

Computer Analysis of the Adsorption Process on Metal-Organic Frameworks

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Adsorption processes are among the widespread applications of Metal-Organic Frameworks (MOFs), which found employment in: removal of harmful substances such as heavy metals from liquid and gaseous streams, storage and sequestration of gases such as carbon dioxide, methane and hydrogen as well as in separation and purification of gases and others. The performance and applicability of MOFs in mentioned processes among others depend on the high specific surface area and adsorption capacity. In this work adsorption properties of N₂, CO₂ and CH₄ on Basosiv M050 sample were determined by a volumetric method. The adsorbed volume values with respect to relative pressure were obtained for all of the gases. The nitrogen adsorption isotherms were studied at 77 K, and carbon dioxide and methane adsorption isotherms were studied at 273 K. The BET and Langmuir surface areas of the samples were determined using N₂ adsorption isotherms. Adsorption capacities for CO₂ and CH₄ are also calculated from their isotherm analysis. Additionally, the new numerical method with the unique fast multivariant identification procedure was employed for the analysis of the adsorption process on a specific type of a MOF sample, Basosiv M050. The proposed tools permit the gathering of a broader spectrum of information on the analyzed structure of MOFs materials and the adsorption processes taking place on their surface as compared with the others methods. Additionally the proposed method with unique numerical procedure can be a good starting point for the development of more advanced tools.

Biography:

Dr. Mirosław Kwiatkowski in 2004 obtained Ph.D. degree from the Faculty of Energy and Fuels at the AGH University of Science and Technology in Krakow (Poland), and in 2018 D.Sc. degree from the Faculty of Chemistry at the Wrocław University of Technology (Poland). His published work includes more than 45 papers in reputable international journals and 80 conference proceedings. Dr. hab. eng. Mirosław Kwiatkowski is the editor in chief of The International Journal of System Modeling and Simulation (United Arab Emirates), an associate editor of Micro & Nano Letters Journal (United Kingdom) and a member of the editorial board of international journals as well as a member of the organizing and scientific committees many international conferences.