ドイツ人工知能研究センター日本研究所 特別セミナー

AI × Materials & Chemistry

AIで拓く、材料・化学の新たな可能性



講師 **Dr. Muhammad Nabeel Asim**

ドイツ人工知能研究センター(DFKI) 上級研究員 / 大阪公立大学客員教授

日時 **2026 11.18 水曜日**

会場 **なかもずキャンパス サイエンスホール A12棟**

対象 **本学の学生・教職員 学外の方**

3限 13:15〜14:45

Navigating Materials Space with AI: From Large-Scale Databases to Property Prediction and Materials Design

The rapidly expanding materials space offers important opportunities for discovering advanced materials, while creating substantial computational and data-management challenges. This workshop talk will present an AI-driven framework that connects large-scale materials databases with property prediction, virtual screening, and the design of new materials. We will discuss how machine-learning models can learn from chemical composition, crystal structure, processing conditions, and experimental measurements to predict properties such as stability, conductivity, mechanical strength, thermal behaviour, and optical performance. The talk will also explore materials language models, graph neural networks, and generative AI for identifying promising candidates and designing materials with targeted properties. Finally, we will discuss benchmarking, explainability, uncertainty estimation, and experimental validation as essential components of a reliable materials-discovery pipeline.

4限 15:00〜16:30

Navigating Chemical Space with AI: From 183 Million Compounds to Predictive Language Models

The rapid expansion of chemical space creates exciting opportunities and substantial computational challenges for modern drug discovery. In this workshop talk, we will present an AI-driven journey through ChEMBase , our well-organized database containing approximately 183 million chemical compounds. We will demonstrate how this resource enables efficient large-scale compound screening and supports the development of data-driven molecular discovery workflows. The talk will also introduce our in-house chemical language model for predicting key absorption, distribution, metabolism and excretion (ADME) properties. Finally, we will present a comprehensive benchmarking framework for evaluating chemical language models and molecular word embeddings through distinct and complementary strategies. Together, these resources provide an integrated foundation for exploring chemical space, assessing molecular representations and accelerating the identification of promising compounds.

参加方法：自由参加 (対面) ※セミナーは、どちらか一方のみ、または両方のいずれでもご自由にご参加いただけます。

オンライン参加及び、後日、録画視聴をご希望の方は、
右のリンクより事前登録をお願いいたします。 https://forms.gle/HnZm6Jm8xLLjY6dp8

主催：ドイツ人工知能研究センター（DFKI Lab Japan）所長 黄瀬 浩一

共催：ASPIRE 先端国際共同研究推進事業
関連プロジェクト：医療×ＡＩの日独重層型研究開発ネットワーク形成と産業創出

協賛：大阪公立大学大学院工学研究科
大阪公立大学大学院情報学研究科

問合せ先：大阪公立大学 協創研究センター 水野 r-mizuno[at]omu.ac.jp