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.

Basic Plan by NEDO

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

Atom → Reaction/ Polymerization → Monomer/ Polymer → Higher Order Structure → Polymer Reaction/ Surface Modification → Hybrid Materials (Org/Org., Org./Inorg.) → Molding and Foaming Processing

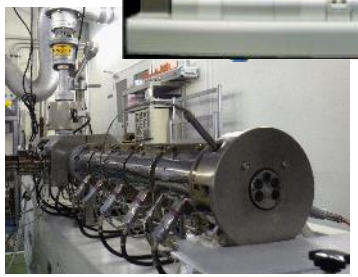
High-Throughput Synthesis

Multiscale Simulators

Super Computer

Computational Material Design (CMD)

Functional Materials Development



Continuous Extruded Foaming

High-Speed/ Innovative Processing

Advanced Nano-Characterization

Electron Spectroscopic Imaging TEM

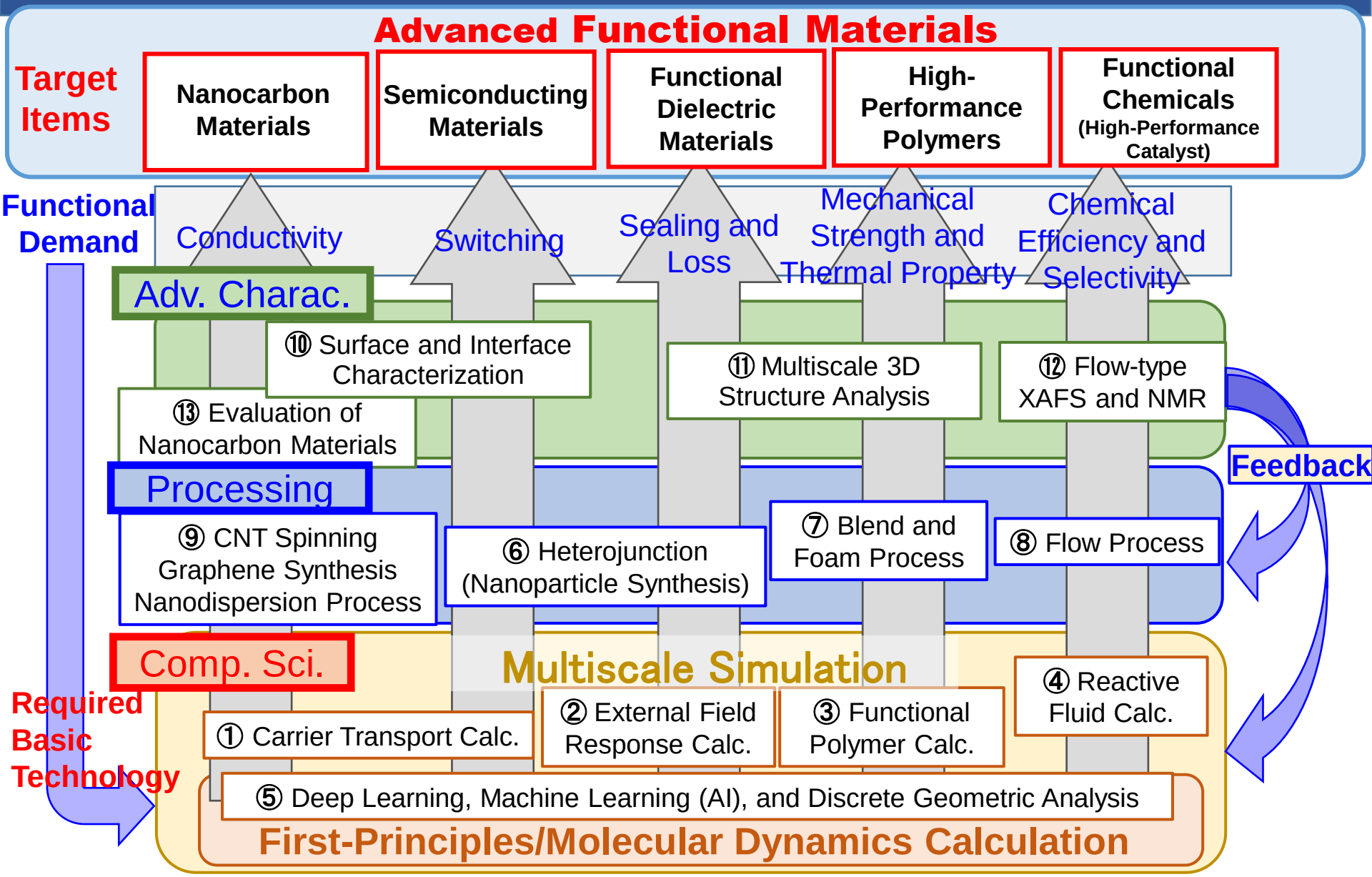
Positron Annihilation

High Speed and Variable Processes

Advanced Characterizations of the Relationship between Structure and Function

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

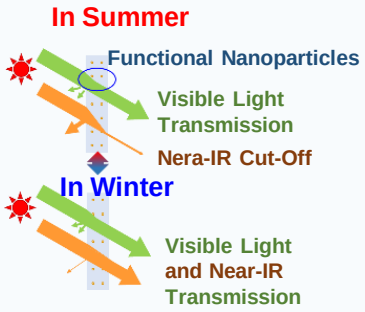
R&D of Advanced Functional Materials by Fundamental Technologies



Assumed Products from U2M Project

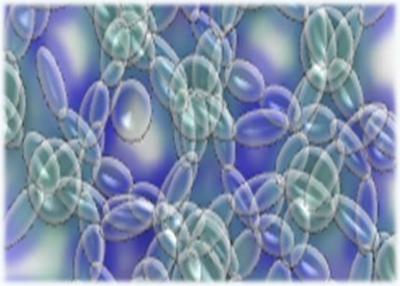
Semiconductors

Transparent Thermochromic Film, Organic Semiconductor



Dielectric Materials

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



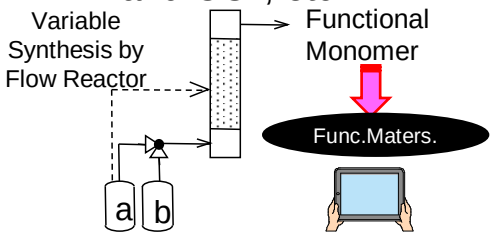
High-Performance Polymeric Materials

High-Performance Composite Materials, Electronic Materials, etc.

Car Components, etc.

Functional Chemicals (High-Performance Catalyst)

Functional Chemicals and Materials from Natural Products and CO_2, etc.



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

Atom → Reaction/ Polymerization → Monomer/ Polymer → Higher Order Structure → Polymer Reaction/ Surface Modification → Hybrid Materials (Org/Org., Org./Inorg.) → Molding and Forming Processing

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

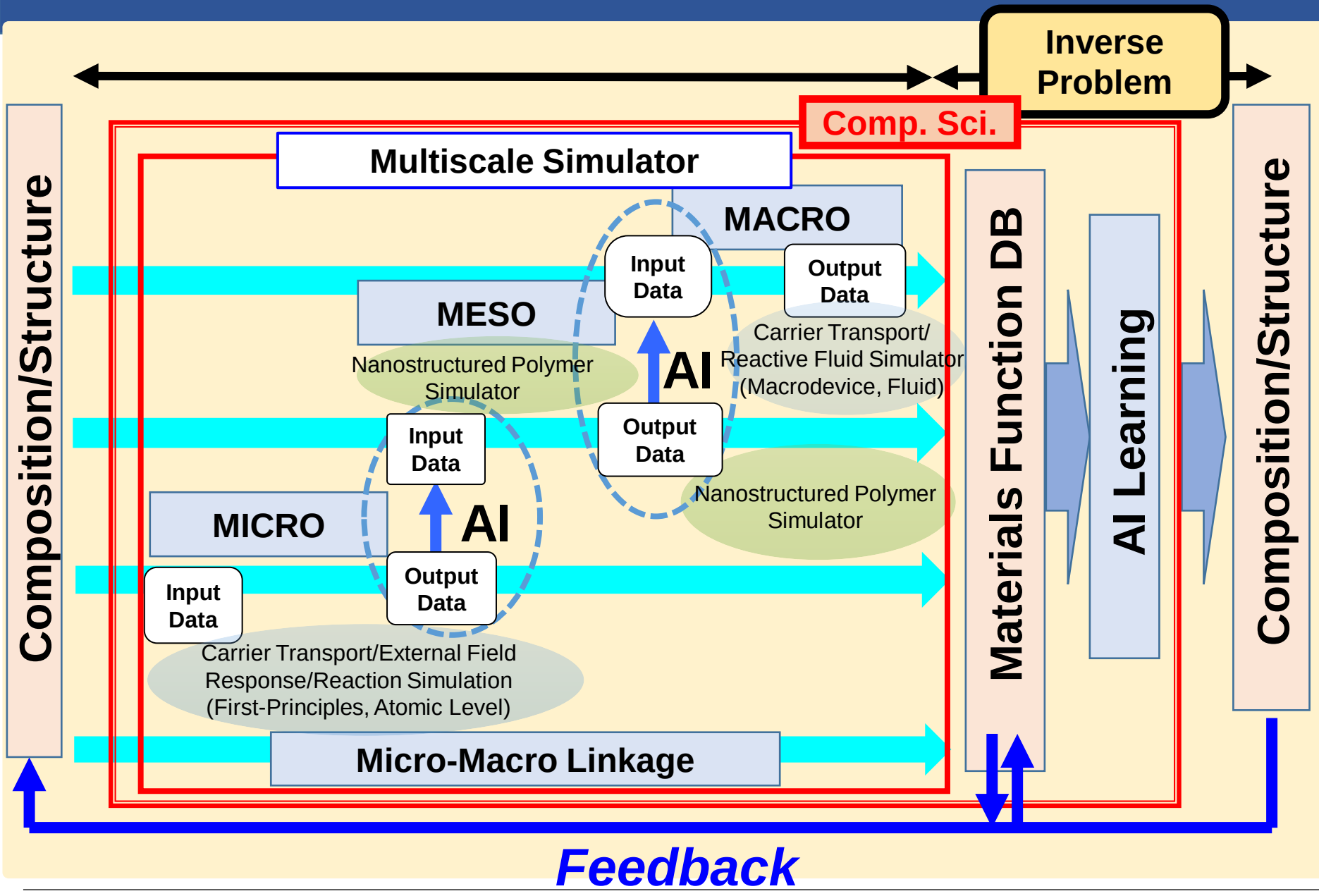
Process

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

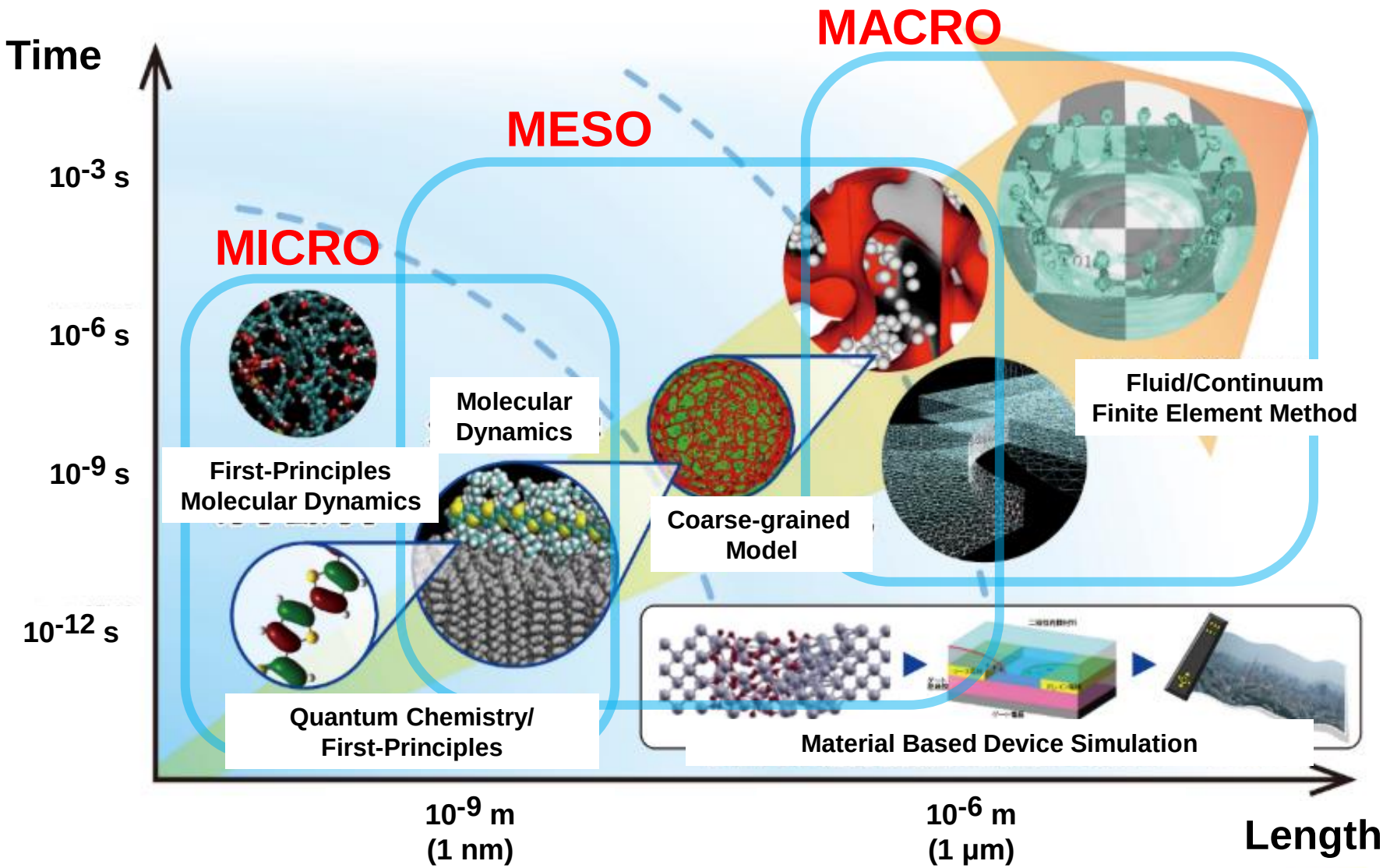
Adv. Charac.

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

Comp. Sci.-1: R&D of Functional Maters. with Comp. Sci.

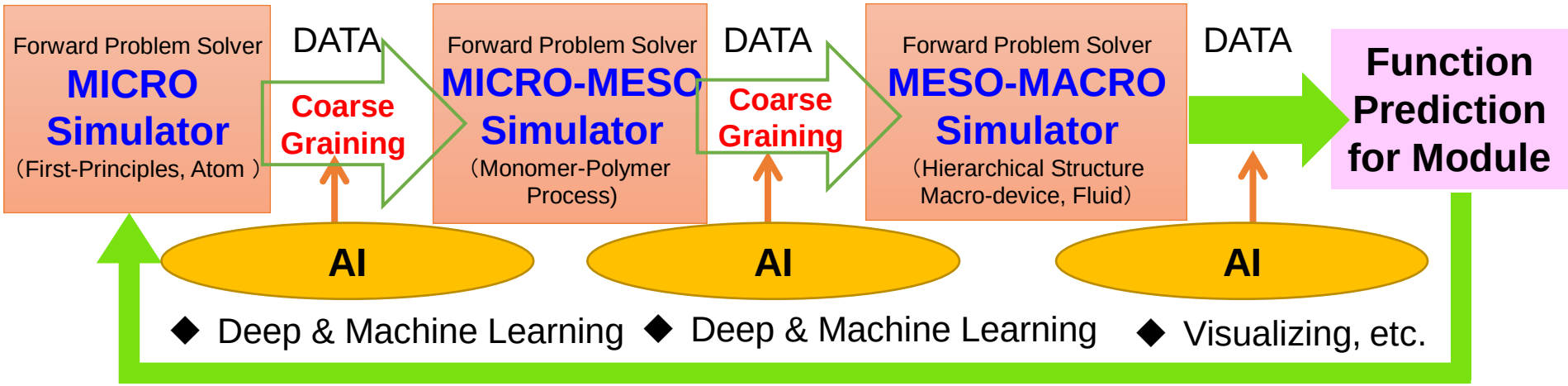


Materials Design by Multiscale Calculations

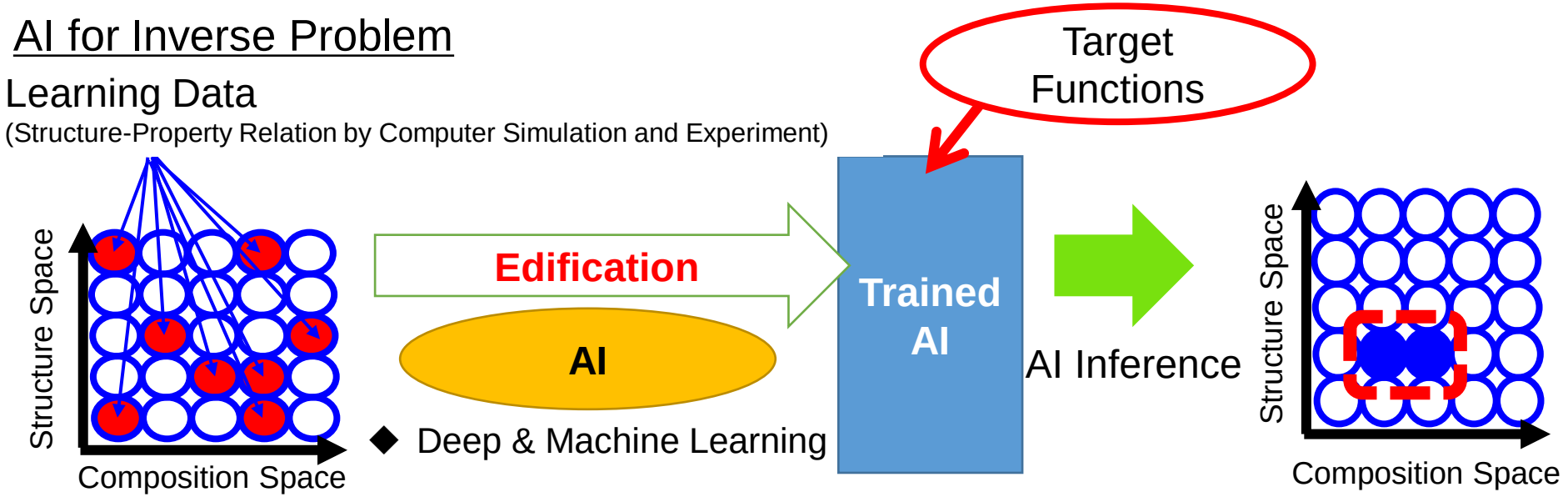


Two Examples of AI Application to Computer Simulation

AI for Forward Problem: AI to Bridge Multiscale Simulations



AI for Inverse Problem

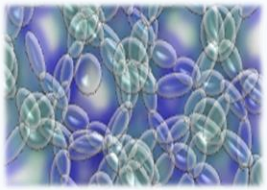


Developed Simulators

- 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



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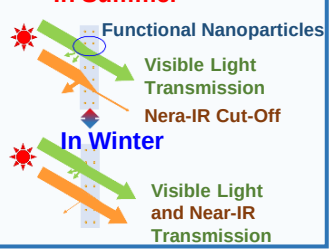

High-Performance Polymeric Materials

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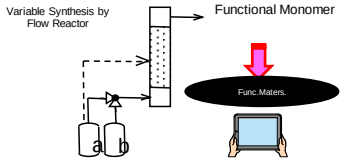

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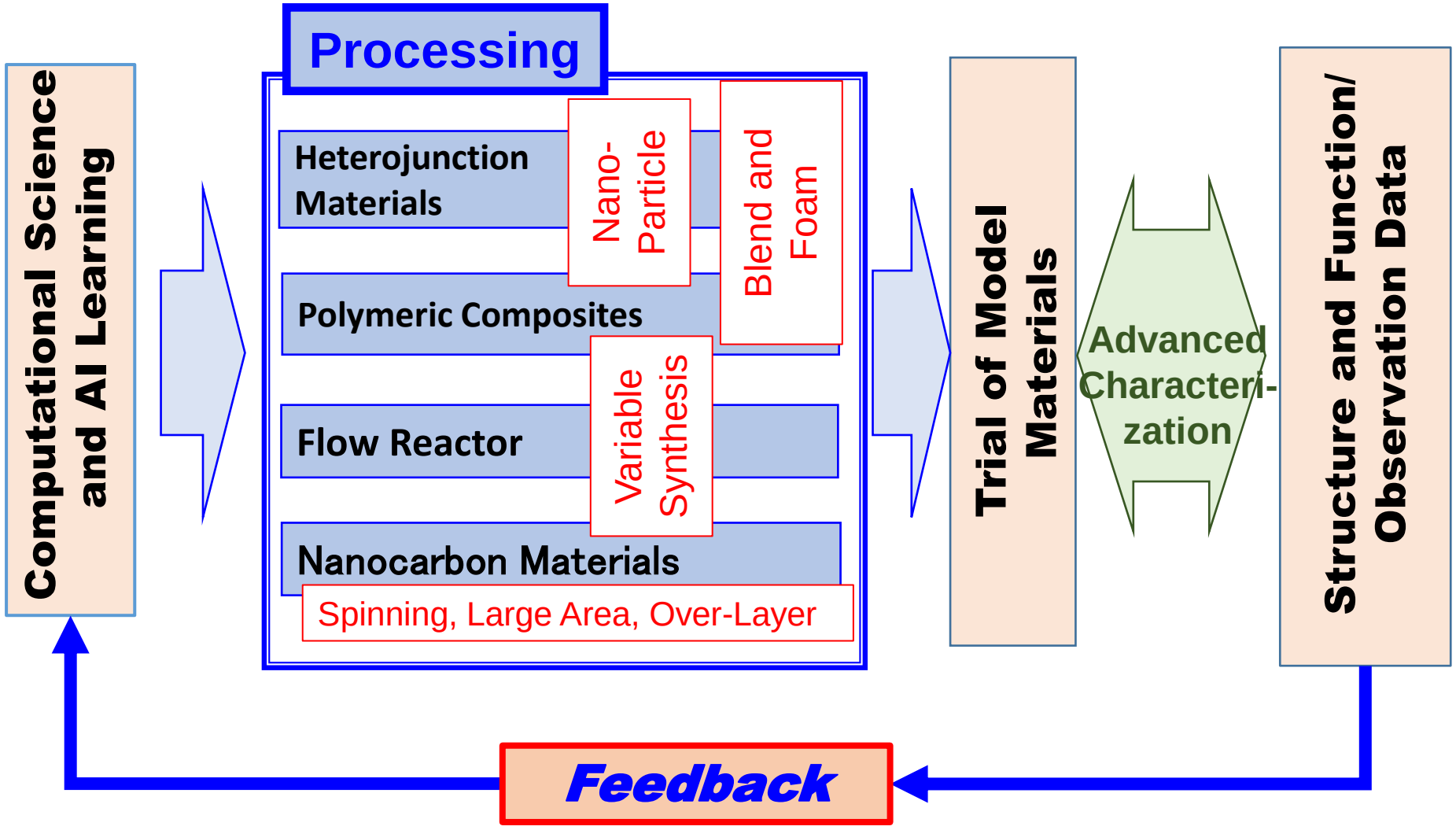
Flexible Display, Lighting Equipment, etc.

Process-1: Process Engineering and R&D for Functional Materials



Process-2: High-Throughput and Innovative Processing

Time

Morphology and Shape Control

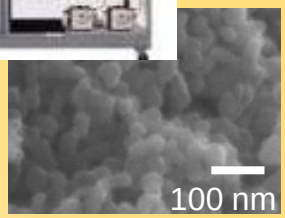
Spinning,
Over-Layer,
Foaming,
Large-area

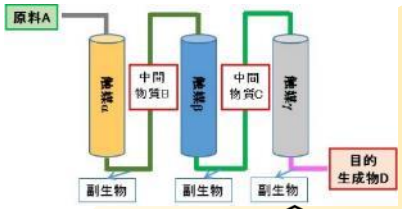
Crystal Growth Control

Chemical Reaction Control

Cracking

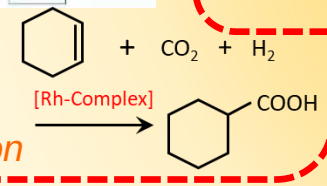
Composite



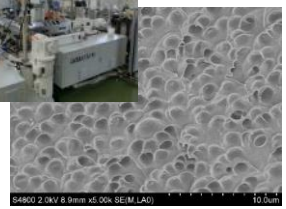


Phase Equilibrium
Mechanical
Operation

Chemical
Operation



Flow Reaction



Kneading

Atom/Molecule

Nanoparticle/Nanocarbon

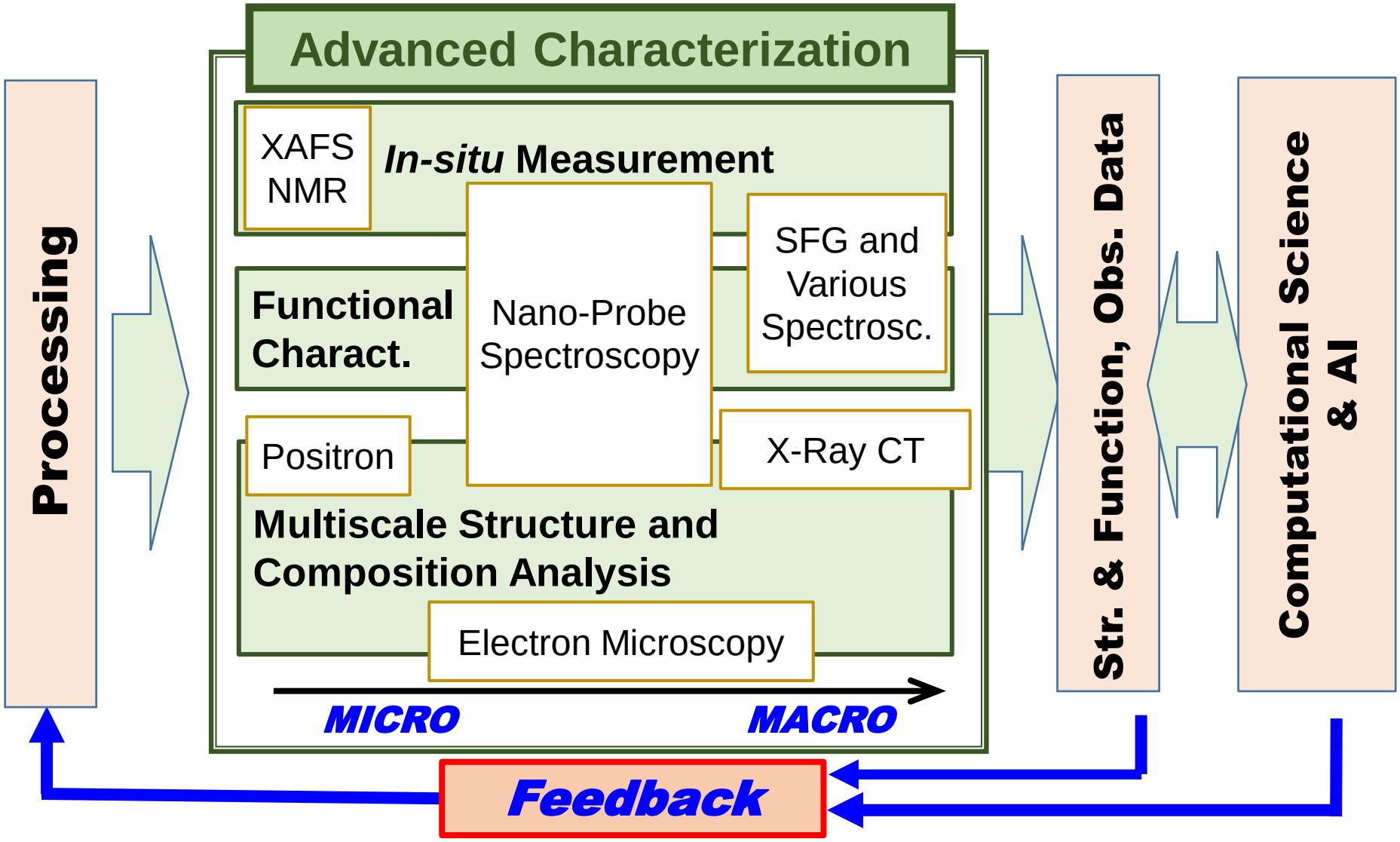
Dispersion Control

10^{-9} m
(1 nm)

10^{-6} m
(1 μm)

Length

Adv. Charact.-1: Adv. Charact. and R&D for Functional Maters.

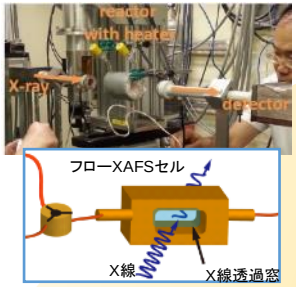


Adv. Charact.-2: Nano Characterization and Evaluation

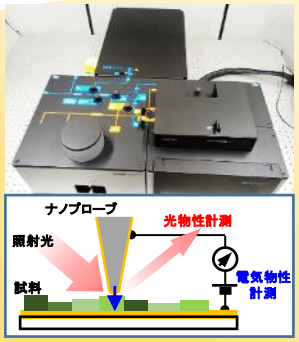
Functional Measurement

Structural Measurement

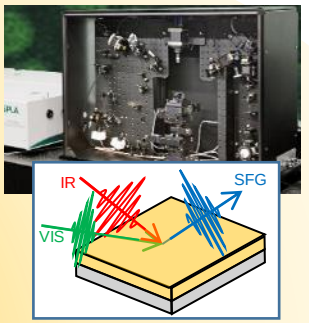
Flow-Type XAFS



Nano-Probe Spectroscopy



SFG Spectroscopy



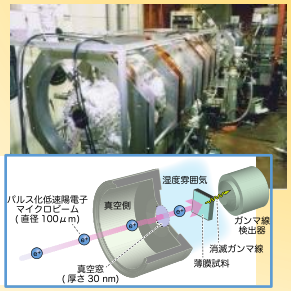
Chemical Reaction *In-situ* Measurement

Characterization of Structure-Function Correlation

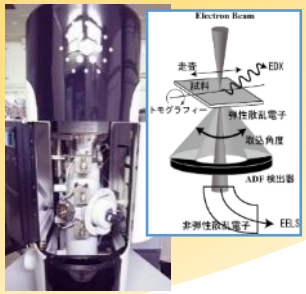
Multiscale Structure-Composition Analysis

DNP-NMR

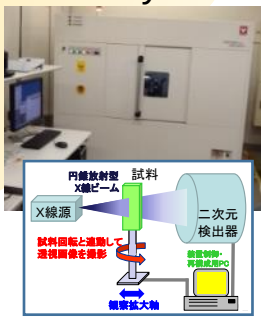
Positron Annihilation



ESI-TEM



X-Ray CT



Atom/Molecule

Composite

Nanostructure, Nanoparticle and Nanocarbon

10^{-9} m (1 nm)

10^{-6} m (1 μm)

Length

Materials Structure Design and Cooperation of Comp. Sci., Process and Charact.

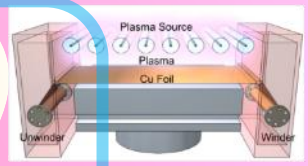
Time
Energy

Multiscale 3D Structure Analysis

In-situ **Measurement**

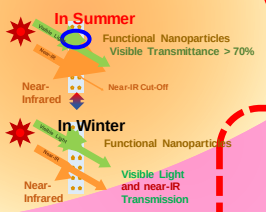
Morphology and Shape Control

Spinning, Over-Layer, Foaming、Large-Area



Dispersion/Orientation/ Interface Structure Control

Nanoparticle



Surface Modification

Chemical Reaction Control

Chemical Operation/Flow Reaction

Hybrid Materials Composite

Dispersion Control

Phase Equilibrium, Mechanical Operation

Cracking & Kneading

Monomer/Polymer

Nano Particle, Nano Carbon

Coarse-grained Model

Atom/Reaction

Quantum Chemistry/

First-Principles/MD

Fluid/Continuum Finite Element Method

MICRO

MESO

MACRO

＜Physical Property Control＞

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

＜Function Control＞

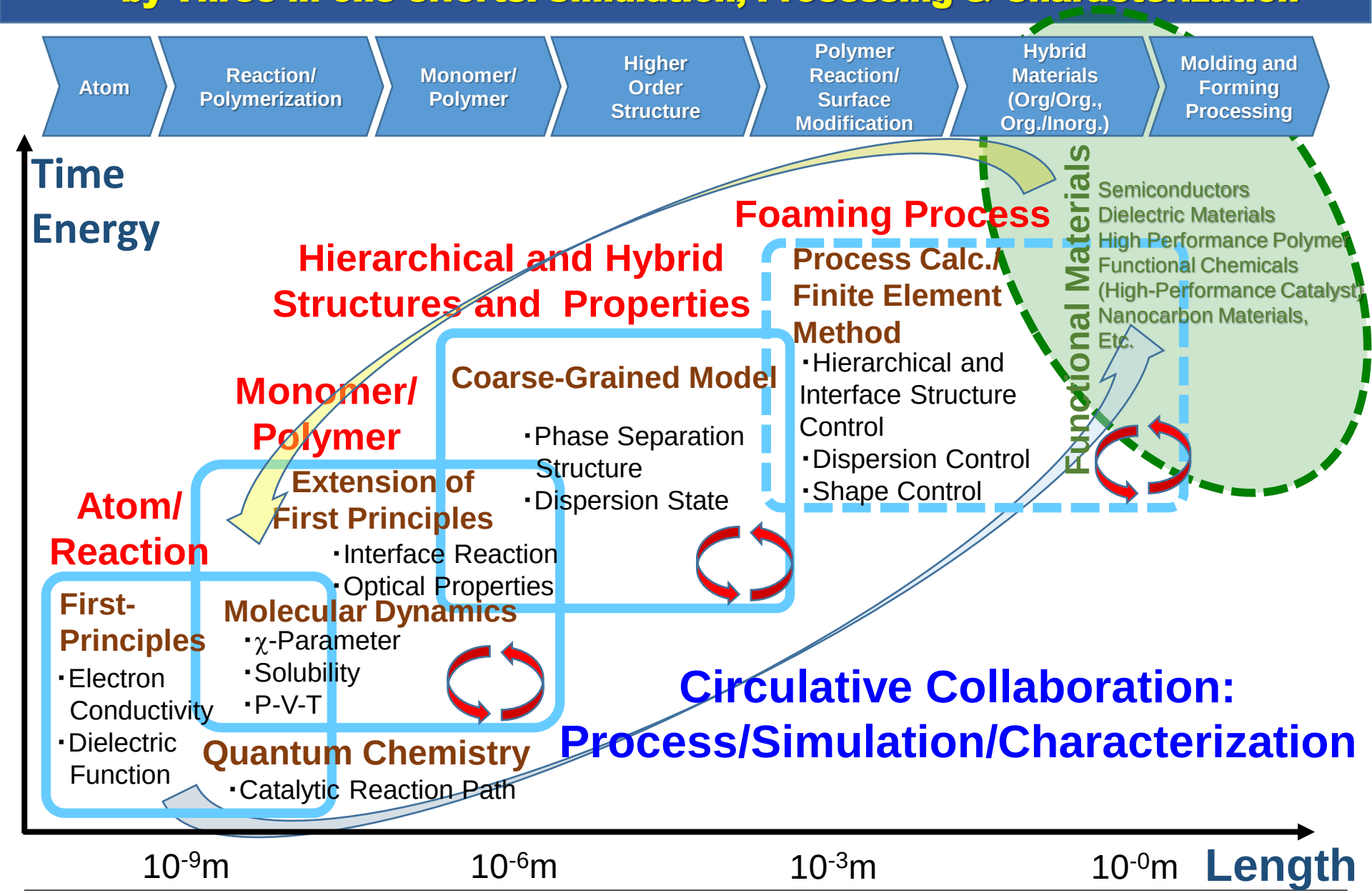
Thermal Insulation, Shading, High Strength, Thermostable, High Voltage Endurance, etc.

Multi Properties Observation of Nanoscale Area (Function Evaluation)

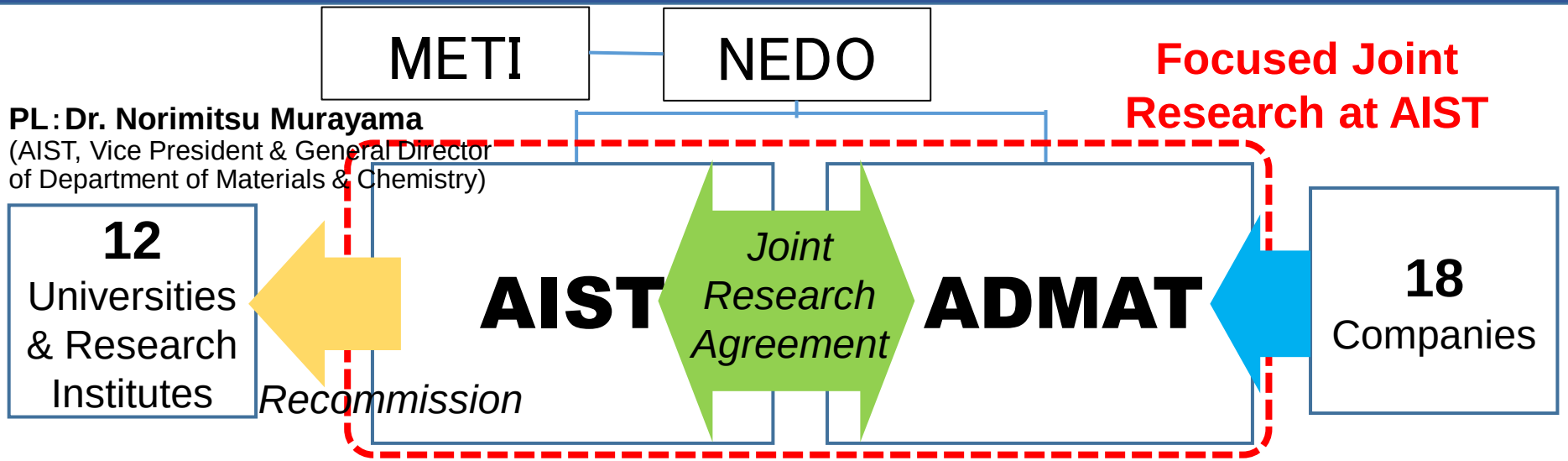
Length

10^{-9} m (1 nm)　　10^{-6} m (1 μm)　　10^{-3}m (1 mm)

Future Image: High Throughput Design of Functional Materials by Three-in-one efforts: Simulation, Processing & Characterization



Implementation System



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

- Establish: July 12, 2016
- President：Kunihiro Koshizuka (KONICA MINOLTA, INC., Senior Technical Advisor)
- Member (18 Companies): Idemitsu Kosan Co., Ltd., Ube Industries, Ltd., KANEKA CORPORATION, KONICA MINOLTA, INC., JSR Corporation, Showa Denko K.K., Showa Denko Materials Co., Ltd., Sekisui Kasei Co., Ltd., DIC Corporation, Tosoh Corporation, Toray Industries, Inc., NIPPON STEEL Chemical & Material Co., Ltd., NIPPON SHOKUBAI CO., LTD., Zeon Corporation, Panasonic Corporation, Furukawa Electric Co., Ltd., Murata Manufacturing Co., Ltd., The Yokohama Rubber Co., Ltd.

Annual Plan

FY 2016 | FY 2017 | FY 2018 | FY 2019 | FY 2020 | FY 2021

Establishing the Elements of the Material Design (MD)

Establishing the Orchestration Scheme for the Elements to Model Materials

Further Improvement of the M.D. Elements

Autonomous Development of Functional Materials

<Contracted Research and Development>

R&D Theme (1)	Computational Material Design
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

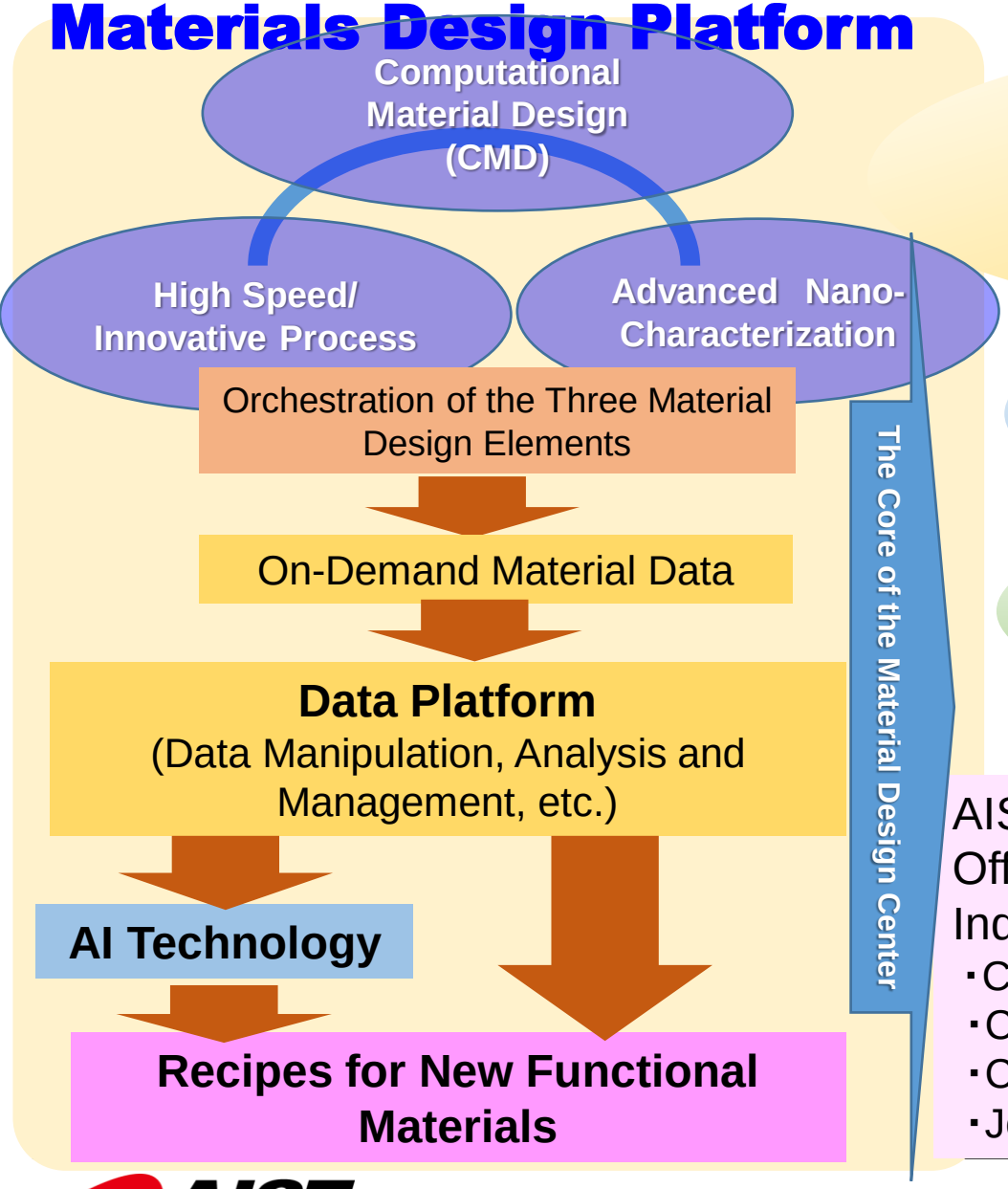
Ex-Post Evaluation

<Grant Development>

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

Future Efforts and Perspective for Application of Results

Materials Design Platform



Closed: Priority Use by ADMAT Partners

DESIGN TECHNOLOGY

Computational Material Design Protocol
- Innovative Process
- Advanced Characterization

Softwares to be Opened

SIMULATORS

- Computational Simulation

AIST Local

EXPRIMENTAL EQUIPMENTS

- Innovative Process
- Advanced Characterization

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.