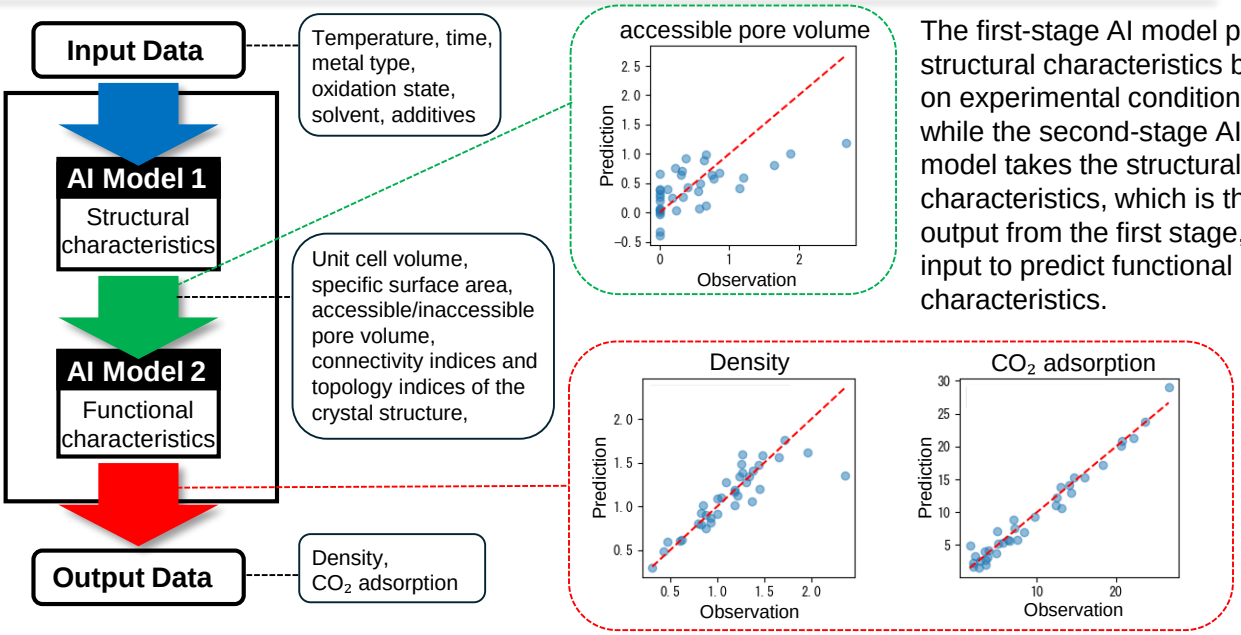
Balancing Density Control and CO_2 Adsorption Capacity in MOF Synthesis using Multi-Sigma®

This case study showcases how AIZOTH's AI analytics platform, Multi-Sigma®, is utilized to optimize the synthesis of Metal-Organic Frameworks (MOFs), achieving both optimal density and high CO_2 adsorption capacity

1. AI Chain Analysis



The first-stage AI model predicts structural characteristics based on experimental conditions, while the second-stage AI model takes the structural characteristics, which is the output from the first stage, as input to predict functional characteristics.

2. Factor Analysis

Impact of Synthesis Conditions

- **Synthesis time (17–20%)**: The strongest factor, with control over extended durations being particularly crucial.
- **Synthesis temperature (16–19%):** The second most influential factor, requiring careful selection of the appropriate temperature range.
- **Oxidation state (9–12%):** A +2 oxidation state consistently yields stable and favorable results.

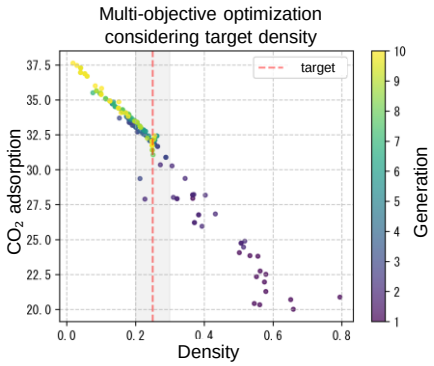
Impact of Structural Characteristics

- CO_2 adsorption capacity strongly depends on **surface area** and **pore volume**.
- Density is influenced by **unit cell volume** and **the connectivity of the crystal structure**.

3. Multi-Objective Optimization for CO_2 Adsorption and Density Control

Using Multi-Sigma's optimization functionality, a multi-objective approach was employed to maximize CO_2 adsorption while maintaining a target density of approximately 0.25 g/cm³. As a result, the following synthesis conditions were identified, achieving a density of 0.25 ± 0.005 g/cm³ and a high CO_2 adsorption capacity of 32.2:

- Synthesis temperature: 174° C
- Synthesis time: 408 hours
- Metal type: Indium
- Oxidation state: +2



(Note 1) Data Source: GitHub (https://github.com/aimat-lab/MOF_Synthesis_Prediction)
(Note 2) The unit of density is (g/cm³) and accessible pore volume is (cm³/g)., and the CO_2 adsorption capacity is measured at a temperature of 298 K and a pressure of 16 bar.

AIZOTH inc. provides a range of AI services, including Multi-Sigma®, AI consulting, experimental condition optimization support, and contract research and development.
Multi-Sigma® is a cloud-based AI software designed for research and development, significantly reducing experimental workload and enabling researchers to discover innovative solutions to real-world challenges with minimal experimental datasets.

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