Creation of a Predictive MOF Performance Indication System Utilizing Synthesis Criteria and Machine Learning

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Infinitely many metal-organic frameworks (MOFs) can be made by combining nodes and organic linkers. As of now, 90,000 MOFs have been successfully synthesized and over 500,000 predicted.The purpose of this investigation is to create an efficient and effective litmus test which can be utilized by scientists to further investigate potential MOFs; it serves as a screening system to determine whether a MOF is feasible and synthesizable in the lab. The program utilizes machine learning to concoct a program that uses the CORE-MOF 2019 and statistical significance to identify viable MOFs. Cavity diameter, surface area, and density were used as synthesis criteria to achieve this task. Using PANDAS, a code was constructed to sort and analyze .cif files taken from the CORE-MOF 2019 database. A MOF was deemed not viable by the system if it exceeded three standard deviations from the collected mean for two or more criteria. The program was designed to analyze data on a rolling basis to create a dynamic approach to keep up with novelty in MOF structures. The aim of the investigation, to create a predictive MOF performance indication system utilizing varying synthesis criteria, was achieved. The program created as a result of iteration two correctly determined CO2 capture MOFs efficacy 91% of the time. With further development, this tool could be used as a litmus test for future MOFs; a scientist looking to synthesize their theoretical MOF could insert their .cif file into the program to get a gauge of whether or not the design will synthesize; this litmus test will allow for materials and funds to be more effectively utilized and distributed.