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Editorial

Coal Molecular Structure Evolution for Methane Adsorption Molecular Mechanism

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Coal is complex as it includes organic matter (macerals) and inorganic matter (minerals). Previous research has mainly focused on the evolution during coal formation, which is the comparison of different mature coal structures [1]. In addition, more research work studies the evolution characteristics of coal chemical structure by thermal simulation technology and coal pyrolysis, which can ensure the same parent material [2–4]. The storage of methane in coal structures (pores and matrix in coal reservoirs) is mainly in an adsorption state. And the macromolecular structural evolution of coal may influence the nanoscale pore configuration and its spatial distribution, which, in turn, may impact the methane adsorption behavior. The coal macromolecular structure is highly complex, and there are significant differences in the adsorption capacity of methane for different rank coals [5]. Moreover, the composition of different aliphatic and aromatic chemical structure groups in the coal macromolecule models may also affect the adsorption properties of methane [6,7]. Some useful experimental techniques can be used to investigate the coal chemical structure, which affects the adsorption capacity, e.g., FTIR spectroscopy, Raman, XRD, 13 CNMR, and HRTEM [8–11]. These experiments can provide a lot about the types of functional groups, crystal structures, carbon types, and aromatic stripes in the chemical structure of coal.

Based on the information on the chemical structure, classical coal structure molecular models have been built. Some three-dimensional macromolecular structure models of coal in different coal ranks have been used to study the application at coal molecular level, which include nano-pores, gas adsorption and desorption, and chemical and physical properties [12,13]. With the development of technology and the advancement of methods, we have gained a better understanding of coal structure, providing new ideas for me to solve methane adsorption molecular mechanisms. It can be used in the areas of clean and efficient utilization of coal, development of coalbed methane, underground coal gasification, and CCUS. As an unconventional clean resource, coalbed methane has been widely concerned and investigated in terms of energy utilization, environmental protection, and mining safety. Regarding the studies of methane adsorption properties in coal, several researchers focused on the role of the macromolecular structure of coal, as well as the pore distribution and its morphology, in controlling them. As for the adsorption capacity of methane in different rank coals, the investigations mainly include characterizing the pore size distribution (combined with adsorption modeling) and modeling the physical and chemical structure of macromolecules (molecular dynamics simulation of methane adsorption). The controlling mechanism of methane adsorption properties by macromolecular structures in coals in different evolutionary degrees is an important scientific research topic of practical significance [14,15]. So, a further exploration of it at the molecular level is also needed.

This editorial refers to the Special Issue "Coal Molecular Structure Evolution for Methane Adsorption Molecular Mechanism". The Special Issue highlights chemical structure, pore structure, and CBM gas content.

Seven manuscripts were submitted for consideration for the Special Issue, and all of them were subject to the rigorous *Sustainability* review process. In total, six papers were

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finally accepted for publication and inclusion in this Special Issue. The contributions are listed below:

Li et al. have taken Lvjiatuo Coal Mine as a case to study the pore and fracture in different coal seams and discuss the adsorption process. Along with the increasing depth, the methane adsorption in coal seam also increases. The results and conclusions are useful for the coalbed methane production and it is also reducing gas outbursts.

Duan et al. investigated the pore structure of different coal seam samples. The research area is located in the eastern and central Qinshui Basin. The results show that many micropores can be found in high-rank coal, while at a medium-rank, coal mesopores and macropores might be higher. It is useful for coalbed methane exploration and production.

Yang et al. chose the Huimin Depression of the Bohai Bay Basin as a research area and analyzed the Sha-4 Member sedimentary facies. The Sha-4 Member's sedimentary environment model might have shallow lake facies and a delta front. This article provides details about sandbody distribution characteristics.

Yang et al. have built a new CBM gas content prediction model by a method with the name Bayesian hyper-parameter optimization. This model is different from other models; the simulated gas content curve shows a good relationship with the measured value. It will be useful for calculating the CBM gas content.

Deng et al. also chose the CBM gas content as a topic. They have calculated lost methane content by a special method. Multiple parameters have given the total gas content. The average error is approximately 7%.

Liu et al. discussed the non-covalent bonds of bituminous coal by deformation simulation. The results show that, along with increasing deformation, π–π bonds and hydrogen bonds were determined by the relaxation stage. This could make the motion ability of the liberated molecular structures much greater. The results are useful for knowing the coal and gas outburst.

As mentioned above the articles list, the authors of these papers are all from China, indicating that coal research has received great attention in China, which is closely related to China's large coal reserves and wide utilization. At present, more molecular models and adsorption models have been proposed, and the applicability and structural characteristics of these models should be given attention.

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List of Contributions

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