

Study of Adsorption–Desorption Isotherms and Pore Structure of an Inorganic Polymer Sorbent Derived from Local Clay

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Abstract In this article, the porous structure of an inorganic aluminosilicate polymer sorbent, synthesized from local clay using the sol-gel method, was investigated via low-temperature nitrogen adsorption-desorption at 77 K. The specific surface area was determined using the BET method, while the pore size distribution was calculated based on Density Functional Theory (DFT). The isotherm resembles a Type IV classification according to IUPAC standards, characterized by a wide hysteresis loop and low-pressure hysteresis. The material exhibited a specific surface area of $\approx 32 \text{ m}^2/\text{g}$ and a total pore volume of $0.0186 \text{ cm}^3/\text{g}$. The DFT distribution is bimodal in nature, showing primary pore widths of $\approx 1.9 \text{ nm}$ (supermicropores) and $\approx 3.6 \text{ nm}$ (mesopores). The pore volumes determined via DFT and adsorption data are consistent with each other.

Keywords Inorganic polymer, Aluminosilicate sorbent, Nitrogen adsorption, BET, DFT, Pore structure, Pore distribution, Hysteresis, Specific surface area

1. Introduction

The specific surface characteristics, porosity parameters, and specific pore volume of inorganic polymer sorbents derived from local raw materials are among the key factors determining their sorption properties [1]. While pore size and pore-size distribution govern the diffusion rate of substances within the porous structure, analysis of the specific pore volume is essential for evaluating the physicochemical properties of inorganic polymer sorbents [2].

To prepare the inorganic polymer sorbent, local clay was first treated with 1 M sulfuric acid at a solid-to-liquid ratio of 1:5 at room temperature for 2 h. The acid-treated clay was then washed with distilled water until neutral conditions were reached, followed by treatment with 3 M NaOH solution at a ratio of 1:3 at room temperature for 4 h [3]. The textural properties of the pristine clay and the resulting sorbent were investigated from nitrogen (N_2) adsorption–desorption isotherms measured at 77 K. Prior to analysis, a 0.0882 g sample was degassed under vacuum at 120°C for

2 h 56 min. Adsorption and desorption isotherms were recorded over the relative-pressure range $P/P_0 = 0.03\text{--}0.99$.

The specific surface area (S_{BET}) was calculated using the Brunauer–Emmett–Teller (BET) equation from adsorption-branch data in the $P/P_0 = 0.05\text{--}0.30$ range [4]:

$$P / [V(P_0 - P)] = 1 / (V_m C) + [(C - 1) / (V_m C)] (P/P_0), \quad (1)$$

where V is the volume of nitrogen adsorbed at the relative pressure P/P_0 , $\text{cm}^3 \text{ g}^{-1}$ (STP); V_m is the monolayer capacity, $\text{cm}^3 \text{ g}^{-1}$ (STP); and C is the BET constant related to the interaction energy between the adsorbate and the adsorbent. Taking the molecular cross-sectional area of nitrogen as 0.162 nm^2 , the specific surface area is calculated as follows:

$$S_{\text{BET}} = 4,353 V_m. \quad (2)$$

From the slope (s) and intercept (i) of the linear BET plot (Figure 3), the monolayer capacity and BET constant were determined as follows:

$$W_m = 1/(s + i), \quad C = s/i + 1. \quad (3)$$

The specific surface area was calculated using the cross-sectional area of the nitrogen molecule ($A_{\text{cs}} = 0.162 \text{ nm}^2$):

$$S_{\text{BET}} = W_m N_A A_{\text{cs}} / M, \quad (4)$$

where N_A is Avogadro's constant, $6.022 \cdot 10^{23} \text{ mol}^{-1}$, and M is the molar mass of nitrogen, $28.013 \text{ g mol}^{-1}$.

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The total pore volume (V_{total}) was determined by converting the volume of nitrogen adsorbed at the relative pressure $P/P_0 = 0.99$ to the equivalent volume of liquid nitrogen:

$$V_{\text{total}} = 0.001547 \cdot V_{0.99}, \quad (5)$$

where 0.001547 is the conversion factor from the volume of gaseous nitrogen at STP to the volume of liquid nitrogen at 77 K. The average pore diameter was calculated assuming a cylindrical-pore model:

$$D = 4V_{\text{total}}/S_{\text{BET}} \quad (6)$$

The pore-size distribution was determined by density functional theory (DFT) from the adsorption branch of the N_2 isotherm at 77 K using an NLDFIT model for cylindrical/slit-shaped pores on the surface of the inorganic polymer sorbent [1,2]. The distribution was expressed as integral pore volume (V) and differential pore volume (dV/dr) as functions of the pore half-width.

2. Results and Discussion

The nitrogen adsorption–desorption isotherms of the inorganic polymer sorbent at 77 K are presented in Figure 1. The adsorption branch does not exhibit a sharp increase in the low-relative-pressure region ($P/P_0 < 0.1$); thus, no distinct stage characteristic of volumetric filling of micropores is observed. As the relative pressure increases, the adsorbed nitrogen volume increases almost linearly and approaches saturation at approximately $8 \text{ cm}^3 \text{ g}^{-1}$ at $P/P_0 \approx 0.9$. The maximum adsorption value ($\approx 8.1 \text{ cm}^3 \text{ g}^{-1}$) is relatively low, indicating limited overall porosity of the material.

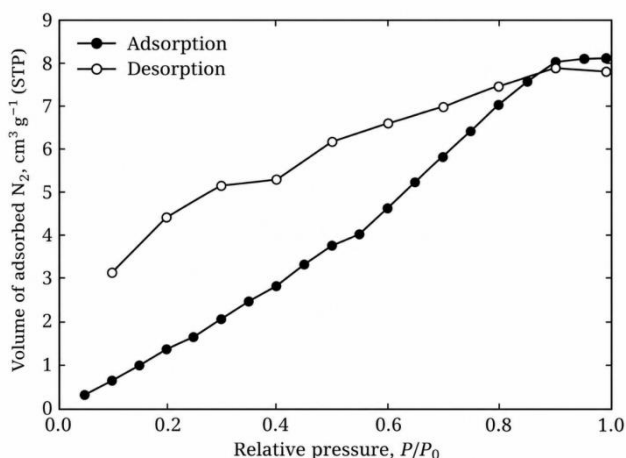


Figure 1. Nitrogen adsorption (●) and desorption (○) isotherms of the inorganic polymer sorbent at 77 K

The saturation uptake at high relative pressures and the presence of a broad hysteresis loop make the isotherm close to Type IV according to the IUPAC classification [4]. The hysteresis loop extends over $P/P_0 \approx 0.1$ – 0.9 , and the desorption branch does not rejoin the adsorption branch even at low pressures (low-pressure hysteresis). This behavior is generally attributed to incomplete equilibration caused by

slow diffusion of nitrogen molecules through narrow pore entrances, partial irreversible retention of nitrogen within the pores, or deformation of the material framework during adsorption [4].

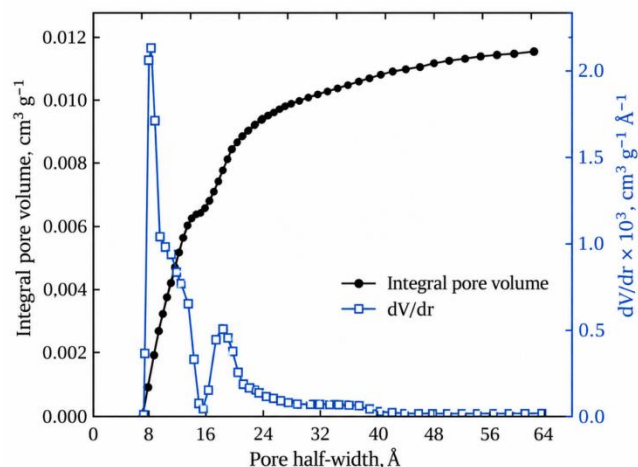


Figure 2. Integral (●) and differential (□) pore-volume distributions of the inorganic polymer sorbent determined by DFT

The pore-size distribution determined by DFT is shown in Figure 2. The differential distribution curve exhibits a bimodal character: the principal and most intense peak corresponds to a pore half-width of approximately 9.5 Å (pore width $\approx 1.9 \text{ nm}$), whereas the second, less intense peak occurs at approximately 18 Å ($\approx 3.6 \text{ nm}$). These results indicate that supermicropores and small mesopores predominate in the material.

The integral pore-volume curve increases sharply over the pore half-width range of 8 – 20 Å , within which approximately 70% of the total DFT pore volume is accumulated. The contribution of pores with half-widths greater than 40 Å (pore width $> 8 \text{ nm}$) is very small, and the curve becomes nearly horizontal. The integral pore volume determined by DFT is close to the total pore volume obtained at $P/P_0 = 0.99$, demonstrating good agreement between the two approaches.

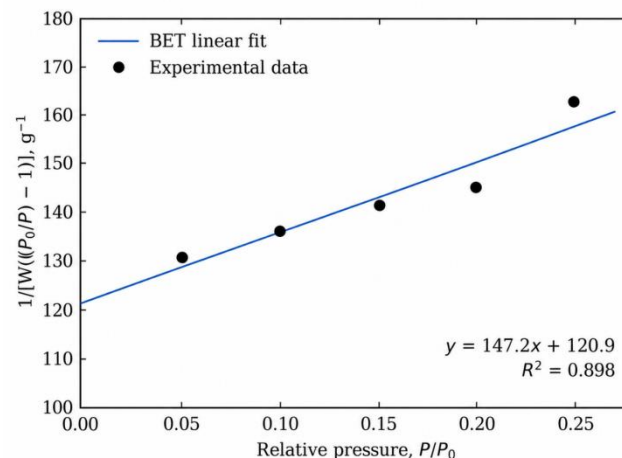


Figure 3. Multipoint BET plot for the inorganic polymer sorbent

The multipoint BET plot is presented in Figure 3, and the calculated parameters are summarized in Table 1. Within the selected range, the experimental points are distributed around a straight line ($R^2 = 0.898$); however, the point at $P/P_0 = 0.25$ deviates upward from the linear trend. Such a deviation indicates that the upper limit of applicability of the BET equation is being approached.

The calculated specific surface area was approximately $32 \text{ m}^2 \text{ g}^{-1}$. The relatively low BET constant ($C \approx 4.2$) indicates weak interactions between the adsorbate and the adsorbent surface, as well as substantial overlap between monolayer formation and multilayer adsorption. Therefore, the S_{BET} value should be regarded as an approximate estimate [4]. This result is consistent with the nitrogen adsorption isotherm and DFT analysis and confirms the limited porosity of the material.

Table 1. BET analysis results, including linear fitting parameters, monolayer capacity, BET constant, and specific surface area of the material

Parameter	Value
Relative pressure range, P/P_0	0.05–0.25
Number of points	5
Slope of the straight line, s, g^{-1}	147.2
Intercept, i, g^{-1}	120.9
Coefficient of determination, R^2	0.898
Monolayer capacity, $W_m, \text{g g}^{-1}$	$3.73 \cdot 10^{-3}$
BET constant, C	4.2
Specific surface area, $S_{\text{BET}}, \text{m}^2 \text{ g}^{-1}$	≈ 32

3. Conclusions

Mesopores in the 15–20 nm range were retained most prominently, which is considered an optimal range for ion exchange and diffusion. The modification preserved the overall pore volume while promoting the formation of active sites for ion exchange. The predominance of mesopores in the 10–20 nm range provides a scientific basis for the high sorption performance of the inorganic polymer sorbent.

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