

キャタリストインフォマティクスの最前線

(北大触媒研¹・京大触媒電池²) ○鳥屋尾 隆^{1,2}

Frontier of Catalyst Informatics

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Recent revolutions made in data science could have a great impact on traditional catalysis research in both industry and academia and could accelerate the development of catalysts. Machine learning (ML), a subfield of data science, can play a central role in this paradigm shift away from the use of traditional approaches. In this talk, recent progress that has been made in utilizing ML to create homogeneous and heterogeneous catalysts will be presented. The focus of the talk is on the design, synthesis, and characterization of catalytic materials/compounds as well as their applications to catalyzed processes.

Keywords : *Catalyst informatics, Catalyst, Machine learning*

触媒研究者は膨大な文献情報を統合して作業仮説をたてるが、触媒関連情報は膨大で多岐にわたるため、実験を行わずに仮説構築・触媒特性予測をすることは困難である。最近、理論・実験材料科学とデータ科学の融合領域が注目されているが、固体触媒のような複合的・化学的現象への展開は萌芽的段階にあり、他の材料分野に遅れをとっている。¹⁻⁵ 本発表では、触媒化学とデータ科学の境界領域研究に関する現状を我々の取り組み⁶⁻¹⁰とともに紹介する。

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