# Article information:

Molecular model construction of Chifeng lignite and analysis of adsorption mechanism of O2 at low temperature - ScienceDirect
<https://www.sciencedirect.com/science/article/pii/S002228602202258X?via%3Dihub>

# Article summary:

1. A macromolecular model of Chifeng lignite was constructed using elemental analysis, 13C NMR and XPS analysis combined with molecular mechanics (MM) and molecular dynamics (MD).

2. The mechanism of oxygen adsorption by coal was studied using Grand Canonical Monte Carlo (GCMC) and Density Functional Theory (DFT) at different temperatures and pressures.

3. Oxygen tends to be adsorbed on each functional group structure of coal in a parallel direction, with the highest adsorption capacity for aromatic rings.

# Article rating:

May be slightly imbalanced: The article presents the information in a generally reliable way, but there are minor points of consideration that could be explored further or claims that are not fully backed by appropriate evidence. Some perspectives may also be omitted, and you are encouraged to use the research topics section to explore the topic further.

# Article analysis:

This article provides an in-depth look into the molecular model construction of Chifeng lignite and its oxygen adsorption mechanism at low temperature. The authors have used a variety of methods such as elemental analysis, 13C NMR, XPS analysis, molecular mechanics (MM), molecular dynamics (MD), Grand Canonical Monte Carlo (GCMC), and Density Functional Theory (DFT) to construct the macromolecular model of Chifeng lignite and study its oxygen adsorption mechanism. The results are presented in a clear manner that is easy to understand.

The article does not appear to be biased or one-sided in its reporting, as it presents both sides equally. It also does not contain any promotional content or partiality towards any particular point of view. All claims made are supported by evidence from the research conducted by the authors, which adds to the trustworthiness and reliability of the article. Furthermore, possible risks associated with coal spontaneous combustion are noted throughout the article, providing readers with a comprehensive understanding of this phenomenon.

The only potential issue with this article is that it does not explore any counterarguments or alternative points of view regarding its findings. While this does not necessarily detract from the overall quality of the article, it would have been beneficial if some counterarguments were discussed in order to provide readers with a more balanced perspective on this topic.

# Topics for further research:

* Coal spontaneous combustion
* Oxygen adsorption mechanism
* Molecular mechanics
* Molecular dynamics
* Grand Canonical Monte Carlo
* Density Functional Theory

# Report location:

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