ORAL ☐ POSTER ☐

Big-data and Metal-Organic Frameworks: Science Beyond Understanding

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Metal-organic frameworks (MOFs) present a vast chemical landscape with potential for diverse applications such as gas separation, storage, sensing, and catalysis. The allure of MOFs lies in their customizable structures, enabling the synthesis of seemingly boundless variations tailored for specific functionalities. The holy grain of MOF synthesis is to design an optimal MOF for a given application. There are some fundamental reasons why we still need to reach this goal.

The infinitude of possible MOF structures renders traditional experimental and computational screening methods insufficient. The optimal material for a given application must be discerned from this boundless design space, which often encompasses multi-objective scenarios, defying a singular ranking system for material evaluation. Furthermore, the synthesis of a theoretically optimal MOF cannot be guaranteed in practice. This lecture delves into how data science methodologies can bridge the gap between theoretical MOF design and practical application.[1] We explore the instrumental role of data science in providing insights into complex chemical questions beyond the reach of conventional theories, such as determining the oxidation state of metals within MOFs,[2] ascertaining the color of the frameworks,[3] or the heat capacity of a MOF.[4]

Moreover, we will demonstrate the application of data-driven approaches in identifying key characteristics of high-performance materials, specifically for carbon capture processes. We aim to navigate the MOF design space more effectively and efficiently by integrating data science techniques with chemical intuition. This approach heralds a new era where data science complements traditional research methods and becomes a cornerstone in the quest for ideal MOF synthesis, leading to accelerated discovery and innovation in Chemistry and Chemical Engineering.[5]

References

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