Supplementary Materials

The effect of the zeolite pore size on the Lewis acid strength of extra-framework cations

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List of Figure and Table

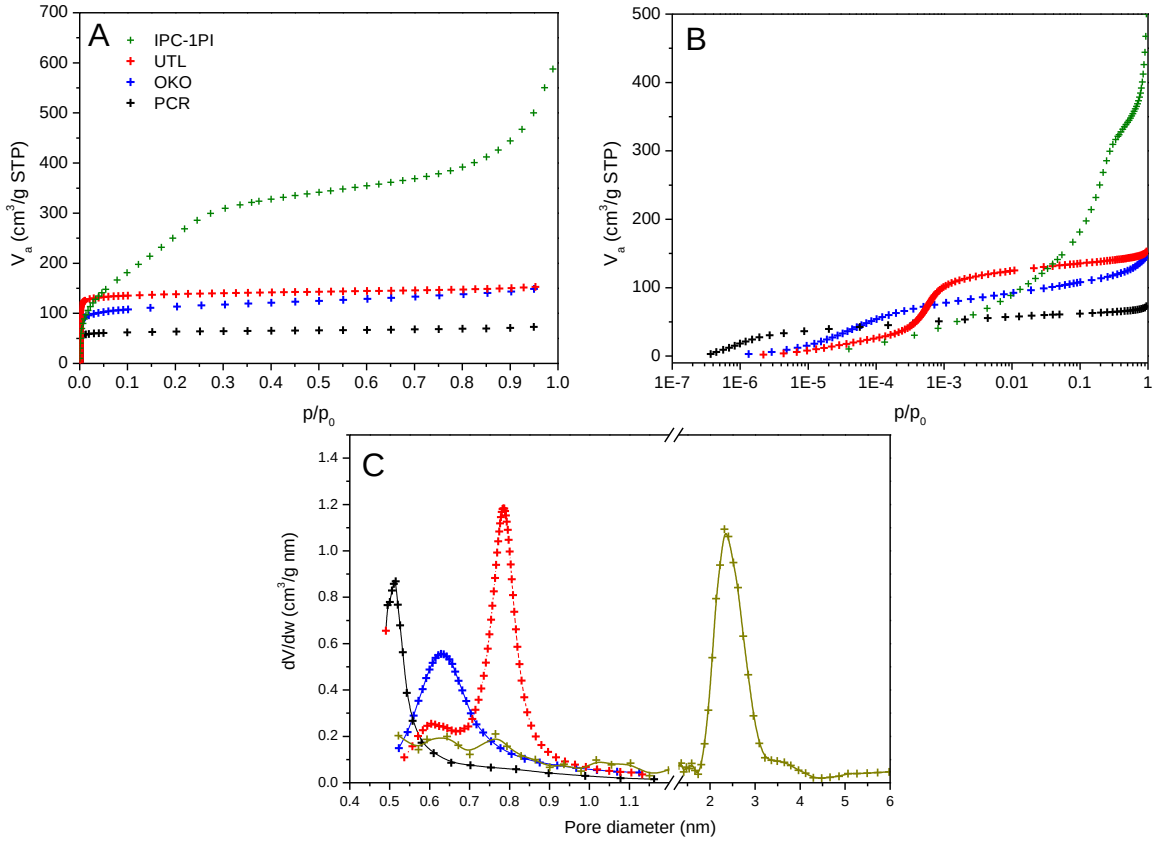

Fig. SI-1 Argon adsorption isotherms measured at -186°C displayed in linear (A) and semilogarithmic scale (B) and pore-size distribution calculated from the adsorption data by SAEIUS software (C).

Table SI-1. The numbering of T sites in IPC-1P, **UTL**, **OKO** and **PCR** was taken from IZA database. The common numbering of the T' sites are chosen following numbering of UTL structure.

Common denotation	IPC-1P	**UTL**	IPC-2 (**OKO**)	IPC-4 (**PCR**)
T1'		T1		
T2'		T2	T6	
T3'	T3	T3	T1	T1
T4'	T4	T4	T2	T3
T5'	T5	T5	T3	T4
T6'	T6	T6	T4	T5
T7'	T7	T7	T5	T2
T8'	T8	T8	T7	T6
T9'	T9	T9	T8	T7
T10'	T10	T10	T9	T8
T11'	T11	T11	T10	T9
T12'	T12	T12	T11	T10

Table SI-2. The most stable Li^+ sites found for all possible Al positions inside the 2D dense layer in Li-IPC-1P, Li-**UTL**, Li-**OKO**, and Li-**PCR**; Li distances to framework oxygen atoms (O_f) smaller than 2.4 Å also reported.[a]

Al location	Al site	r(Li^+…O_f)			
		IPC-1P	UTL	OKO	PCR
layer sites	T3'	*P8bb* *1.98, 2.02, 2.19*	*M8b* *1.86, 1.97, 2.16*	*M8b* *1.87, 2.02, 2.05*	*M8b* *1.88, 2.10, 2.19*
	T4'	*P8bb* *1.87, 1.88*	*I2*[b] *1.86 ,1.88*	*I2* *1.86 1.87*	*I2* *1.87, 1.89*
	T5'	*M8b* *1.93, 1.96, 2.08*	*M8b* *1.94, 1.95, 2.08*	*M8b* *1.91, 1.94, 2.15*	*M8b* *1.92, 1.93, 2.03*
	T8'	*P8bb* *1.92, 1.95, 2.18*	*M8b* *1.91, 1.93, 2.02*	*M8b* *1.93, 1.94, 2.03*	*M8b* *1.94, 1.94, 2.10*
	T9'	*M8b* *1.94, 2.01, 2.02, 2.23*	*M8b* *1.94, 1.99, 2.07, 2.18*	*M8b* *2.00, 2.05, 2.12, 2.13*	*M6b* *1.98, 2.00, 2.12, 2.20*
	T11'	*M6b* *1.93, 1.93, 2.07*	*M6b* *1.97, 2.00, 2.21*	*M6b* *1.95, 2.01, 2.32*	*M6b* *1.97, 1.97, 2.31*
inter-layer sites	T6'	*P5* *1.90, 1.90, 2.04*	*I2* *1.86, 1.87*	*M8b* *1.89, 2.01, 2.04*	*P6* *1.94, 2.06, 2.16, 2.24*
	T7'	*M5'* *1.88, 1.91, 1.99*	*I2* *1.85, 1.88*	*I2* *1.87, 1.91*	*P6'* *1.92, 2.10, 2.17, 2.20*
	T10'	*S8b* *1.93, 2.07, 2.11, 2.11*	*P5'p* *1.90, 1.94, 1.95*	*P5'* *1.83, 2.01, 2.04*	*P6'* *1.97, 1.97, 2.24, 2.24*
	T12'	*P5* *1.92, 1.99, 2.07*	*M8b* *1.89, 1.98, 2.10*	*M8b* *1.89, 2.03, 2.09*	*P6* *1.96, 1.96, 2.16, 2.16*

[a] Distances are in Å

[b] This site was denoted P8bb in Ref. [1]

Table SI-3. DFT/CC correction energies without Li^+ interation [a]

Al location	Al site	ΔEcor			
		IPC-1P	UTL	OKO	PCR
layer sites	T3'	-11.4	-10.7	-9.9	-16.7
	T4'	-8.0	-10.0	-10.3	-15.4
	T5'	-11.7	-11.3	-12.2	-16.8
	T8'	-12.9	-12.3	-11.8	-16.7
	T9'	-13.6	-13.5	-14.6	-15.1
	T11'	-9.6	-8.4	-8.6	-15.1
inter-layer sites	T6'	-9.2	-8.5	-9.8	-15.7
	T7'	-5.8	-7.7	-10.9	-15.6
	T10'	-7.2	-12.8	-11.0	-15.7
	T12'	-9.1	-13.1	-12.3	-15.7

[a] Energies are in kJ mol^{-1}

1. Thang, H. V.; Rubes, M.; Bludsky, O.; Nachtigall, P., Computational Investigation of the Lewis Acidity in Three-Dimensional and Corresponding Two-Dimensional Zeolites: Utl Vs Ipc-1p. *J Phys Chem A* **2014**, *118*, 7526-7534.