



Article

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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Table of Contents Learning Guide Predicting Gas Behavior

1. Understanding the eBook Learning Guide Predicting Gas Behavior
 - The Rise of Digital Reading Learning Guide Predicting Gas Behavior
 - Advantages of eBooks Over Traditional Books
2. Identifying Learning Guide Predicting Gas Behavior
 - Exploring Different Genres
 - Considering Fiction vs. Non-Fiction
 - Determining Your Reading Goals
3. Choosing the Right eBook Platform
 - Popular eBook Platforms
 - Features to Look for in a Learning Guide Predicting Gas Behavior
 - User-Friendly Interface
4. Exploring eBook Recommendations from Learning Guide Predicting Gas Behavior
 - Personalized Recommendations
 - Learning Guide Predicting Gas Behavior User Reviews and Ratings
 - Learning Guide Predicting Gas Behavior and Bestseller Lists

5. Accessing Learning Guide Predicting Gas Behavior Free and Paid eBooks
 - Learning Guide Predicting Gas Behavior Public Domain eBooks
 - Learning Guide Predicting Gas Behavior eBook Subscription Services
 - Learning Guide Predicting Gas Behavior Budget-Friendly Options
6. Navigating Learning Guide Predicting Gas Behavior eBook Formats
 - ePub, PDF, MOBI, and More
 - Learning Guide Predicting Gas Behavior Compatibility with Devices
 - Learning Guide Predicting Gas Behavior Enhanced eBook Features
7. Enhancing Your Reading Experience
 - Adjustable Fonts and Text Sizes of Learning Guide Predicting Gas Behavior
 - Highlighting and Note-Taking Learning Guide Predicting Gas Behavior
 - Interactive Elements Learning Guide Predicting Gas Behavior
8. Staying Engaged with Learning Guide Predicting Gas Behavior
 - Joining Online Reading Communities
 - Participating in Virtual Book Clubs
 - Following Authors and Publishers Learning Guide Predicting Gas Behavior
9. Balancing eBooks and Physical Books Learning Guide Predicting Gas Behavior
 - Benefits of a Digital Library
 - Creating a Diverse Reading Collection Learning Guide Predicting Gas Behavior
10. Overcoming Reading Challenges
 - Dealing with Digital Eye Strain
 - Minimizing Distractions
 - Managing Screen Time
11. Cultivating a Reading Routine Learning Guide Predicting Gas Behavior
 - Setting Reading Goals Learning Guide Predicting Gas Behavior
 - Carving Out Dedicated Reading Time
12. Sourcing Reliable Information of Learning Guide Predicting Gas Behavior
 - Fact-Checking eBook Content of Learning Guide Predicting Gas Behavior
 - Distinguishing Credible Sources
13. Promoting Lifelong Learning

- Utilizing eBooks for Skill Development
 - Exploring Educational eBooks
14. Embracing eBook Trends
- Integration of Multimedia Elements
 - Interactive and Gamified eBooks

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