Electronic Supplementary Material (ESI) for RSC Advances.

Supplementary Information

Physicochemical characterization to assess Ni and Zn incorporation into zeotype SAPO-34 nanoparticles synthesized with different mixing methods through ultrasound-promoted crystallization

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Table S1. Characterization techniques of the synthesized samples.

Subject to measure	Measurement method	Instrument	Remarks
Crystal phase, crystallinity, and crystallite size	XRD (Powder X-ray diffraction)	Equinox 3000	operated at 40 kV and 30 mA with a Cu Kα X-ray source (λ=1.541874Å) at room temperature.
Crystal size and morphology	SEM (Scanning electron microscopy)	VEGA\\ TESCAN	equipped with an energy dispersive X-ray spectrometer.
	TEM (Transmission electron microscopy)	Philips, CM30	operated at 300 kV.
Elemental analysis	EDX (Energy dispersive X-ray)	VEGA\\ TESCAN	
Coordination state of metal	UV-Vis DRS (Ultraviolet visible-Diffuse reflectance spectroscopy)	Avantes, AvaSpec-ULS3648	$BaSO_4$ was used as the reflectance standard.
Framework structures, active sites, and adsorbed species	FTIR (Fourier transform infrared spectroscopy)	Thermo Scientific, Nicolet iS10	operated at room temperature with KBr pellet.
Changes in weight of material	TGA (Thermo-gravimetric analysis)	Shimadzu, TGA-50	recorded under air with a heating rate of 20°C/min.

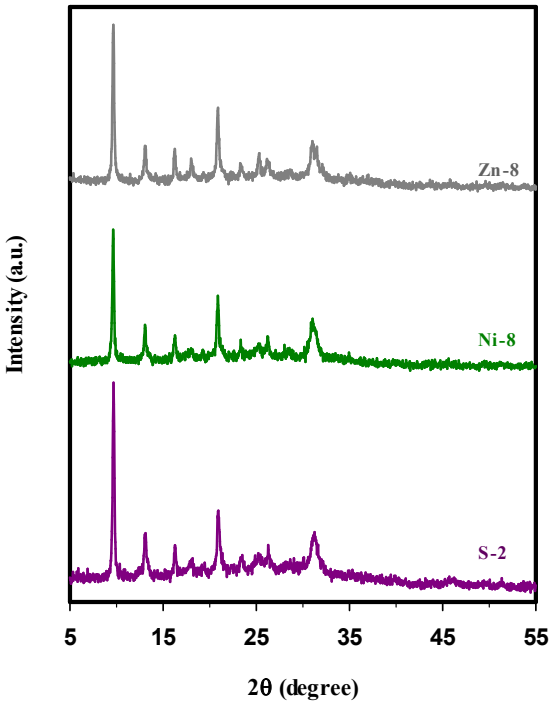

Fig. S1. XRD patterns of parent (S-2), nickel (Ni-8), and zinc (Zn-8) containing SAPO-34 samples synthesized hydrothermally for 5h.

Unit cell calculation

In an attempt to calculate the unit cell parameters, the type of crystal system in a sample of interest should be initially specified and thereafter lattice parameters are determined according to the type of crystal structure. A detailed investigation on the SAPO-34 lattice parameters (*a, b, c, α, β, and* γ) reveals that SAPO-34 is made up of a unit cell with the hexagonal crystal structure. It is known that [1] in hexagonal crystal system, a unit cell is given by a rectangular prism with a vertical axis, *c*, perpendicular to a rhombus-shaped base and the equal edges of which are at 60° and 120° with respect to each other. The length of the rhombus edge is designated by two equal vectors, *a* and *b*, (i.e. $a = b \neq c$, $\alpha = \beta = 90°, \gamma = 120°$), as shown in Fig. S2.

The unit cell parameters are measured by analysis of the powder diffraction data, according to the following equation based on the hexagonal crystal system [1]:

$$\frac{1}{d^2} = \frac{4\,sin^2\theta}{\lambda^2} = \frac{4}{3}\left(\frac{h^2 + hk + k^2}{a^2}\right) + \frac{l^2}{c^2}$$

where *a* and *c* represent the unit cell parameters, *d*-spacing is the distance between similar atomic planes, θ is the diffraction angle, λ is the wavelength of the incident X-ray, and (*h, k, l)* are the Miller indices.

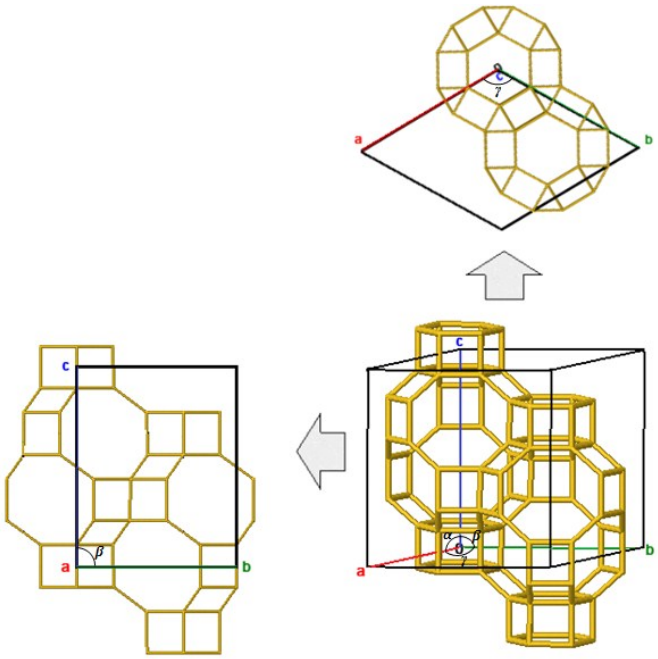

Fig. S2. Schematic representation of chabazite (CHA) framework in the unit cell (Adapted from the IZA database, namely www.iza-online.org).

References

1. Y. Waseda, E. Matsubara, K. Shinoda, *X-Ray Diffraction Crystallography (Introduction, examples and solved problems),* Springer, Heidelberg Dordrecht, London, New York, 2011.