Evolution of Electron Structure of the Methane-Coal Sorption System Components and Properties

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- Chapter
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Abstract

It is shown that metastable state of the carbon matter and variability of properties associated with it are a consequence of the adaptive ability of carbon atoms to change the degree of hybridization depending on external thermodynamic conditions. Mechanisms of evolution of the coal structural and functional characteristics during interphase interaction in the coal-gas system are visualized by a qualitative assessment of the change in the distribution of carbon atoms between the sp

–sp

states. A stepwise adsorption scheme is proposed, starting from the macroscale and ending with the transformation of methane molecules and fragments of the coal aromatic structures. The results of the theoretical methods used for determining the evolution of the structure and, along with it, the reactivity of the system components in the conditions of changing characteristics of external factors confirm the substantial possibility and efficiency of the quantum-chemical modeling for identifying the peculiarities of the course of interphase interaction. The obtained results are consistent with the data of molecular spectroscopy, and the generalization of the information set is decisive for determining the driving forces of adsorption under the conditions of mechanical loading. A comprehensive approach to the systematic research allows obtaining fundamental data on the patterns of transformations of organic compounds and formation of their properties and will serve as a basis for the formation of a strategy for new-generation nanosynthesis processes and development of mechanochemistry.

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