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SYNTHESIS AND INVESTIGATION OF THE PHYSICAL-CHEMICAL PROPERTIES OF MOFS AS THE POTENTIAL MATERIALS FOR HYDROGEN STORAGE

Abstract. *MOFs (Metal-Organic Frameworks) materials* MOF-5 (*$Zn_4O(1,4$-benzenedicarboxylate)$_3$* и MOF-177 (*$Zn_4O(4,4',4''$-benzene-1,3,5-triyltribenzoate*) were synthesized by different methods such as *electrochemical, solvothermal, microwave-assisted.* Physical-chemical properties of the MOFs (crystal structure, thermal stability) were investigated.

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СИНТЕЗ И ИССЛЕДОВАНИЕ ФИЗИКО-ХИМИЧЕСКИХ СВОЙСТВ МОКС КАК ПОТЕНЦИАЛЬНЫХ МАТЕРИАЛОВ ДЛЯ АККУМУЛИРОВАНИЯ ВОДОРОДА

Аннотация. *МОКС (металл-органические каркасные структуры) типа MOF-5* (Zn$_4$O(1,4-бензендикарбоксилат)$_3$ и MOF-177 (Zn$_4$O(4,4',4"-бензен-1,3,5-триил трибензоат)$_2$ *синтезированы различными методами (сольвотермальным, электрохимическим, микроволновым). Исследованы физико-химические свойства (кристаллическая структура, термостойкость), полученных МОКС.*

The development goals and technological route plans of hydrogen storage in the United States and the European Union all point to high-safety and high-efficiency hydrogen storage based on materials, such as the MOFs.

MOF-5 samples were produced by solvothermal and electrochemical methods. Firstly, based on the XRD results of the solvent-thermal method synthesis of MOF-5 represented in the figure1, it is perfectly consistent with the reference [1]. The sharp peak values indicate high crystallinity, and the diffraction peaks at $2\theta=6.8°$, $9.6°$, $13.8°$, $15.4°$ correspond to the (200), (220), (400), (420) crystal planes of the cubic crystal system.
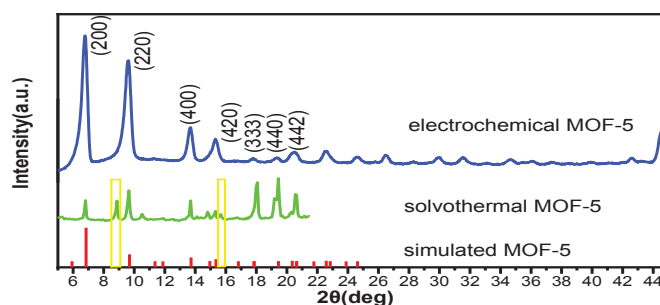

Fig. 1 - Powder X-ray diffraction patterns collected using Cu Kα radiation for MOF-5 produced by solvothermal and electrochemical methods

From the fig.1, peaks at $2\theta=8.9°$ and $15.8°$ appear, which are not present in standard cards. According to the literature [2] by the Yaghi team it is known that this is due to the fact that the samples were stored in the air for a certain time, leading to the partial decomposition of the sample due to the presence of water vapor.

Fig. 2 - Compare the XRD results of MOF-5(EL1) and MOF-5(EL2)	**Fig. 3 - The FT-IR results of MOF-5**
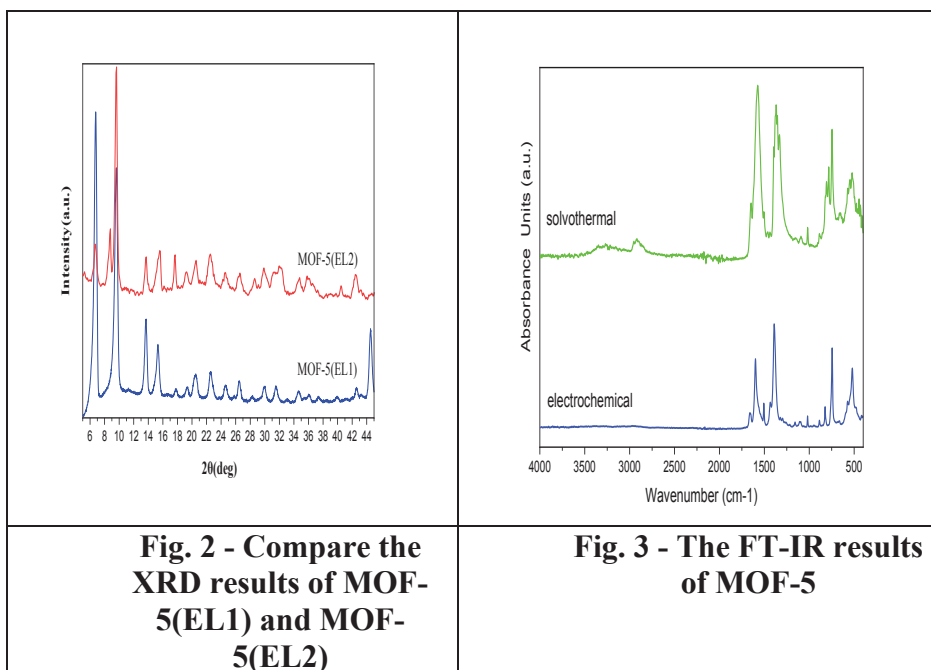
The XRD results comparison of two electrochemically prepared MOF-5 samples are shown in fig. 2. Firstly, it can be observed that the characteristic peaks of the two samples overlap significantly. Secondly, it is evident that MOF-5 (EL2) exhibits a peak at $2\theta=8.79$, similar to the solvothermal result. Under the same experimental conditions, we know that this peak is caused by residual solvent within the framework pores. Comparing these results with the BET surface area, it can be concluded that the difference in reaction current can affect the framework pore size, thereby impacting the temperature required for solvent evaporation within the pores. In other words, as the reaction current increases, the framework pore size decreases, resulting in a higher temperature requirement for drying the solvent within the pores.

The FT-IR spectrum of the MOF-5 prepared by solvothermal and electrochemical methods after vacuum degassing can be summarized into five regions [3].

a) In the first region (3600-3300 cm^{-1}), as revealed by the Bordiga team [4], the broad band centered at 3500 cm^{-1} associated with H-bonded $\nu_{(OH)}$ groups used for water adsorption almost disappears due to vacuum degassing at 393K. However, a weak absorption persists, indicative of the presence of carboxylic acid complexes $\nu_{(OH)}$ arising from the outer surface or internal defects (e.g. 1,4-benzenedicarboxylate vacancies). This weak feature of the band precisely reflects the very low defectivity of the studied material.

b) In the second region (3200-2850 cm^{-1}), again referring to the results of the Bordiga team [4], it is known that the sharp peak in this region is due to the aromatic and aliphatic ν(CH) modes of the benzene ring and DMF. Additionally, the second harmonic of the extremely intense ν(CO) vibration in this range may also have an impact on the peak value.

c)In the fourth region (1700-1300 cm^{-1}), the Raman double peak resulting from the asymmetric and symmetric modes of carboxylate salt is evident (two curves are observed near 1580 cm^{-1} and 1504 cm^{-1}, respectively). The peak near 1650 cm^{-1} is attributed to hydroxyl group, and the peak at 1388 cm^{-1} is due to the symmetric stretching vibration of the carboxylic acid group in the BDC molecule.

d)In the fifth region (1300-700 cm^{-1}), the peaks are assigned to skeletal modes and out-of-plane vibration modes of BDC, as well as to the stretching mode of benzene ring and C-H bonding vibration, which show strong peaks in the 800-750 cm^{-1} range.

Furthermore, the Yang team [5] suggests that regarding the differences between electrochemical and solvothermal methods, the peak shape of the electrochemical results at 1580 cm^{-1} is less sharp than that of the solvothermal results due to the template effect of the ionic liquid.

According to the summary from the literature, new spectral bands appear at 3610, 3200, 1300, 1230, and 660 cm^{-1} after storing for a period of time in humid conditions. These spectral bands are related to the collapse of MOF-5 structure due to the change of carboxyl groups and zinc oxide in the environment. The peaks at around 660 cm^{-1}, 1300 cm^{-1}, 3200, and 3610 cm^{-1} can be seen in the MOF-5 results prepared by the solvent thermal method. It is concluded that this sample has partially collapsed due to improper storage.

Thermal stability of MOF-5 was studied by TGA (fig. 4). From the curve, it can be seen that there are three obvious stages of weight loss in the temperature range from 73.6 ^{o}C to 600 ^{o}C. The first stage, within the temperature range of 73.6-216 ^{o}C, the mass loss is 2.43%, that is attributed to solvent mass loss. The second stage, within the temperature range of 216-340 ^{o}C, the mass loss is 21.59%, and 293 ^{o}C has a maximum mass loss rate, that is attributed to the guest organic molecule DMF release in MOF-5. The third stage, within the temperature 340-600 ^{o}C, the mass loss is 32.4%, it is a maximum mass loss rate, it marks the collapse of the frameworks structure. After decomposition, the residual mass is 43.58%, which is close to the theoretical decomposition residue 42.42%. So it shown that 340 ^{o}C is the maximum temperature for remaining the crystal MOF-5 stable, and the purity was high.
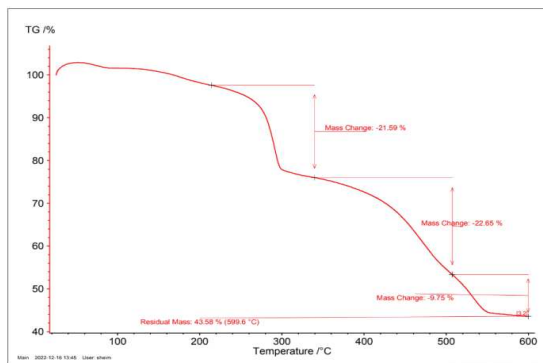
Fig. 4 - TGA of the crystal MOF-5 (solvothermal method) under nitrogen atmosphere
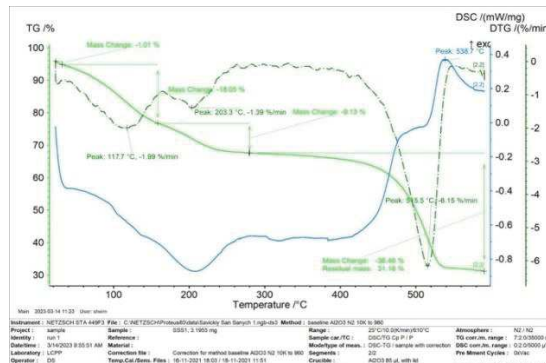

Fig. 5 - TGA of the crystal MOF-5(solvothermal method) under nitrogen atmosphere

The TG-DSC curve of MOF-5 prepared by electrochemical synthesis exhibited three weight losses, with the first two occurring in the temperature range of 30-280°C, accounting for 27.18% of the total weight loss, which could be attributed to the release of solvent molecules from the pores of MOF-5, including water, DMF. The third weight loss occurred in the temperature range of 380-538.7 °C, with the largest weight loss of 36.46%, mainly due to the destruction of the MOF-5 framework and decomposition at high temperature. After 538.7 °C, the weight remained almost unchanged, indicating that only ZnO was left as the final product. Based on the TG-DSC characterization, the thermal stability temperature range of electrochemically synthesized MOF-5 is between 280-380 °C.
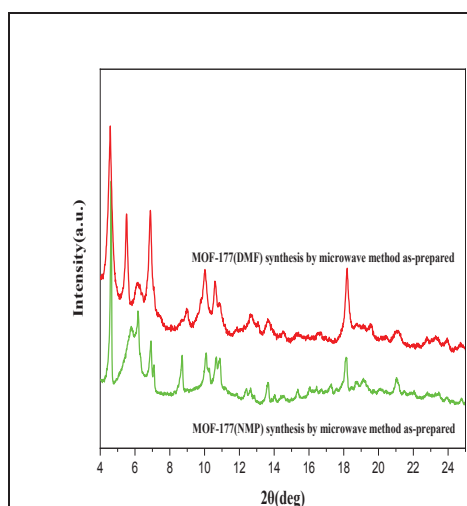

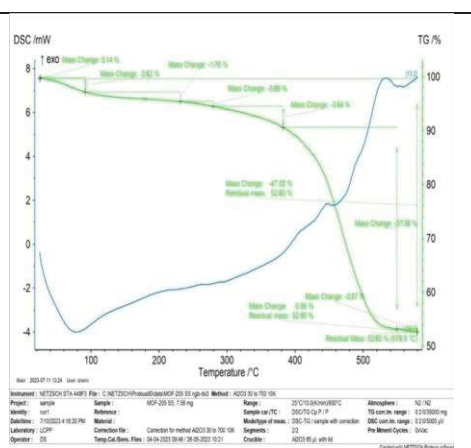| **Fig. 6 - The XRD results of MOF-177 by microwave method as-prepared**	**Fig. 7- The TGA results of MOF-177 by solvothermal method and microwave method after vacuum drying at 200 °C for 15h**

The conclusion drawn from XRD analysis of MOF-205 indicates that an improved microwave synthesis method was employed to prepare MOF-177. Two different organic solvents, DMF and NMP, were respectively used to dissolve the reactants, resulting in the formation of MOF-177 (DMF) and MOF-177 (NMP). The results obtained from the graph clearly demonstrate a significant level of crystallinity. This confirms the notion that improving the crystallinity of the microwave synthesis method is indeed the correct direction.

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РАСЧЕТ КОРРОЗИОННОГО СОСТОЯНИЯ ЭЛЕМЕНТОВ ЗАЗЕМЛИТЕЛЕЙ

Аннотация. В статье рассматривается применение действующего метода оценки состояния заземляющих устройств. Определение потери массы заземляющих электродов и изменение сопротивления растекания тока, а также общая длина и масса заземляющих устройств. Приводятся пример расчета коррозионного состояния элементов заземлителей.