

The Institute of Statistical Mathematics, Research Organization of Information and Systems

Research Center for Materials Informatics

## **Call for Researchers on Materials Informatics**

### **Outline**

We are developing the world's largest database of polymer properties in collaboration with several universities and companies, using automated all-atom classical molecular dynamics simulation systems. We are currently recruiting one researcher with expertise in materials science, data science, or computational chemistry (molecular simulation). The maximum term of appointment is five years.

### **Research subjects**

1. Research on materials informatics for polymeric materials (required skills: materials science or machine learning)
2. Development of algorithms that combine machine learning and molecular simulation (required skills: molecular dynamics simulation or machine learning)
3. Development of algorithms and software for automated calculation of polymer properties (required skills: molecular dynamics simulation and programming)

### **Research project**

You are expected to carry out your own research theme while participating in the following projects. Please feel free to contact us if you would like to know more about our research.

We have formed an industry-academia consortium consisting of 6 universities and 33 companies to jointly develop the world's largest polymer property database through high-throughput computational experiments. In this project, we are advancing the development of integrated analysis techniques for simulation and experimental data (such as SIM2REAL transfer learning, meta-learning, Bayesian optimization, and active learning) as well as automation technology for computational experiments on polymeric materials. Additionally, we can promote collaborative research with various researchers in the field of materials science, including the utilization of robots for automated and autonomous experiments.

Particularly, on April 1, 2024, we have launched the new research project about the bio-based polymers such as polypeptides. This project aims at open science and open innovation of biodegradable and bioadaptive polymers. A variety of researchers from academia in the fields of materials science, data science, and computational chemistry will participate in the project to promote interdisciplinary research. This project will conduct research on materials informatics of

bio-based polymers and on the fusion analysis of molecular simulation and machine learning.

**Position available**

1 position for postdoctoral researcher (job title: Project Assistant Professor or Project Associate Professor, depending on qualification)

**Working place**

The Institute of Statistical Mathematics (ISM)  
Research Organization of Information and Systems

[http://www.ism.ac.jp/index\\_e.html](http://www.ism.ac.jp/index_e.html)

Research Center for Materials Informatics

<https://monozukuri.ism.ac.jp/en/>

**Working conditions and contract period**

Full-time (nontenured)

Fixed term employee. The initial contract is for 1 fiscal year, but it can be renewed for a second fiscal year or later depending on performance evaluation and financial condition. Salary will be competitive in accordance with ISM's bylaws, with consideration of the academic qualifications and demonstrated research skills of the candidate.

**Closing date**

May 24, 2024

**Application procedure**

In the application, please include application materials listed below and we will handle them carefully based on the strict rules in our institute to protect your private information. Personal information received during the recruiting process will be used only for recruitment screening and appointment procedures, and not for any other purposes.

**Selection method**

Candidates will be selected based on submitted application materials and a possible follow up interview.

**Application materials**

- (1) Curriculum vitae
- (2) List of publications

- (3) Statement of past researches and research plan (maximum 2 pages)
- (4) Names and contact addresses (email) of two references (recommendation letters may be required to propose in later)

**Please send applications by email with the subject “Application to a researcher position at ISM”.**

### **Contact**

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