Introduction of Ultra-High-Throughput Design and Prototyping Technology for Ultra-Advanced Materials Development Project (U2M)

Research Association of High-Throughput Design and Development for Advanced Functional Materials (ADMAT)

National Institute of Advanced Industrial Science and Technology (AIST)
Target and Output of U2M PJ

<Target>
In our National Project, we develop a data-based material design scheme for organic materials on the basis of advanced computational simulation, artificial intelligence (AI) and experiments such as innovative material processing and advanced characterization. It will replace the traditional material development protocol ever based on hunch and experience with an AI based one, which is expected to largely increase competitiveness of materials industries.

<Output Aim>
The main focus of this project is to enhance the quality of material data to increase prediction the reliability of AI, which is achieved by the cutting-edge methodology development for computational simulations, high-throughput processing and advanced characterization as well as the combination between theory and experiment. On the basis of these, the cycle number and tact time will be reduced to one-twentieth as compared with present numbers.
Features and Expected Effects of U2M

Features: Computational Science + AI for R&D of Functional Materials

<List of Items for Implementation>
✓ Computer Simulator Development for ‘in Silico’ Prediction of Structure-Property Relation in Organic/Polymer Materials
✓ Precise Simulation and Multiscale Simulation for the Prediction.
✓ AI based Design of Functional Organic Materials Using Materials Data
✓ Materials Data from High-Throughput Processing and Advanced Characterization as well as Computer Simulations

<Expected Effects>
✓ Game Changer in Functional Material Development: From Hunch and Experience to AI based Predictions
✓ Bringing Competitiveness to Materials Industries
Concept of U2M: Three-in-one efforts: CMD, Processing & Characterization

Multiscale Simulators

Computational Material Design (CMD)

Functional Materials Development

High-Speed/Innovative Processing

Advanced Nano-Characterization

Advanced Characterizations of the Relationship between Structure and Function

R&D by Orchestration/Collaboration of Simulation/AI, Processing and Characterization

High-Throughput Synthesis

Continuous Extruded Foaming

Super Computer

Electron Spectroscopic Imaging TEM

Positron Annihilation
R&D of Advanced Functional Materials by Fundamental Technologies

**Target Items**
- Nanocarbon Materials
- Semiconducting Materials
- Functional Dielectric Materials
- High-Performance Polymers
- Functional Chemicals (High-Performance Catalyst)

**Advanced Functional Materials**
- Conductivity
- Switching
- Sealing and Loss
- Mechanical Strength and Thermal Property
- Chemical Efficiency and Selectivity

**Functional Demand**
- Processing
- Comp. Sci.

**Adv. Charac.**
- Evaluation of Nanocarbon Materials
- Multiscale 3D Structure Analysis
- Flow-type XAFS and NMR

**Processing**
- CNT Spinning
- Graphene Synthesis Nanodispersion Process
- Heterojunction (Nanoparticle Synthesis)
- Blend and Foam Process
- Flow Process

**Comp. Sci.**
- Carrier Transport Calc.
- External Field Response Calc.
- Functional Polymer Calc.
- Reactive Fluid Calc.
- Deep Learning, Machine Learning (AI), and Discrete Geometric Analysis

**Multiscale Simulation**
- First-Principles/Molecular Dynamics Calculation

**Feedback**
Assumed Products from U2M Project

**Semiconductors**
- Transparent Thermochromic Film, Organic Semiconductor
  - In Summer: Functional Nanoparticles, Visible Transmittance > 70%
  - Near-Infrared: Functional Nanoparticles
  - In Winter: Functional Nanoparticles, Visible Light and near-IR Transmission

**Dielectric Materials**
- Organic/Inorganic Hybrid Condenser with High Voltage Endurance and High Dielectric Constant

**High-Performance Polymeric Materials**
- High-Performance Composite Materials, Electronic Materials, etc.
- Car Components, etc.

**Functional Chemicals (High-Performance Catalyst)**
- Functional Chemicals and Materials from Natural Products and CO₂, etc.
  - Variable Synthesis by Flow Reactor
  - Functional Monomer
  - Display Materials, Functional Rubber Materials, etc.

**Nanocarbon Materials (CNT, Graphene)**
- Light & High-Performance Wire Harness, Electric Cable, Heat Release Materials for Vehicles
  - Wire Harness, Wiring of Motor for Motorcar
  - Conductive Rubber, Thermostable Resin, Exothermic Materials, etc.
  - Flexible Display, Lighting Equipment, etc.
R&D Theme: Linkage for High Speed Development

Comp. Sci.

① Multiscale Simulator for Carrier Transport
② Large-scale Simulator for Complex Material and its External Field Response
③ Multiscale Simulator for Functional Nano-polymeric Material
④ Multiscale Simulator for Reactive Fluid
⑤ Deep Learning, Machine Learning and Discrete Geometric Analysis for Materials Data

Process

⑥ Variable Processes for Heterojunction Materials (Nanoparticle Synthesis)
⑦ Blend and Foam of Polymer Composites
⑧ Flow Reactor for Variable Synthesis (High Throughput)
⑨ Nanocarbon Processes

Adv. Charac.

⑩ Structural Characterization of Surface and Interface/Multi Properties
   Characterization in Nanoscale Area (Sum Frequency Generation Spectroscopy and Nano-Probe)
⑪ Three-dimensional Structure Analysis of Organic (Inorganic) Composite Materials (TEM, Positron Annihilation and X-Ray CT)
⑫ Highly Sensitive in-situ Measurement in Flow Process (XAFS and NMR)
⑬ Structure and Property Evaluation of Nanocarbon Materials

Inverse Problem

Feedback

Composition/Structure

Multiscale Simulator

Micro-Macro Linkage

Input Data

Output Data

Nanostructured Polymer Simulator

Carrier Transport/Reactive Fluid Simulator (Macrodevice, Fluid)

Nanostructured Polymer Simulator

Nanostructured Polymer Simulator

Macro

MESO

Input Data

Output Data

Micro

AI

AI Learning

Materials Function DB

External Field Response/Reaction Simulation (First-Principles, Atomic Level)
Materials Design by Multiscale Calculations

- **MICRO**
  - First-Principles Molecular Dynamics
  - Quantum Chemistry/First-Principles

- **MESO**
  - Molecular Dynamics
  - Coarse-grained Model

- **MACRO**
  - Fluid/Continuum Finite Element Method
  - Material Based Device Simulation

**Length**

- $10^{-9}$ m (1 nm)
- $10^{-6}$ m (1 μm)

**Time**

- $10^{-12}$ s
- $10^{-9}$ s
- $10^{-6}$ s
- $10^{-3}$ s
Two Examples of AI Application to Computer Simulation

AI for Forward Problem: AI to Bridge Multiscale Simulations

- Forward Problem Solver: MICRO Simulator (First-Principles, Atom)
- DATA: Coarse Graining
- Function Prediction for Module

- Forward Problem Solver: MICRO-MESO Simulator (Monomer-Polymer Process)
- DATA: Coarse Graining
- Visualizing, etc.

- Forward Problem Solver: MESO-MACRO Simulator (Hierarchical Structure Macro-device, Fluid)
- DATA: Coarse Graining
- Deep & Machine Learning

AI for Inverse Problem

Learning Data
(Structure-Property Relation by Computer Simulation and Experiment)

- Structure Space
- Composition Space
- Deep & Machine Learning

Edification
- Trained AI
- AI Inference
- Deep & Machine Learning

Target Functions
- Structure Space
- Composition Space
- Deep & Machine Learning
Developed Simulators

- Carrier Transport Simulator (Extended-CONQUEST)
- Interfacial Dynamics of Atoms and Reaction Simulator (I) (ESM-RISM)
- Interfacial Dynamics of Atoms and Reaction Simulator (II) (HybridQMCLT)
- Monte Carlo Full-Band Device Simulator
- External Field Response Simulator
- Voltage-Controlled Coarse Grained Molecular Dynamics Simulator (I, II) (Extended-COGNAC, LAMMPS)
- Multi-Task Interface (Extended-OCTA)
- Filler-Polymer Composite Simulator (Extended-KAPSEL)
- Nanocarbon Composite Simulator (SOBA)
- Reactive Fluid Simulator

Dielectric Materials
Organic/Inorganic Hybrid Condenser with High Voltage Endurance and High Dielectric Constant

Semiconductors
- Transparent Thermochromic Film, Organic Semiconductor
- Dielectric Materials
- Organic/Inorganic Hybrid Condenser with High Voltage Endurance and High Dielectric Constant

High-Performance Polymeric Materials
High-Performance Composite Materials, Electronic Materials, etc.
- Car Components, etc.

Nanocarbon Materials (CNT, Graphene)
- Light & High-Performance Wire Harness, Electric Cable, Heat Release Materials for Vehicles
- Conductive Rubber, Thermostable Resin, Exothermic Materials, etc.
- Flexible Display, Lighting Equipment, etc.

Variable Synthesis by Flow Reactor
- Functional Chemicals and Materials from Natural Products and CO\textsubscript{2}, etc.
- Functional Monomer
- Display Materials, Functional Rubber Materials, etc.
Process-1: Process Engineering and R&D for Functional Materials

- Heterojunction Materials
- Polymeric Composites
- Flow Reactor
- Nanocarbon Materials
  - Spinning, Large Area, Over-Layer
- Variable Synthesis
- Nano-Particle
- Blend and Foam

Processing

Feedback

Computational Science and AI Learning

Trial of Model Materials

Advanced Characterization

Structure and Function/Observation Data

AIST
Process-2: High-Throughput and Innovative Processing

- Chemical Reaction Control
- Crystal Growth Control
- Dispersion Control
- Composite
- Phase Equilibrium
- Mechanical Operation
- Morphology and Shape Control

Time

Chemical Operation
Flow Reaction

Atom/Molecule → Nanoparticle/Nanocarbon

10^{-9} m (1 nm) → 10^{-6} m (1 μm)

Kneading
Spinning, Over-Layer, Foaming, Large-area

Composite

Advanced Characterization

In-situ Measurement

Nano-Probe Spectroscopy

SFG and Various Spectrosc.

X-Ray CT

Electron Microscopy

Functional Charact.

XAFS NMR

Positron

Multiscale Structure and Composition Analysis

Micro-Macro Processing

Str. & Function, Obs. Data

Computational Science & AI

Feedback

AIST

Nano-Probe Spectroscopy

Flow-Type XAFS

Chemical Reaction
In-situ Measurement

DNP-NMR

Characterization of Structure-Function Correlation

Multiscale Structure-Composition Analysis

Positron Annihilation

ESI-TEM

Nanostructure, Nanoparticle and Nanocarbon

X-Ray CT

Composite

10^-9 m (1 nm)

10^-6 m (1 μm)

**Time**

**Energy**

**In-situ** Measurement

Chemical Reaction Control

Chemical Operation/Flow Reaction

Quantum Chemistry/First-Principles/MD

**DISP**

Dispersion/Orientation/Interface Structure Control

Nanoparticle

Surface Modification

Monomer/Polymer Nano Particle, Nano Carbon

Coarse-grained Model

**Meso**

Micro Properties Observation of Nanoscale Area (Function Evaluation)

**Micro**

Heat Transfer/Conductivity, Thermal Response, Elastic Modulus, Dielectric Constant

**Function Control**

Thermal Insulation, Shading, High Strength, Thermostable, High Voltage Endurance, etc.

**MACRO**

Fluid/Continuum Finite Element Method

**Macro**

Dispersion Control

Phase Equilibrium, Mechanical Operation

Cracking & Kneading

**Morphology and Shape Control**

Spinning, Over-Layer, Foaming, Large-Area

**Multiscale 3D Structure Analysis**

**Length**

<table>
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<th>10^{-3} m (1 mm)</th>
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Hierarchical and Hybrid Structures and Properties

- Monomer/Polymer
  - Molecular Dynamics
    - \(\chi\)-Parameter
    - Solubility
    - P-V-T
  - Quantum Chemistry
    - Catalytic Reaction Path
- Coarse-Grained Model
  - Phase Separation Structure
  - Dispersion State
- Extension of First Principles
  - Interface Reaction
  - Optical Properties

Foaming Process
- Process Calc./Finite Element Method
  - Hierarchical and Interface Structure Control
  - Dispersion Control
  - Shape Control

Circulative Collaboration: Process/Simulation/Characterization

- First-Principles
  - Electron Conductivity
  - Dielectric Function

Length

- 10^{-9} m
- 10^{-6} m
- 10^{-3} m
- 10^{0} m

Energy

- Time
Research Association of High-Throughput design and Development for Advanced Functional Materials (ADMAT)

- **Establish**: July 12, 2016
- **President**: Kunihiro Koshizuka (KONICA MINOLTA, INC., Director)
Establishing the Orchestration Scheme for the Elements to Model Materials

<Contracted Research and Development>

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<tr>
<th>R&amp;D Theme (1)</th>
<th>Computational Material Design</th>
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| R&D Theme (2) | High-Throughput and High-Precision Manufacturing Process |

| R&D Theme (3) | High-Throughput and High-Resolution Characterization |

Establishing the Elements of MD
Orchestration / Collaboration among (1), (2) and (3)

Mid-Term Evaluation

Validation and Application of the MD Protocol to Accelerate Model Materials Development
- Augmenting Material Function Prediction Software Module (Optimum Search, etc.)
- High-Throughput Experiments based on Automated Material Process and Characterization
- Validation of the AI based Material Design

Ex-Post Evaluation

<Grant Development>

| Grant Theme (4) | Functional Materials Development using the Computational Material Design |

Grant Development
Future Efforts and Perspective for Application of Results

**Materials Design Platform**

- **Computational Material Design (CMD)**
- **High Speed/Innovative Process**
- **Advanced Nano-Characterization**

**Orchestration of the Three Material Design Elements**

**Data Platform**
(Data Manipulation, Analysis and Management, etc.)

**AI Technology**

**Recipes for New Functional Materials**

**DESIGN TECHNOLOGY**
Computational Material Design Protocol
- Innovative Process
- Advanced Characterization

**SIMULATORS**
- Computational Simulation

**EXPERIMENTAL EQUIPMENTS**
- Innovative Process
- Advanced Characterization

Closed: Priority Use by ADMAT Partners

Softwares to be Opened

**AIST to be Material Design Center**
Offering Design Protocols and Rules to Industries in Some Ways as Follows:
- Consortium
- Cooperative Research
- Consulting
- Joint Facilities, etc.