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ELEMENTS TOOLKIT



ZEOLITE SCIENCE: KEY TERMS

Adsorption Adsorption is a physical-chemical process where gas or liquid molecules (the adsorbate) interact with the extensive internal and/or external surfaces of a zeolite (the adsorbent) without changing its crystal structure. This phenomenon in zeolites is primarily driven by physisorption (weak van der Waals or electrostatic forces) and can facilitate a highly precise molecular sieving mechanism.

Adsorption isotherm An adsorption isotherm illustrates how the amount of an adsorbate (the substance being adsorbed) on a solid changes with the concentration of that substance in the liquid or gas phase at a constant temperature. It can be used to describe the equilibrium between the adsorbate and the adsorbent and can elucidate adsorption mechanisms.

Alkalinity The capacity of water to neutralize acids, primarily due to the presence of bicarbonate, carbonate, and hydroxide ions.

Amorphous A material that lacks a long-range, ordered crystal structure such as glass.

Authigenic mineral A mineral that forms in situ within sediments or rocks via precipitation or recrystallization during or after deposition through chemical or biological processes, rather than being transported from elsewhere.

Bentonite A clay-rich rock consisting predominantly of smectite. It forms mainly from alteration of pyroclastic and/or volcanoclastic rocks.

Bonding strength The measure of the force or energy required to break the bond between atoms and molecules.

Cage A three-dimensional cavity with a closed form within a zeolite framework that can trap, store, or selectively adsorb molecules and ions based on their size, charge, and shape.

Cation-exchange capacity (CEC) A measure of the ability of zeolites to hold and exchange positively charged ions (cations) into their pores.

Cavity An internal pore (or void) within a zeolite framework that provides a volume for the adsorption, diffusion, and exchange of ions and molecules.

Channel In a zeolite structure, a channel is defined as a continuous, one-dimensional tunnel confined by interconnected rings of tetrahedra (TO₄, where T is usually Si or Al) that allows the diffusion and selective transport of molecules and ions between cavities and the external surface. Systems of interconnected channel pathways can be one-, two-, or three-dimensional within the same structure.

Charge density The concentration of negative charge within the zeolite framework, determined by the distribution of Al³⁺ ions and balanced by exchangeable cations. It strongly influences the zeolite's ion-exchange capacity, adsorption selectivity, and affinity for polar molecules.

Colloid A system of finely divided particles, ~1 to 1,000 nm in size, dispersed within a continuous medium in a manner that prevents them from being filtered easily or settling rapidly.

Concrete Composite material of (Portland) cement and fine and coarse aggregates that flows when first mixed with water and that then sets and hardens to a solid, rock-like material.

C – S – A – F – H Cement shorthand notation referring to the main chemical components: C = CaO, S = SiO₂, A = Al₂O₃, F = Fe₂O₃, H = H₂O.

Denaturation The structural alteration of a protein or other biomolecule by breaking weak non-covalent bonds, caused by physical or chemical factors, resulting in the loss of its native structure and biological activity.

Diagenesis The physical, chemical, and biological processes that alter sediments after deposition, leading to their transformation into sedimentary rock.

Dimensionality Describes the connectivity of channel systems (e.g., one-, two-, or three-dimensional) in zeolite structures.

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Diatomaceous earth Naturally occurring, soft, siliceous sedimentary material composed of the fossilized remains of microscopic aquatic algae called diatoms. The cell walls of diatoms are made primarily of amorphous silica (SiO_2).

Electrostatic interaction The attractive or repulsive force between electrically charged particles or surfaces that plays a key role in adsorption, ion exchange, and molecular binding.

External CEC The cation-exchange capacity associated with the external surface of a zeolite, representing the amount of exchangeable cations available outside the internal pore structure.

Extra-framework cation A positively charged ion located within the pores (or cavities) of a zeolite where it balances the framework's negative charge and can participate in cation exchange.

Flocculation The process by which suspended particles (colloids) aggregate into larger clusters (flocs), making them easier to settle or separate from a liquid.

Framework The three-dimensional network of interconnected atoms that forms the fundamental structure of a material. In natural zeolites, the framework consists of SiO_4 and AlO_4 tetrahedra, linked through oxygen atoms, creating cavities in the form of channels or cages.

Free diameters "Free diameters" refer to the effective, net dimensions of the pore openings through which guest molecules can diffuse. In zeolites, the free diameters of the cavities determine molecular accessibility and size selectivity. They are determined by: 1) measuring the distance between opposite oxygen atoms that form the ring of tetrahedra confining a cavity; and 2) subtracting the conventional van der Waals radius of oxygen, 1.35 Å. For elliptical pores, usually the shortest and the longest free diameters are reported.

High-density amorphous phase An amorphous material with a compact, disordered atomic structure and a higher density than its low-density amorphous counterpart, resulting from closer atomic packing.

Hydration energy The energy released when an ion interacts with H_2O molecules during hydration. It influences ion mobility, stability in solution, and ion-exchange behavior in materials such as zeolites.

Hydrophilic Having a strong affinity for water, allowing a material or surface to readily attract, interact with, or be wetted by H_2O molecules.

Hydrophobic Having a low affinity for water, causing a material or surface to repel water and preferentially interact with nonpolar substances.

Hydrothermal Processes, systems, or conditions involving the combined action of water (hydro-) and heat (thermal).

Hygrothermal Combined effects of moisture (hygro-) and temperature (thermal) on a material, structure, or environment.

Isotypic Referring to compounds that share the same framework structure but differ in chemical composition, through substitution of one or more constituent elements.

Low-density amorphous phase An amorphous material with a relatively open, disordered atomic structure and lower density than its crystalline or high-density amorphous counterpart. In silica-based materials, LDA materials are characterized by a porous, low-density network.

Metamorphism Metamorphism is the geological process where pre-existing rocks (protoliths) are transformed by heat, pressure, and fluids. This process fundamentally alters the rock's mineral composition and texture in the solid state without melting it.

Micelle A spherical aggregate of surfactant molecules formed in solution, with hydrophobic tails oriented inward and hydrophilic heads facing outward, enabling the encapsulation of nonpolar substances.

Molecular sieve A porous material with internal pores that selectively adsorb or separate molecules based on their size and shape.

Mortar Composite material comprising (Portland) cement, sand, and water that is mainly used to bind building blocks.

Natural pozzolan Any natural material, e.g., volcanic tuff, pumice, diatomaceous earth, that exhibits cementitious properties when combined with lime.

Negative thermal expansion Property of a material that causes its structural dimensions (length, area, or volume) to decrease as its temperature increases.

Palagonitization The alteration of basaltic volcanic glass, commonly through interaction with water, into palagonitized glass—a yellowish-brown, hydrated material composed of altered glass and secondary minerals.

Polarity The unequal distribution of electrical charge within a molecule or bond, resulting in regions of partial positive and negative charge that influence intermolecular interactions and adsorption.

Polymerization The chemical process in which small molecules (monomers) join to form larger molecules known as polymers.

Pore An internal cavity (or void) within a zeolite framework that provides volume for the adsorption, diffusion, and exchange of ions and molecules. For zeolitic structures, "pore" and "cavity" are synonyms.

Portland cement A material composed of ground Portland clinker and minor additions of calcium sulfates that sets and hardens when combined with water and that can be used to bind materials together.

Portland clinker Nodular material produced by high-temperature sintering (1450°C) of clays and limestone in a rotary kiln. The clinker is mainly composed of high-temperature calcium silicates (C_3S and C_2S), aluminate (C_3A), and ferrite (C_4AF). For notation, see "C-S-A-F-H."

Pozzolan A siliceous or siliceous-aluminous material that reacts with $\text{Ca}(\text{OH})_2$ or a $\text{Ca}(\text{OH})_2$ -producing material in the presence of water to form cementitious compounds with binding properties.

Pyroclastic Referring to fragmented volcanic material, such as ash, pumice, or rock fragments, produced and ejected during explosive volcanic eruptions.

Rigid unit mode A low-energy structural deformation in which predominantly rigid polyhedral units (e.g., SiO_4 or AlO_4 tetrahedra) rotate or tilt without significant distortion of their internal bond lengths or angles.

Selectivity The ability of a material (zeolite) to preferentially adsorb, separate, or exchange one molecule or ion over others based on differences in size, shape, charge, or chemical affinity.

Si/Al The molar ratio of silicon to aluminum atoms in a zeolite framework, which influences its charge density, hydrophilicity, acidity, thermal stability, and ion-exchange properties.

Sorption The general process by which a substance is taken up by another material through adsorption, absorption, or both. Cation exchange is an example of a sorption process.

Supplementary cementitious materials (SCM) Siliceous or siliceous-aluminous materials added to cement or concrete to partially replace Portland cement, improving mechanical properties, durability, and sustainability through pozzolanic or (latent) hydraulic reactions.

Surfactant A surface-active compound that reduces surface or interfacial tension by accumulating at interfaces, typically containing both hydrophilic and hydrophobic groups.

Surfactant modified zeolite (SMZ) A zeolite whose surface has been coated or functionalized with surfactant molecules to enhance its sorption capacity and selectivity, particularly for organic contaminants and anions.

Tectosilicate A class of silicate minerals with a three-dimensional framework of interconnected SiO_4 tetrahedra, in which each oxygen atom is shared between adjacent tetrahedra. Zeolites, quartz, feldspathoids, and feldspars are common examples.

Topology In a zeolitic structure, topology defines the fundamental, three-dimensional connectivity of the crystalline framework, independent of its specific chemical composition (such as the Si/Al ratio), constituent atoms, or slight variations in unit-cell dimensions. Essentially, it serves as the "geometric blueprint" or graph of the framework, mapping exactly how tetrahedral nodes are linked together in space to form rings, channels, and cages.

Vitric tuff A pyroclastic rock composed predominantly of volcanic glass fragments (glass shards) produced during explosive volcanic eruptions.

Void An internal space within the zeolite framework, in the form of channels or cages that accommodates molecules and ions and facilitates adsorption, diffusion, and ion exchange. For zeolitic structures, "void," "pore," and "cavity" are synonymous.