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Deep Learning Models for Predicting Gas Adsorption Capacity of Nanomaterials

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Abstract: Metal–organic frameworks (MOFs), a class of porous nanomaterials, have been widely used in gas adsorption-based applications due to their high porosities and chemical tunability. To facilitate the discovery of high-performance MOFs for different applications, a variety of machine learning models have been developed to predict the gas adsorption capacities of MOFs. Most of the predictive models are developed using traditional machine learning algorithms. However, the continuously increasing sizes of MOF datasets and the complicated relationships between MOFs and their gas adsorption capacities make deep learning a suitable candidate to handle such big data with increased computational power and accuracy. In this study, we developed models for predicting gas adsorption capacities of MOFs using two deep learning algorithms, multilayer perceptron (MLP) and long short-term memory (LSTM) networks, with a hypothetical set of about 130,000 structures of MOFs with methane and carbon dioxide adsorption data at different pressures. The models were evaluated using 10 iterations of 10-fold cross validations and 100 holdout validations. The MLP and LSTM models performed similarly with high prediction accuracy. The models for predicting gas adsorption at a higher pressure outperformed the models for predicting gas adsorption at a lower pressure. The deep learning models are more accurate than the random forest models reported in the literature, especially for predicting gas adsorption capacities at low pressures. Our results demonstrated that deep learning algorithms have a great potential to generate models that can accurately predict the gas adsorption capacities of MOFs.

Keywords: metal–organic framework; gas adsorption; deep learning



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1. Introduction

Nanomaterials have been widely studied in various fields, such as food science, energy, electronics, and drugs, due to their advantageous physical, chemical, optical, and electrical properties [1–6]. In contrast to other rigid nanoparticle carriers, metal–organic frameworks (MOFs) have gained attention in recent years due to their well-defined structure, ultrahigh surface area, high porosity, tunable pore size, and easy chemical functionalization. In a MOF, metal ions or clusters of ions are linked by organic molecules to form a repeating, cage-like hollow structure. The unique structure diversity and exceptionally large surface area make MOFs promising candidates for many applications including intracellular delivery of drugs, proteins, and nucleic acids; sensing; bioimaging; and energy storage [7]. In contrast to other rigid nanoparticles, MOF nanocarriers have a high drug loading capacity and controlled drug release properties, which contributes to the growing attention on MOFs for pharmaceutical applications [8].

The industrial and biomedical applications using MOFs have increased over the past few years, including catalysis, gas storage, and gas separation. By carefully selecting metal clusters and organic linkers, researchers can synthesize MOFs to selectively adsorb specific gases [9–11]. To find good performing materials for some specific applications, gas adsorption data are typically used to screen a diverse MOF database. Due to the large number of

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