World Premier International Research Center Initiative

AIMR

TOHOKU UNIVERSITY

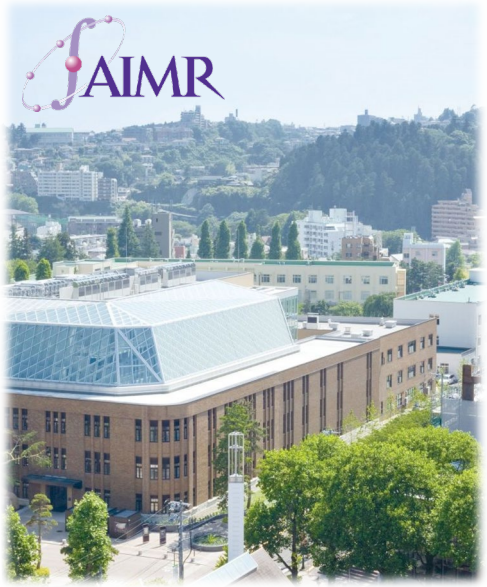
to Tohoku University and AIMR

Prof. Motoko Kotani
Director
Pure mathematician
(Geometer)

Susumu Ikeda

Associate Professor
earch Support Division (Administrative Director)

l Institute for Materials Research (WPI-AIMR)
Tohoku University, Japan



My visits to **France** so far

Minerals Tour
Musée de minéralogie MINES ParisTech
Collection of Univ. Pierre et Marie Curie
Muséum national d'Histoire naturelle

1998 Orléans (**mineralogy** conference), **Paris** (Quartier Latin)

13 WPI Centers

World Premier International Research Center Initiative

Sendai City



Univ. Tsukuba IIIS
Sleep

Hokkaido Univ. ICReDD
Chemical Reaction Design


Kanazawa Univ. NanoLSI
Nano life


Kyoto Univ. iCeMS
Cells & Materials

Tohoku Univ. AIMR
Materials (Math-Mate)


Kyoto Univ. ASHBi
Human Biology

NIMS-MANA
Nanotechnology


U. Tokyo Kavli IPMU
Universe (Phys-Math)

U. Tokyo IRCN
Neurointelligence

Osaka Univ. IFReC
Immunology

Tokyo Tech ELSI
Earth-Life

Kyushu Univ. I²CNER
Energy

Nagoya Univ. ITbM
Bio-Molecules




- Founded in 1907 as the 3rd Imperial University in Japan
- "Research First" and "Open-Door" Policy
- The first university which accepted women students, foreign students in Japan

TOHOKU UNIVERSITY

First Women Students in 1913 Tohoku University

President
Dr. Hideo OHNO

Tohoku University

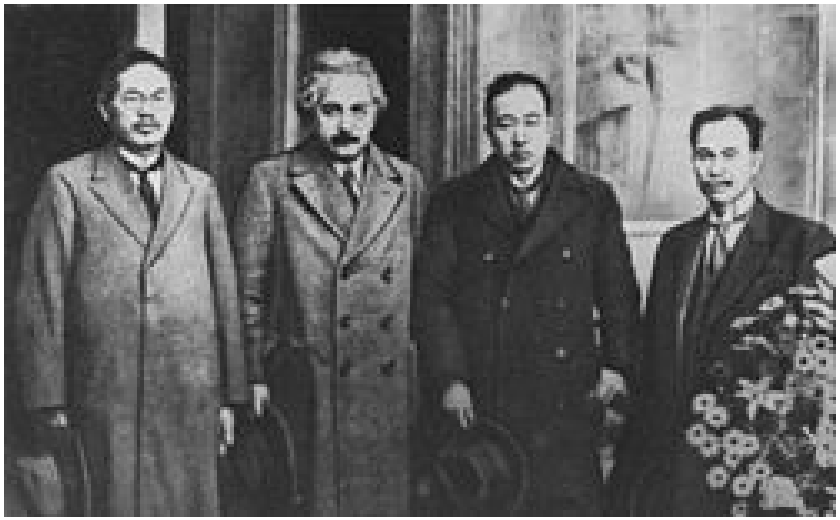
Dr. Kotaro HONDA "god of steel"

1917 Invention of **KS Steel**, the strongest magnet in the world

1916-22 Establishment of ***Institute for Materials Research (IMR)***

1931-40 President of Tohoku University

1937 First recipient of **Order of Culture**, the Japan's highest cultural honor



With **Albert Einstein** in 1922 at Tohoku Univ.

KS Steel

Dr. Honda laid the **foundation of materials science** of not only Tohoku University but also Japan**.**

Historical Inventions

Yagi-Uda Antenna

invented by
Prof. Shintaro UDA and
Prof. Hidetsugu YAGI
in 1926

Invented by

Prof. Jun-ichi NISHIZAWA 1926-2018

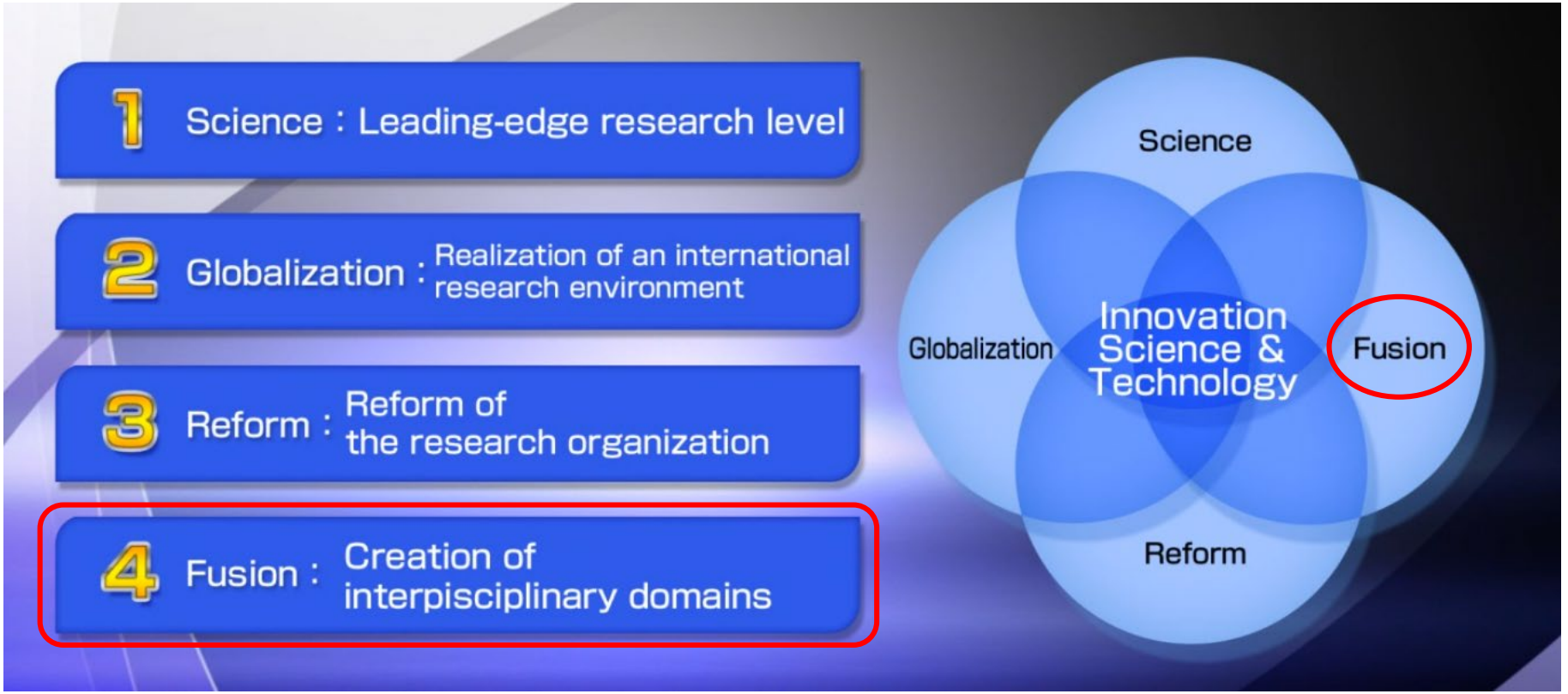
- Light-focusing Glass Fibers (1964)
- Polarization Fibers (1974)
- Avalanche Photodiode (1952)
- PIN Photodiode (1953)
- Semiconductor Lasers (1957)
- Static Induction Thyristor (1970)

IEEE Jun-ichi Nishizawa Medal
was established in 2002 in honor of Jun-ichi Nishizawa's lifetime of outstanding achievements.

Advanced Institute for Materials Research

Missions of WPI Research Centers

to attract excellent researchers from around the world

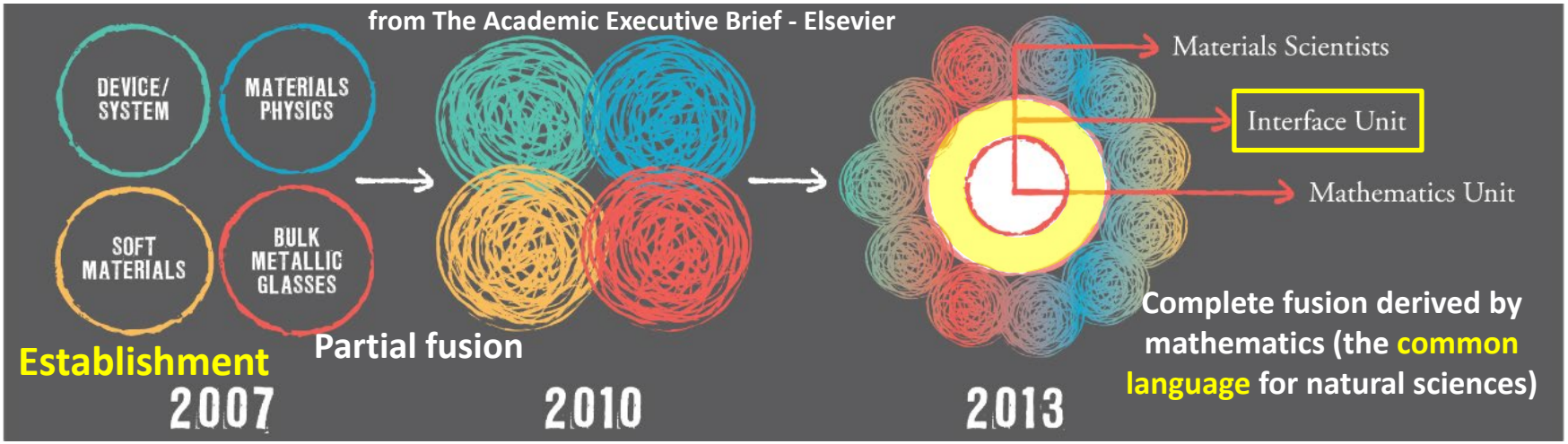


Motoko Kotani
Director
Pure mathematician (Geometer)

Prof. Kotani in a photograph taken at the reception held at Rennes City Hall with Deputy Mayor of Rennes (**NanoMat2015**). Our Sendai City is a sister city of Rennes.

Toward the predictive materials science based on mathematics-materials science collaboration

History of Math-Mate Collaboration at AIMR



2007 2009 2011-12 2016 2019

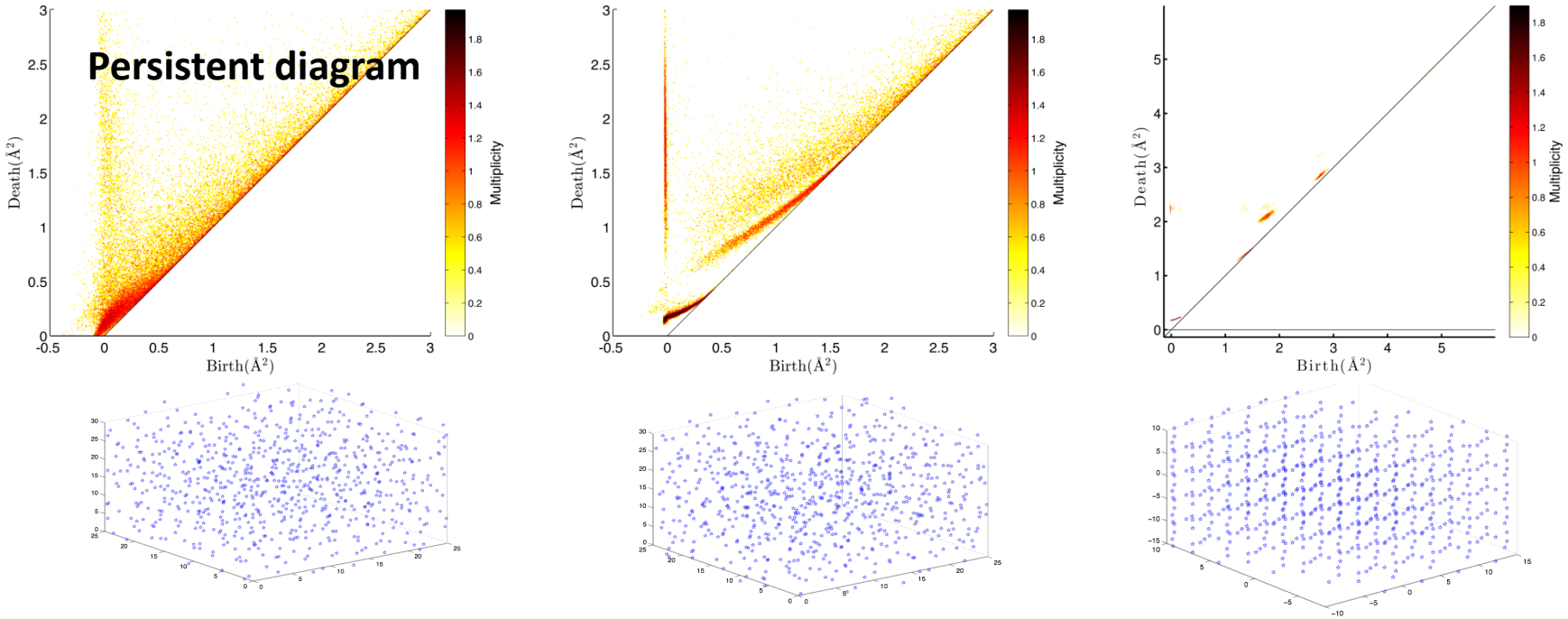
~25% of the AIMR researchers are mathematicians or theoretical physicists

Experimental laboratory

Math Group
WPI-AIMR SINCE2012

Structure analysis of **amorphous materials** using **persistent homology**

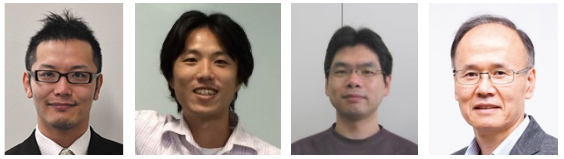
liquid **amorphous** **crystalline**



Persistent homology can extract some order hidden in random structures.

Y. Hiraoka, T. Nakamura, A. Hirata, E. G. Escolar, K. Matsue and Y. Nishiura, Hierarchical structures of amorphous solids characterized by persistent homology. *Proceedings of the National Academy of Sciences* **113**, 7035-40 (2016).

T. Nakamura, Y. Hiraoka, A. Hirata, E.G. Escolar and Y. Nishiura, Persistent homology and many-body atomic structure for medium-range order in the glass. *Nanotechnology* **26**, 304001 (2015).

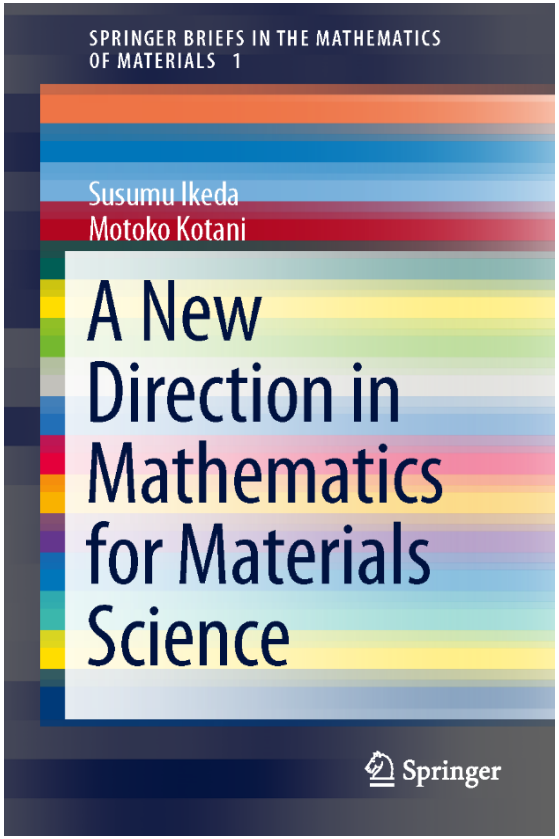


A series of monographs for math-mate collaboration

"**SspringerBriefs in the Mathematics of Materials**"

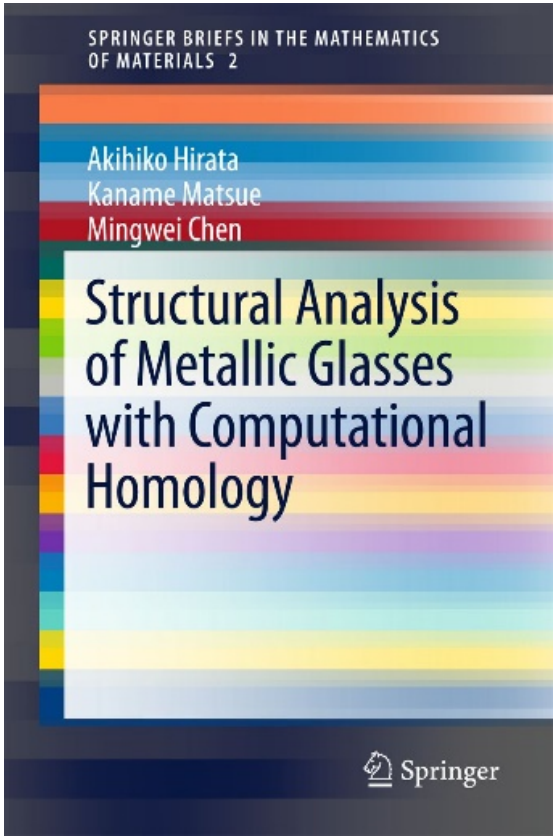
ISSN: 2365-6336

Vol. 1



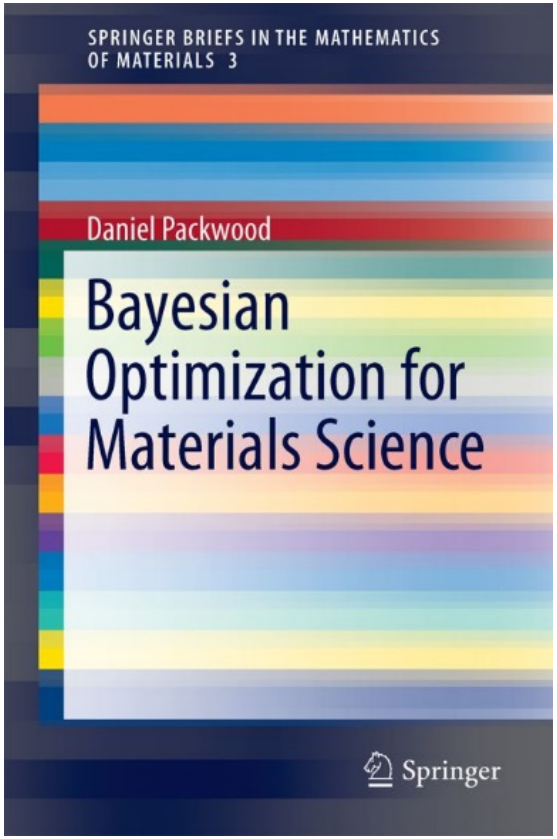
2015

Vol. 2



2016

Vol. 3



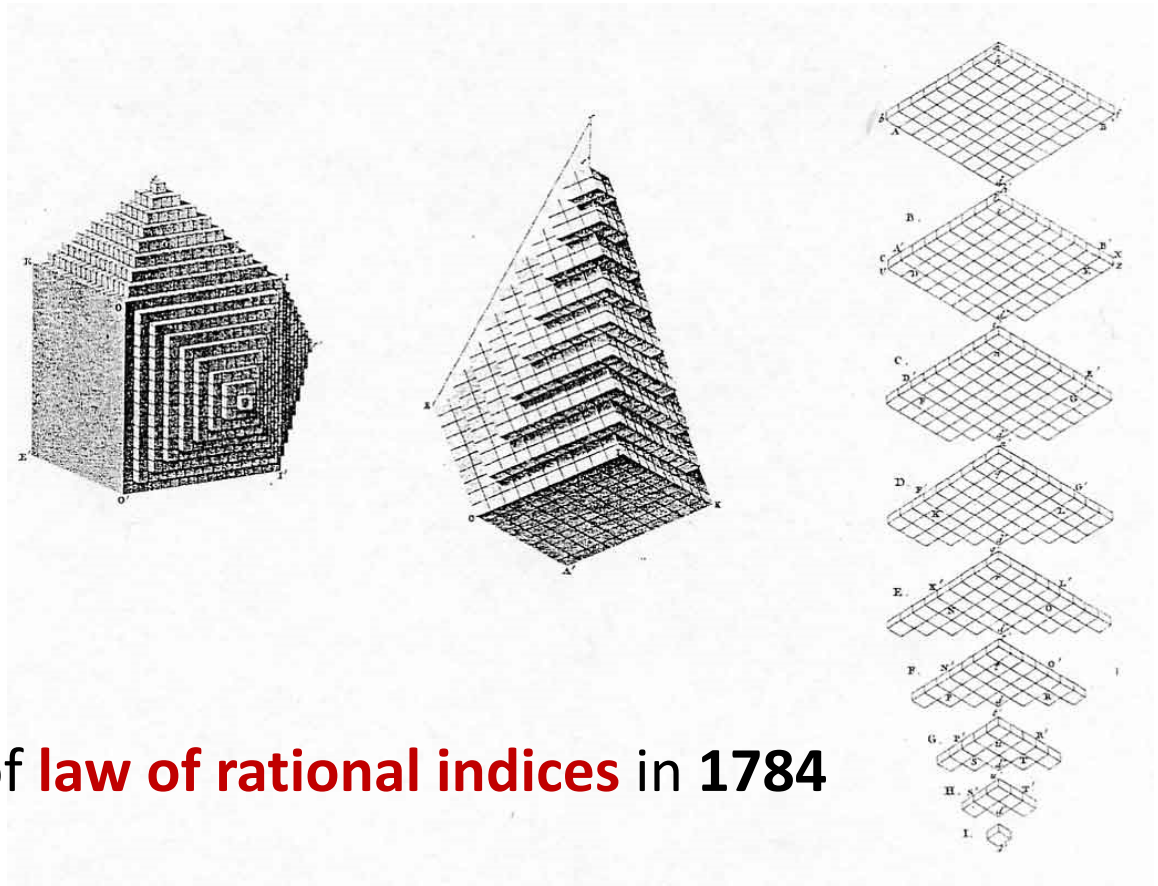
2017

Please refer to these books if you wish to get further information about our math-materials collaboration.

René-Just Haüy (1743–1822)

French mineralogist

"Father of Modern Crystallography"



Discovery of **law of rational indices** in **1784**

Materials (crystals) can be expressed based on the mathematical language **"geometry"**.

Workshop franco-japonais nanomatériaux

***Five** researchers are participating in this **NanoMat2019** from*

Advanced Institute for Materials Research, Tohoku University

Oral speakers from AIMR at NanoMat2019

Assoc. Prof. **Hiroshi Yabu**
Junior Principal Investigator

Nanocomposite materials based on catechol-containing adhesive and reductive polymers

Assoc. Prof. **Akichika Kumatani**

Nanoscale Electrochemical Imaging on Energy Materials: From Lithium-ion (De)intercalation Process to Electrocatalytic Reaction

Poster presenters from AIMR at NanoMat2019

Dr. **Tang Ma**
Assist. Professor

Functional bio-hybrid membranes through self-assembly

Dr. **Hiroya Abe**
Assist. Professor

Fe Azaphthalocyanine for Realizing Highly Active Oxygen Reduction Reaction (ORR) Catalytic Electrodes

Assoc. Prof. **Susumu Ikeda**
Administrative Director

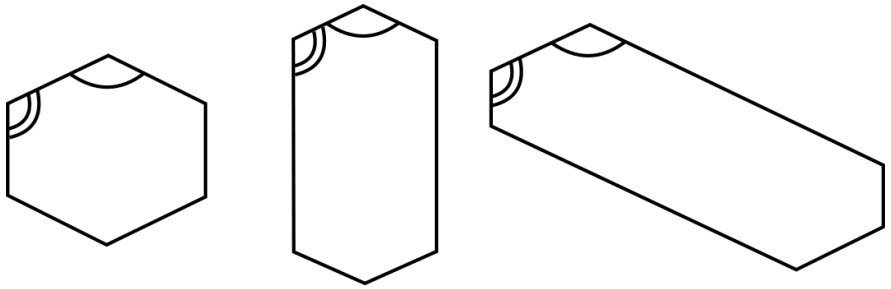
Molecular dynamics simulations of organic semiconductor thin film growth

Create predictive materials science based on mathematics-materials science collaboration

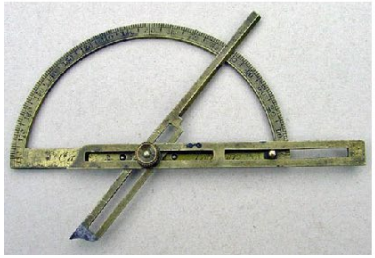
Nicolas Steno (1638–86)

Danish scientist

Discovery of **law of constant angles** in **1669**



First discovery of geometrical characteristics of materials.
This paved the way for the **Haüy's discovery** in 1784.



Apparatuses to measure an angle which two faces form

230 space groups

Group theory

Évariste Galois
(1811–32)

M. Sophus Lie
(1842–99)

mathematical means to describe the regularities

- point symmetries
- periodicities (translation symmetries)

Proof of the classification of the 230 space groups (in 3D)

was independently established by two mathematicians and one crystallographer.

mathematician
E.S. Fedorov
in 1890

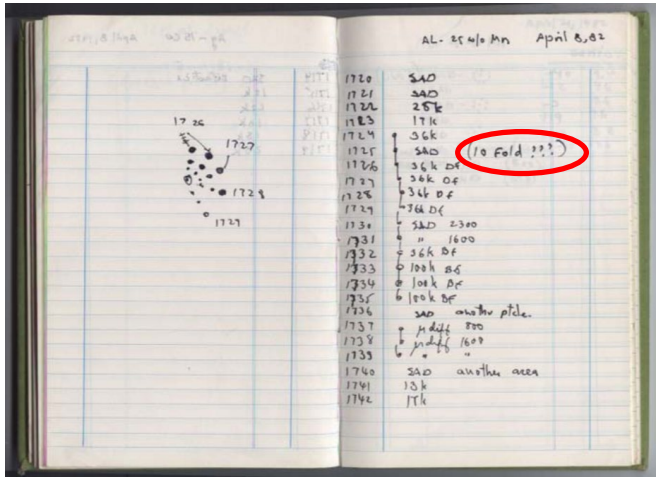
mathematician
A.M. Schoenflies
in 1891

crystallographer
W. Barlow
in 1894

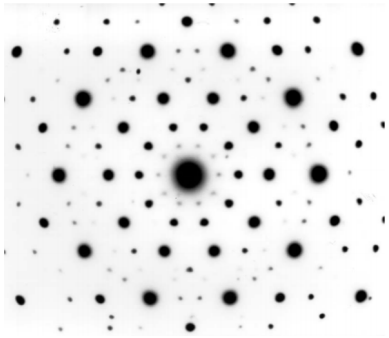
Clearly, mathematics is contributing significantly to the development of materials science.

Quasicrystals

In 1982, Daniel Shechtman observed pentagonal symmetry in the electron diffraction pattern of an aluminum alloy sample.

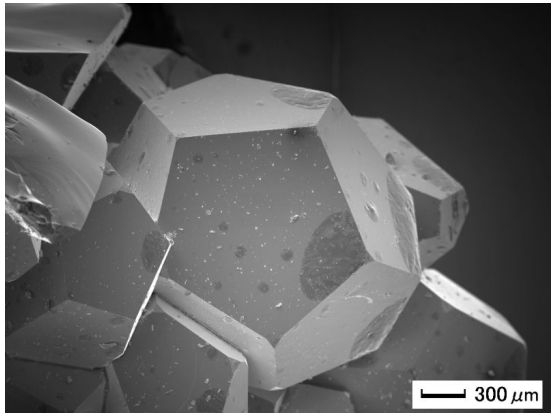


his experimental notebook

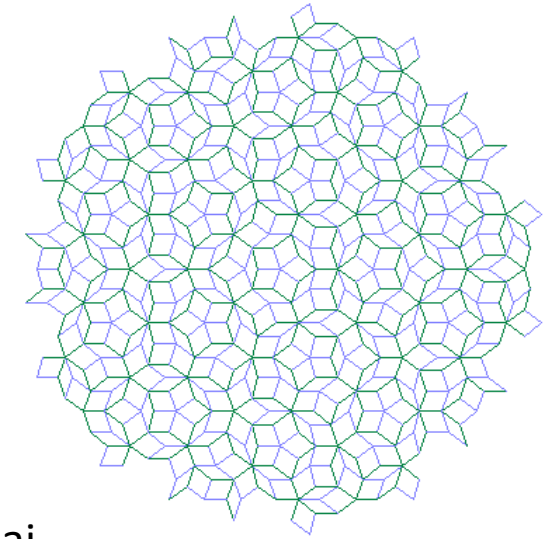


10-fold electron diffraction pattern
(from Shechtman's presentation file)

Daniel Shechtman
(Lecture at Tohoku University)



Zn-Mg-Dy quasicrystals,
courtesy of the late Prof. An-Pang Tsai,
Tohoku University



Penrose tiling
(Wikimedia Commons)

1600 1700 1800 1900 2000 2100

Materials science

Earthenware
Metal ware

Mineralogy

Crystallography

Metallurgy

Ceramics

Surface Science

Semiconductor

Device engineering

Solid State Physics

Spintronics

Steno

1669

Bartholinus

Symmetry

Law of constant angle

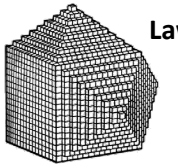
Double refraction
(Birefringence)

Crystal

Optics

Haüy

Periodicity



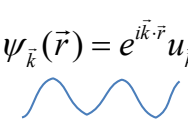
Law of rational indices

Space Group

Wave of electrons

Bloch's theorem

$$\psi_{\vec{k}}(\vec{r}) = e^{i\vec{k}\cdot\vec{r}} u_{\vec{k}}(\vec{r})$$



Quantum mechanics

$$H\mathbf{x} = \varepsilon\mathbf{x}$$

Electronic properties

Kohn

Density functional theory (DFT)

$$\rho(\mathbf{r}) = \sum_i^N |\phi_i(\mathbf{r})|^2.$$

Group Theory

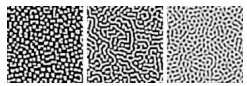
Galois

Lie

Self organization

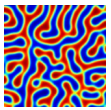
Turing

Pattern formation



Prigogine

Phase separation



Cahn

Allen-Cahn equation

Cahn-Hilliard equation

$$\frac{\partial c}{\partial t} = D\nabla^2\left(c^3 - c - \gamma\nabla^2 c\right)$$

Mathematics

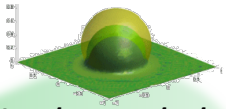
Euclidean Geometry

Eigenvalue problem

$$|A - \lambda E| = 0$$

$$\frac{\partial u}{\partial t} = f(u,v) + D_u\Delta u$$

$$\frac{\partial v}{\partial t} = g(u,v) + D_v\Delta v$$



Level set methods

Osher

Leibniz

Linear Algebra

$$(\widetilde{\mathbf{A}}\mathbf{W}\mathbf{A})\mathbf{x} = \widetilde{\mathbf{A}}\mathbf{W}\mathbf{y}$$

Infinitesimal calculus

$$\frac{d}{dx}\int_a^x f(t)dt = f(x)$$

Newton

Euler

Gauss

Modern Geometry

$$e^{i\theta} = \cos\theta + i\sin\theta$$

Quantum Hall effect

Connes

Noncommutative geometry

Advanced Geometry

Advanced numerical techniques

Research groups

FY2019

- Materials Physics
- Soft Materials
- Non-equilibrium Materials
- Device / System
- Mathematical Science

Management

Director : **M. Kotani**
Deputy Director : **S. Orimo**
Adm. Director: **S. Ikeda**
Deputy Adm. Director : **M. Funada**

Executive Advisor

Masaru Tsukada
Yasumasa Nishiura

International Advisory Board

J.G. Bednorz, IBM Zurich
1987 Physics Nobel laureate

H. Gleiter, Karlsruhe Inst. Tech.

V. Narayanamurti, Harvard Univ.

E. Negishi, Purdue Univ.
2010 Chemistry Nobel laureate

S. Mori, Kyoto Univ.
1990 Fields Medalist

M. Kotani
(Institute Director)

G Leader

S. Orimo
(AIMR)

S. Mizukami
(AIMR)

S. Samukawa
(AIMR)

S. Fukami
(AIMR)

Device/System

H. Yabu
(AIMR)

G Leader

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(AIMR)

T. Fukumura
(AIMR)

T. Sato
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Materials Physics

Y.P. Chen
(Purdue U)

T. Dietl
(Polish Acad Sci)

A.L. Shluger
(UCL)

Q.-K. Xue
(Tsinghua U)

Mathematical Science

G Leader

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(AIMR)

M. Kotani
(AIMR)

H. Chiba
(AIMR)

C. Pickard
(U Cambridge)

Nonequilibrium Materials

G Leader

M.W. Chen
(Johns Hopkins U)

D. Louzguine
(AIMR)

A.L. Greer
(U Cambridge)

G Leader

T. Adschiri
(AIMR)

M. Yamashita
(AIMR)

A. Hirano
(AIMR)

T.P. Russell
(UMass Amherst)

Soft Materials

13 WPI Centers

Origins of Universe/ Earth · Life/ Intelligence

Origin of Earth and Life

Tokyo Tech 2012

Origin of Universe

U. Tokyo 2007

Origin of Intelligence

U. Tokyo 2017

Life Science

Immunology

Osaka U. 2007

Sleep

U. Tsukuba 2012

Human biology

Kyoto U. 2018

Plant biology&chemistry

Nagoya U. 2012

Nano life science

Kanazawa U. 2017

Materials/ Energy

Materials & mathematics

Tohoku U. 2007

Cell biology & materials

Kyoto U. 2007

Nanoarchitectonics

NIMS 2007

Energy

Kyushu U. 2010

Hokkaido U. 2018

chemistry

Data/Information Science