Supplementary Materials

Adsorption mechanism of high-concentration ammonium by Chinese natural zeolite with experimental optimization and theoretical computation

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Table S1. The representative equations of the studied kinetic and isotherm model and their parameters

Kinetic models		
Model	**Equation**	**Parameters**
Pseudo-first-order	$q_t = q_e(1 - e^{-k_1 t})$	q_t (mg/g) is the adsorption capacities at time t (min), and k_1 (min^{-1}) is the rate constant of the kinetic model.
Pseudo-second-order	$\frac{t}{q_t} = \frac{1}{k_2 q_e^2} + \frac{t}{q_e}$	q_e (mg/g) is the sorption capacity at equilibrium, and k_2 is the rate constant (g/mg·min).
Isotherm models		
Model	**Equation**	**Parameters**
Langmuir	$q_e = \frac{q_m K_L C_e}{1 + K_L C_e}$	C_e is the aqueous-phase adsorbate equilibrium concentration (mg/L), K_L (L/mg) is Langmuir isotherm constant, and q_m (mg/g) is the monolayer capacity.
	$R_L = \frac{1}{1 + K_L C_i}$	K_L = Langmuir isotherm constant (L/mg), C_i = Initial adsorbate concentration (mg/L)
Freundlich	$q_e = K_F C_e^{\frac{1}{n}}$	K_F is the Freundlich constant and 1/n is the heterogeneity factor. K_F and n are generally temperature dependent.

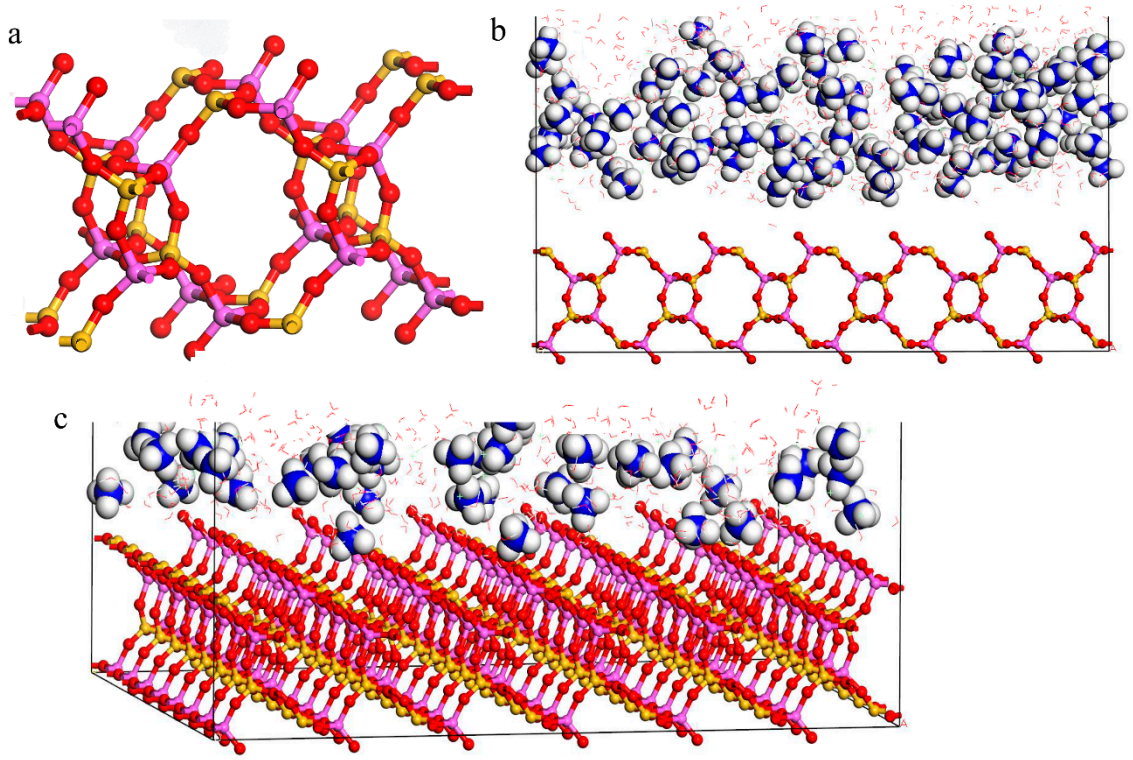

Figure S1. The optimized structures of high-ammonium adsorption onto the natural zeolite. (a) structure of the Chinese natural zeolite; (b) the initial model with 2-nm-high vacuum layer in the upper periodic lattice; (c) the distribution of the random positions of ammonium on the pore surface. Yellow represents Si atoms, pink = Al, red = O, white= H, blue= N.

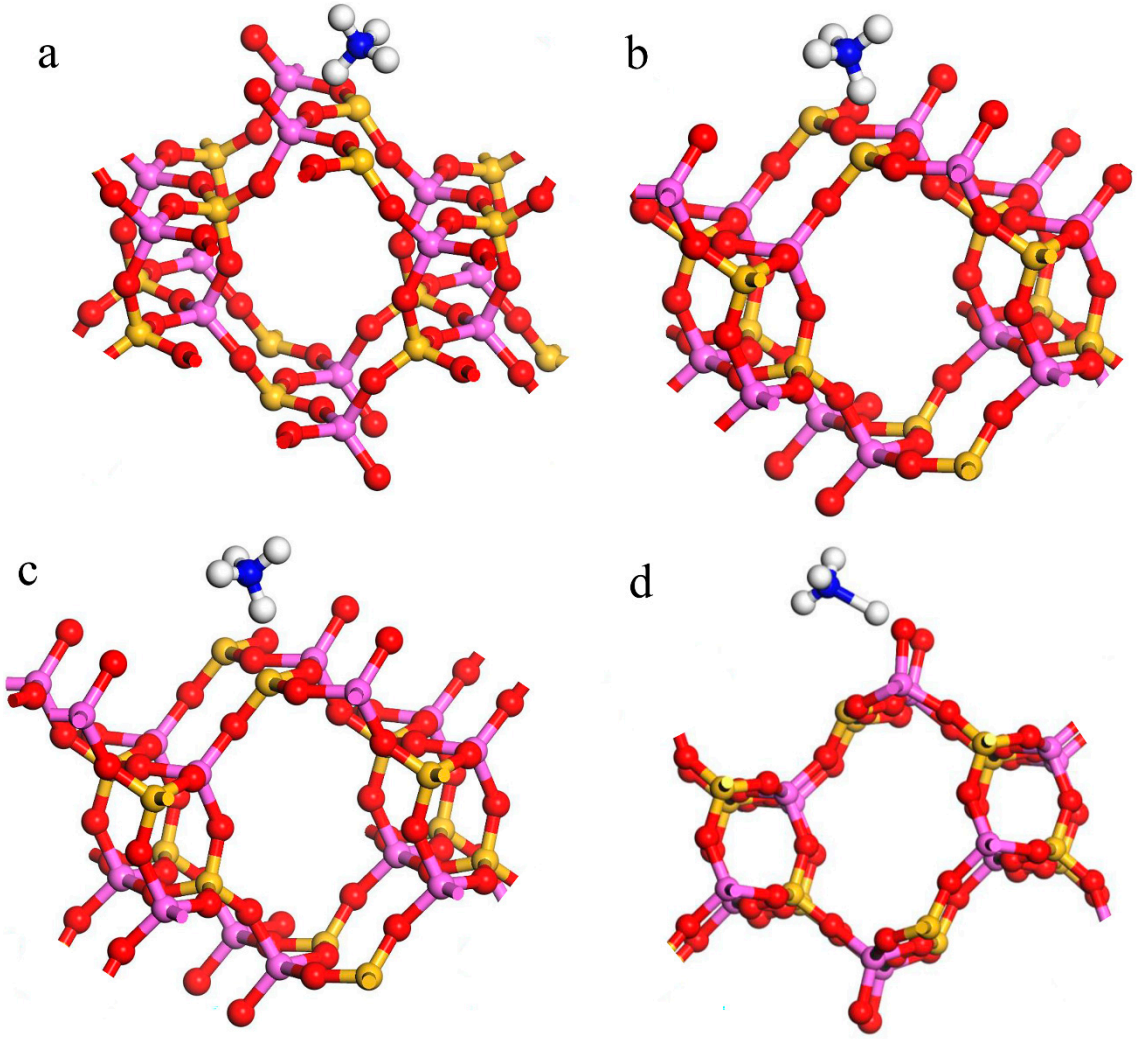

Figure S2. Visualization of ammonium ions adsorbed on different sites of the zeolite framework. (a) and (b) on Al and Si atoms, respectively, (c) and (d) on bridged and unbonded O atom.