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Accelerating the Experimental Search of Nanoporous Catalytic Materials: A Data-Driven Approach

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Reference:Nanoporous materials have been widely used in several practical applications, for example, as adsorbents and catalysts. They have found their central places in chemical industries as one of the most key materials over past decades. To discovery suitable materials for sustaining our human lives and planet, development of materials should be made in a more rapid pace. However, the discovery of new materials and their property optimizations for targeted applications have heavily relied on a trial-and-error search, which is a highly time-consuming approach. To overcome this experimental challenge, a data-driven approach by applying data science techniques to experimental and computational data enables us to extract the most significant material descriptors over the complex chemical/materials space with a high dimension and massive entries, which is sometimes very difficult to be handled by human [1,2].
In this talk, the applications of data science techniques to the exploratory search of nanoporous materials for catalysis-related application are presented. This can make the synthesis–structure–property relationship more apparently, thereby providing some guidelines for design and selection of efficient materials. In particular, several machine learning algorithms are used to extract the (most) influential materials descriptors of nanoporous carbon electrocatalysts for oxygen reduction reaction to rationalize the structure–property relationship, which subsequently suggests the better catalysts [2]. Furthermore, experimental exploration can be accelerated by an active learning pipeline coupling with Bayesian optimization, which is demonstrated in the synthesis of nanoporous PtPdAu alloys for electrocatalytic methanol oxidation [3]. Clearly, the data-driven approach is highly efficient and would be applicable to accelerate the discovery of nanoporous materials and beyond.

[1] Science 374 (2021) 257.
[2] Adv. Mater. 34 (2022) 2107212.
[3] Nano Energy 94 (2022) 106868.
[4] J. Mater. Chem. A 8 (2020) 13532.