

# Kyoto University On-site Laboratory: Center for Integrated Data-Material Sciences (iDM)



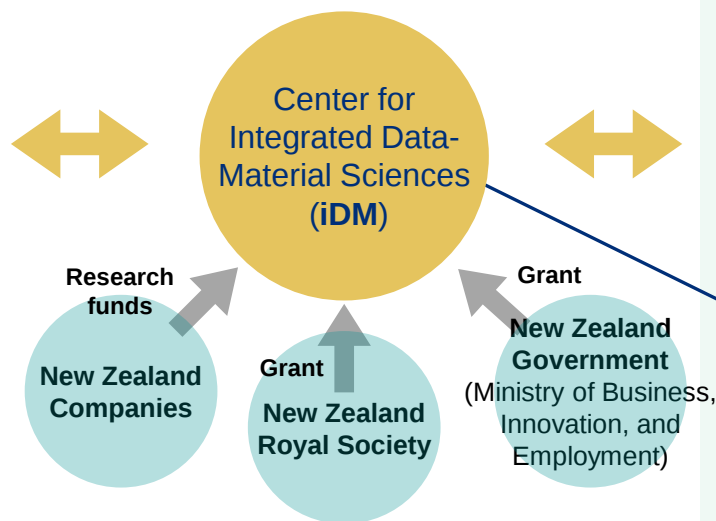
## General Information

- ◆ Approved in FY 2021
- ◆ Established in January 2022
- ◆ Established by the Institute for Integrated Cell-Material Sciences (iCeMS), Kyoto University Institute for Advanced Study (KUIAS)
- ◆ Partner institution: The MacDiarmid Institute for Advanced Materials and Nanotechnology, New Zealand
- ◆ Purpose: Perform integrative data science-materials science research
- ◆ Location: Wellington University, Wellington, New Zealand (outbound)
- ◆ Functions: Deepen research on material sciences using computational science and data science, and internationalize Kyoto University's research and education activities by enhancing collaboration with industry and local research institutions.

## Positive ripple effects to the university's activities

- Development of interdisciplinary fields combining data science and material science.
  - International industrial application of materials developed at Kyoto University
  - Cultivating the perspective of contributing to the international community through basic research among students and early-career researchers.
  - Raising the profile of the Kyoto University brand in Oceania.
- Expanding local research networks and enhancing the brand recognition of Kyoto University and KUIAS through establishing a policy for research on semiconductor materials and porous materials with local research institutions, which is anticipated to contribute to the achievement of a decarbonized society.
- Creating networks with local companies and Japanese companies, which can lead to research collaboration.
- Encouraging exchanges among early-career researchers and international students.
- Promoting the fusion of the humanities and sciences through research plans that fully respect the beliefs and customs of the Maori (indigenous people of New Zealand).

## Activity Overview



### The MacDiarmid Institute for Advanced Materials and Nanotechnology (MDI), New Zealand



New Zealand's largest-scale and highest-level virtual research institute in material science  
(31 laboratories from 5 major universities participate)

University of Auckland  
(7 laboratories)

Massey University  
(2 laboratories)

Victoria University of Wellington  
(12 laboratories + Administrative office)

Space provided by MDI  
Researchers assigned by MDI  
Researcher dispatched from iCeMS

University of Canterbury (6 laboratories)

University of Otago (4 laboratories)



- Accelerating research collaboration in **computing and data science**, with a focus on **material science**, which is a strength of both Kyoto University and MDI.
- Promoting research exchange and brain circulation as a hub of the Kyoto University-MDI network.

## Main activities in FY 2024

### ① Dispatch / acceptance of researchers

#### 【Kyoto → MacDiarmid Institute】

- 1-month stays by faculty (1) and postdocs (2) at MacDiarmid research groups for collaboration
- Participation and presentations at the MacDiarmid Symposium by postdocs (2)
- 1-month Internship at the MacDiarmid venture company Advemto by an undergraduate student (1)

#### 【MacDiarmid Institute → Kyoto】

- 1-month stays at iCeMS by young researchers (4) from the MacDiarmid Institute
- 2-week stays by MacDiarmid faculty (2)
- Acceptance of MacDiarmid young researcher (1) as a JSPS Foreign Postdoctoral Fellow (host institute: iCeMS)

### ② Organic semiconductor research with data science

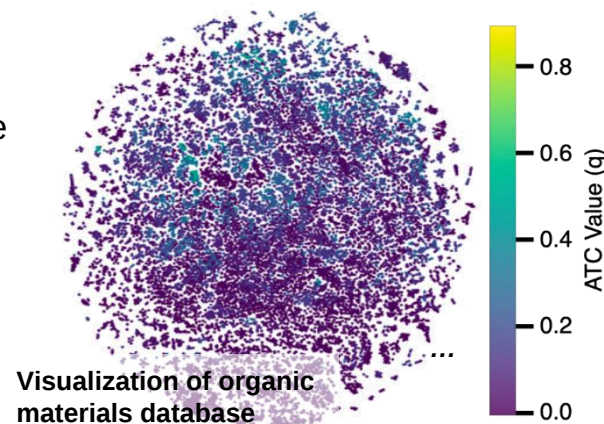
- Trained a graph neural network with high universality using New Zealand material data; reproduced exciton diffusion in organic materials with high accuracy.
- Opened the way to virtual screening of novel semiconductor materials.



Lecture by visiting  
young MacDiarmid  
scientist



Lecture by visiting  
MacDiarmid PI



Accurate reproduction  
of atom-level properties  
in organic materials  
using graph neural  
network

