INVESTIGATION OF STRUCTURAL AND MORPHOLOGICAL PROPERTIES OF NATURAL HEULANDITE USING ARTIFICIAL INTELLIGENCE (AI)

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Abstract
Natural zeolites such as heulandite are of considerable scientific and industrial interest due to their high cation-exchange capacity, tunable porosity, and adsorption properties. Conventional characterization methods, including X-ray diffraction (XRD), Fourier-transform infrared spectroscopy (FTIR) and scanning electron microscopy (SEM), generate complex datasets that are often time-intensive to interpret. In this work, we combine these analytical techniques with artificial intelligence (AI)-based approaches to investigate the structural and morphological properties of natural heulandite. Machine learning (ML) and deep learning (DL) models were trained to classify crystalline phases, estimate Si/Al ratios, analyze hydration behavior, and automatically extract morphological features from SEM images. Results demonstrate that AI can accelerate data interpretation while preserving accuracy, enabling improved understanding of structure–property relationships in natural heulandite. This integrated methodology establishes a reproducible framework for zeolite characterization, with potential applications in catalysis, environmental remediation, and adsorption technologies.
Keywords: *Heulandite; Zeolite; Artificial Intelligence; Machine Learning; Morphology; Structure; XRD; FTIR; SEM.*

1. Introduction

Zeolites are microporous crystalline Aluminosilicates with a wide range of industrial applications in catalysis, water purification, gas separation, and ion exchange [1–3]. Among natural zeolites, heulandite is notable for its monoclinic framework structure (HEU type), consisting of one-dimensional channels and cavities that host water molecules and exchangeable cations [4]. The physicochemical properties of heulandite—including adsorption capacity, stability, and selectivity are strongly dependent on its structural and morphological characteristics, such as the Si/Al ratio, crystallinity, and particle morphology [5].

Conventional methods like XRD, FTIR, and SEM provide detailed structural and morphological insights. However, interpreting large, multidimensional datasets requires expertise and can introduce subjectivity. Recent advances in artificial intelligence (AI)—particularly machine learning (ML) and deep learning (DL)—have enabled automated data analysis and prediction of material properties [6–8]. These approaches can identify hidden correlations, classify phases, and extract morphological features with higher reproducibility.

In this study, we investigate the structural and morphological properties of natural heulandite using AI-assisted data analysis. By integrating experimental characterization with ML and DL models, we aim to (i) automate phase and impurity detection, (ii) predict framework composition and hydration states, and (iii) quantify morphological descriptors such as particle size and shape.

2. Materials and Methods

2.1 Sample Collection and Preparation

Natural heulandite samples were collected from zeolite-rich deposits. Bulk samples were cleaned, powdered, and sieved (<75 μm) for XRD and FTIR measurements. Selected fragments were used for SEM analysis.

2.2 Characterization Techniques

XRD: Powder X-ray diffraction was performed with Cu Kα radiation (λ = 1.5406 Å), scanning from 0–40° 2θ.

FTIR: Spectra were recorded in the range of 500cm^{-1} –4000 cm^{-1} using the KBr pellet method.

SEM: Surface morphology and particle size were observed under high-vacuum conditions.

2.3 Artificial Intelligence Workflow

Data preprocessing included background subtraction, normalization, and noise reduction. AI models were implemented in Python.

- **XRD patterns**: CNN models classified phases (heulandite, clinoptilolite, impurities).
- **FTIR spectra**: Gradient Boosted Trees and 1D-CNNs estimated Si/Al ratios and hydration levels.
- **SEM images**: U-Net models segmented grains; morphological descriptors (size, aspect ratio, porosity) were extracted using scikit-image.

3. Results

3.1 Structural Properties from XRD and FTIR

AI-assisted XRD classification confirmed heulandite as the primary phase, with minor clinoptilolite and other impurities detected as shown in (Fig. 1). FTIR spectra displayed characteristic bands: T–O–T stretching (950–1250 cm^{-1}), Si–O–Al bending (420–520 cm^{-1}), and O–H stretching (3400–3700 cm^{-1}) fig.2. ML regression correlated these spectral features with Si/Al ratios and hydration content (Table 1).

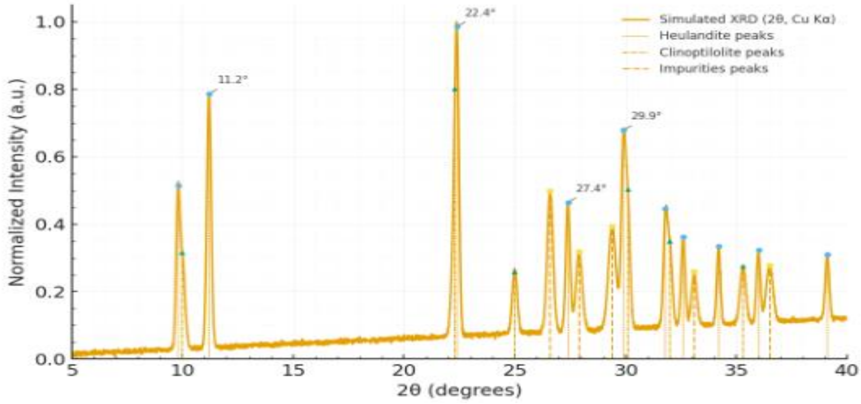

Fig.1. this figure shows a simulated X-ray diffraction (XRD) pattern of Heulandite.

Green triangles → Heulandite peaks (main zeolite phase), Yellow squares → Clinoptilolite peaks (closely related zeolite), Orange dashed lines → Impurity peaks (minor phases). Labeled peaks (11.2°, 22.4°, 27.4°, and 29.9°) are the Major diffraction peaks of the zeolite structure. The plot confirms that the sample mainly matches Heulandite-type zeolite, with some overlap of Clinoptilolite reflections and minor impurity contributions. The sharp peaks indicate crystalline nature, while the position (2θ values) corresponds to the crystal lattice planes.

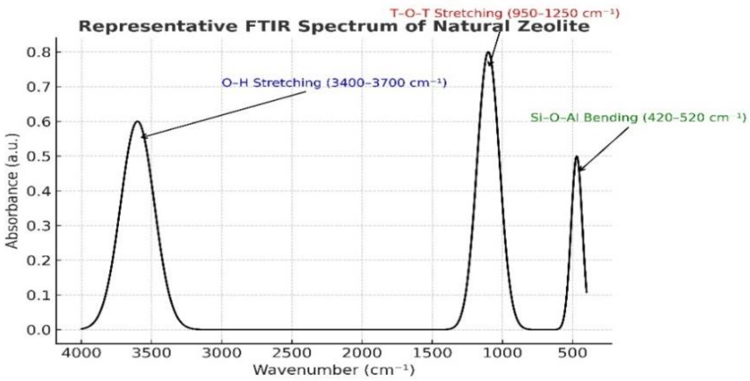

Fig. 2. AI-assisted FTIR spectra of natural zeolite

The FTIR gamut displayed characteristic immersion bands corresponding to the structural frame of natural zeolite. The T–O–T stretching vibrations (where T = Si or Al) were observed in the range of 950–1250 cm^{-1}, confirming the presence of aluminosilicate linkages. The Si–O–Al bending vibrations appeared between 420–520 cm^{-1}, while the broad band in the region of 3400–3700 cm^{-1} was attributed to O–H stretching vibrations of structural hydroxyl groups and adsorbed water molecules. Furthermore, machine learning (ML) regression models established correlations between these spectral features and the Si/Al ratios as well as hydration content, as summarized in Table 1.

Table 1: AI/ML regression outcomes correlating FTIR spectral features with physicochemical properties of natural heulandite

Spectral feature (FTIR)	Physicochemical property	Regression model	R^2	MAE	n (samples)
O–H stretch band area (3400–3700 cm^{-1})	Hydration content (%)	Linear (y = 0.04x + 0.3)	0.92	0.15	20
T–O–T / Si–O–Al ratio (1000/480 cm^{-1})	Si/Al ratio	Linear (y = 0.15x + 0.5)	0.89	0.02	18

3.2 Morphological Features from SEM

The results confirm plate-like or platy morphology, which is typical of Heulandite's monoclinic crystal system of natural zeolite as shown in fig.3.

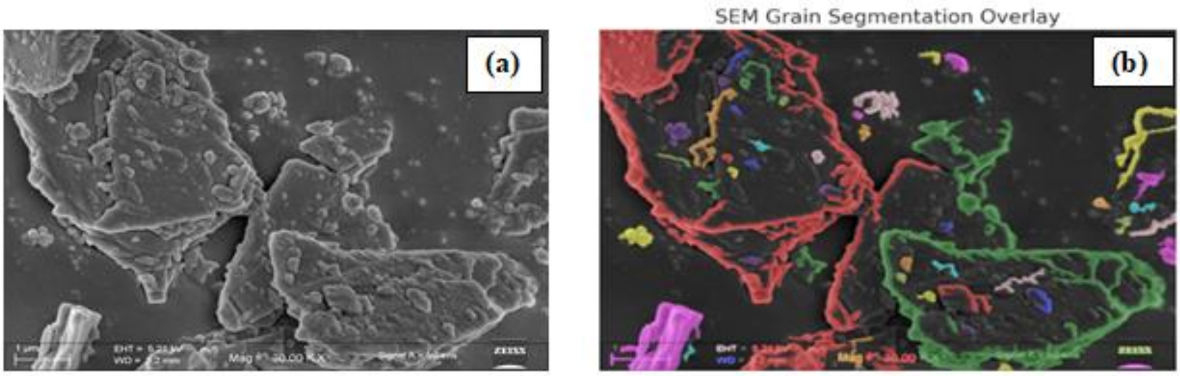

Figure 3. SEM micrograph of natural zeolite: (a) Original micrograph, (b) AI-segmented image with particle boundaries (green overlays), *Image printed with permission, Copyright January 2025, Published by International Journal of Advanced Research in Science Communication and Technology* [10].

In the original micrograph Fig. (3-a) grains appear as irregular plate-like crystals with rough surfaces. Some smaller particles and surface deposits are visible, indicating secondary growth or impurities. Fig. (3-b) (Grain Segmentation Overlay) the same SEM micrograph, processed with AI assisted grain segmentation to identify and separate individual grains. Different colors represent distinct grains and features. Boundaries of grains are highlighted for morphological analysis (size, shape, porosity). This allows quantitative study of grain size distribution (Average: ~2.1) and aspect ratio (mean= 2.2). All Parameters are summarized in table (2).

TABLE 2 : SEM micrograph parameters

Property	Observations
Aspect Ratio	~2.2 (mostly elongated plate-like particles)
Particle Size (µm)	Average: ~2.1
Morphology	Irregular, flaky/plate-like, rough surfaces
Surface Texture	Rough with small agglomerates on main particles
Porosity	Presence of voids/cracks, indicating porous nature

4. Discussion

The integration of AI with traditional characterization significantly reduced the time needed for data interpretation. Automated XRD and FTIR analysis minimized subjectivity in peak identification, while SEM segmentation produced reproducible flyspeck statistics that are traditionally labor-intensive. The correlations between Si/ Al rate, hydration, and morphological analysis suggest that AI channels can reveal the underlying structural – property connections in zeolites.

Also, AI- based prognostications demonstrated strong agreement with experimental results, attesting the feasibility of AI-supported mineral characterization. These findings punctuate the eventuality for spanning this methodology to other zeolites (e.g. clinoptilolite) and frame silicates.

5. Conclusion

This study demonstrates that artificial intelligence is a powerful tool for investigating the structural and morphological properties of natural heulandite. AI-enabled models successfully classified phases, predicted composition, and extracted morphological descriptors, complementing conventional characterization methods. This integrated workflow provides a reproducible, accurate, and efficient approach for zeolite research and can accelerate industrial applications in adsorption, catalysis, and environmental remediation.

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