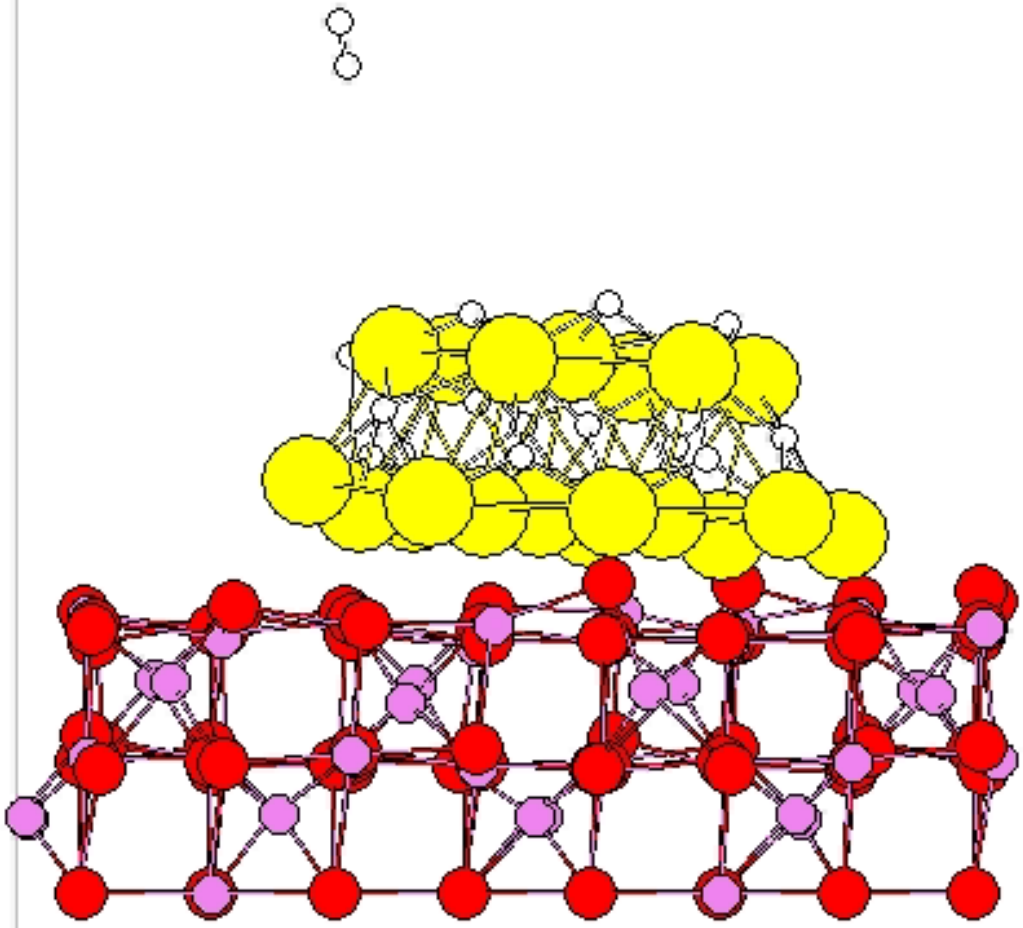
Industry-Academia-Government Innovation for Next Generation Automobile
– Overall Mechanism of Regional Innovation Strategy –



Role of Pt: Formation of Atomic H from H_2 demonstrated by UA-QCMD

Understanding roles of Pt, Pd, or Rh is highly important to decrease or replace the use of precious metals



H_2

Pt_{19} cluster

Al_2O_3

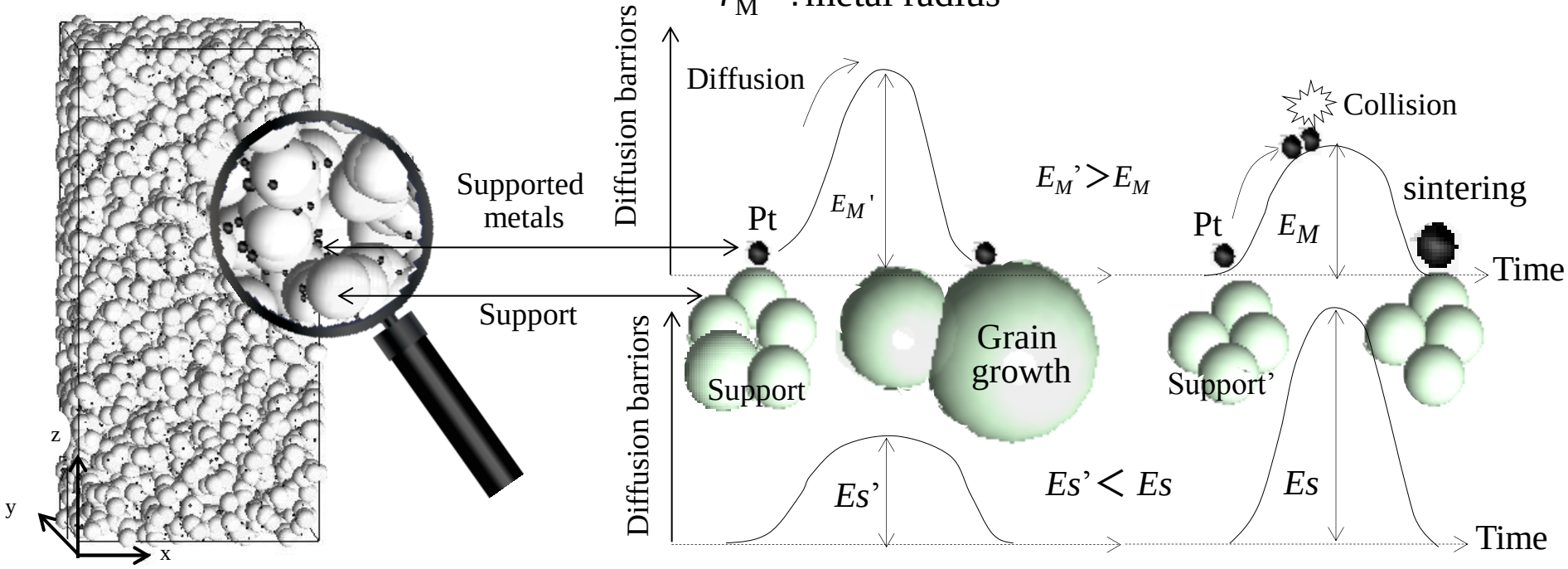
573K

Sintering Simulator of Supported Metals and Supports

Diffusion of Supported Metals: Pt, Pd, Rh

$$D_M(r) = D_{M0}(2r_M)^{-n}\exp(-\frac{E_M}{RT})$$

D_{M0} : Diffusion coefficient of supported metals
E_M : Activation energy for sintering of metals
r_M : metal radius



Diffusion of Supports: Al_2O_3, ZrO_2, CeO_2

$$D_S(r) = D_{S0}(2r_S)^{-n}\exp(-\frac{E_S}{RT})$$

D_{S0} : Diffusion coefficient of supports
Es : Activation energy for grain growth of supports
r_S : support radius

n : Grain-size exponent R : Universal gas constant T : Absolute temperature

Chassis Dynamometer Evaluation of Catalytic Performance under a Variety of Driving Conditions such as JC08 mode, by Dr. Furutani et al., AIST, Japan

JC08mode Chassis Dynamometer Emission Testing