The Rise of Catalyst Informatics: Realities and Key Concepts

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Abstract: Catalyst design is on the verge of reformation due to the recent rise of catalyst informatics. However, the process of applying catalyst data towards the design process of a catalyst is not well-established. Here, three important concepts in catalyst informatics are proposed along with examples of materials and catalyst informatics.

Keywords: Catalyst Informatics, Machine learning, Data Science

1. Introduction

Catalyst informatics has garnered much attention over the past several years due to rapid development of data acquisition techniques such as high throughput experiments and computational science. A similar movement is occurring within the field of materials science with the emergence of materials informatics. However, the manner in which catalysts and materials are designed using materials and catalyst data remains uncertain and thus not established. Here, three important concepts within catalyst informatics are proposed along with examples of materials and catalyst informatics.

2. Method

Three concepts are introduced for catalyst informatics: database, data to knowledge, and platform. In particular, how data science and machine learning are implemented in order to discover catalysts.

3. Results and discussion

Three successful applications of materials informatics are presented.

1: Prediction of lattice constant[2].

2: Discovery of hidden two dimensional magnets[3]

3: Discovery of hidden perovskite materials for solar cells[4].

In addition to the material informatics, strategies for catalyst design using data science are addressed.

4. Conclusions

Catalyst informatics can be a game changer within the field of catalysis; however, it remains unclear what role data science will play within the field of catalysis. Three important concepts for catalyst informatics are introduced along with successful applications of informatics in materials science and catalysis. Additionally, strategies for catalysts informatics are also proposed and discussed.

References

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