

## STUDY OF INTERACTION OF INORGANIC GASES WITH THE SURFACE OF COBALT-CONTAINING POLYACRYLONITRILE IN THE PRESENCE OF WATER MOLECULES

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**Abstract** – Molecular modeling studies and quantum chemical calculations were applied for examining the possibility of interaction of inorganic gases with the surface of a cluster of cobalt-modified polyacrylonitrile (PAN), in the presence of water molecules in air. The simulation results showed the highest probability of interaction of cobalt-containing PAN with molecules of the following gases: sulfur dioxide, chlorine, and carbon dioxide. On the contrary, a low probability of interaction of cobalt-containing PAN in the presence of water molecules with molecules of methane and ammonia was revealed. The developed approach can be used for predicting gas-sensitive properties of gas sensors based on polyacrylonitrile and other materials.

*Keywords:* polyacrylonitrile, quantum chemical calculations, molecular modeling, formation energy, surface cluster, water molecule, gas molecule, gas sensors.