機械学習を利用した固体触媒開発

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Machine learning assisted developments of heterogeneous catalysts
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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, I will show our recent contributions to establishing “Catalysis Informatics”.
Keywords : Catalysis informatics, Heterogeneous catalysts, 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。本発表では、触媒化学とデータ科学の境界領域研究(触媒インフォマティクス)に関する我々の最近の取り組み [1–4] を紹介する。

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