第474回触媒科学研究所コロキウム

Describing Heterogeneous Catalysis via the “Materials Genes” Concept

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The intricate interplay of several underlying processes governing certain materials’ properties and functions prevents the explicit, atomistic modelling and hinders the efficient design of new materials. In this talk, I will discuss AI approaches to identify the key descriptive parameters (“materials genes”) correlated with the materials performance and reflecting the physical processes that trigger, facilitate, or hinder the materials’ behavior.[1] The symbolic-regression sure-independence-screening-and-sparsifying-operator (SISSO) [2] and the subgroup-discovery (SGD) AI methods leverage the typically small high-quality experimental or theoretical datasets in materials science. They identify nontrivial relationships between multiple key descriptive parameters and the performance of exceptional materials, guiding the design of new, improved materials. The “materials genes” concept and its impact will be illustrated for heterogeneous catalysis as an example of a complex materials’ function.[1,3,4]

References:
1. Foppa, L., et al. ″Materials Genes of Heterogeneous Catalysis from Clean Experiments and Artificial Intelligence″ MRS Bulletin (2021), 46, 1016–1026.
2. Ouyang, R., et al. “SISSO: A Compressed-Sensing Method for Identifying the Best Low-Dimensional Descriptor in an Immensity of Offered Candidates” Physical Review Materials (2018), 2, 083802.
3. Foppa, L., et al. ″Learning Design Rules for Selective Oxidation Catalysts from High-Throughput Experimentation and Artificial Intelligence″ ACS Catalysis (2022), 12, 2223–2232.
4. Miyazaki, R., et al. ″Materials Genes of CO2 Hydrogenation on Supported Cobalt Catalysts: An Artificial Intelligence Approach Integrating Theoretical and Experimental Data″ Journal of the American Chemical Society (2024), 146, 5433–5444.

Lucas Foppa received his PhD from ETH Zurich in Switzerland. His doctoral research focused on the first-principles-based multiscale modelling of heterogeneous catalysts. After his PhD, he moved to the Fritz Haber Institute of the Max Planck Society in Germany as a Swiss National Science Foundation postdoc fellow. At the Fritz Haber Institute, he works on artificial-intelligence concepts and methods and their application to computational and experimental materials science and catalysis. Since 2021, he is the head of the group ″ab initio and AI methods for heterogeneous catalysis″ at the Fritz Haber Institute.

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