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Construction of a macromolecular structural model of Chinese lignite and analysis of its low-temperature oxidation behaviour☆

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Abstract: The aim of this paper is to analyze the change in the active structure of lignite during the process of low-temperature oxidation by constructing a molecular structure model for lignite. Using quantum computation combined with experimental results of proximate analysis, ultimate analysis, Fourier transform infrared spectroscopy (FTIR) and X-ray photoelectron spectroscopy (XPS), a structural model for the large molecular structure was constructed. By analyzing the bond lengths in the model molecule, the evolution law for the active structure of lignite was predicted for the process of low-temperature oxidation. In low-temperature oxidation, alkanes and hydroxyls are the primary active structures observed in lignite, though ether may also react. These active functional groups react with oxygen to release heat, thereby speeding up the reaction between coal and oxygen. Finally, the content of various functional groups in the process of lignite low-temperature oxidation was analyzed by infrared analysis, and the accuracy of the model was verified.

Keywords: Chinese lignite, coal combustion, molecular simulation, low-temperature oxidation process, environment

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