Supplementary material

Table S1 Crystal data and refinement parameters of Ag-levyne and Ag-erionite.

Crystal data	**Ag-levyne**	**Ag-erionite**
a (Å)	13.4169(3)	13.29919(19)
c (Å)	22.5926(6)	15.19312(19)
V (Å^3)	3522.09(18)	2327.17(7)
Z	3	1
Space Group	*R*-3*m*	*P*6$_3$/*mmc*
Refined Chemical formula	$Ag_4(Si, Al)_{18}O_{36}\cdot 12.74\ H_2O$	$Ag_{7.15}K_{2.08}(Si, Al)_{36}O_{72}\cdot 35.3\ H_2O$
Crystal size (mm)	0.180 × 0.150 × 0.100	0.05 × 0.03 × 0.015
Intensity measurement		
Diffractometer	APEX II SMART	Synergy-S
X-ray radiation	Mo$K\alpha$ λ = 0.71073 Å	Cu$K\alpha$ λ = 1.54184 Å
X-ray power	50 kV, 30 mA	50 kV, 1mA
Monochromator	Graphite	Mirror Optics
Temperature (K)	296(2)	293(2)
Time per frame (s)	10	6-26
Max. 2θ (°)	58.63	152.25
Index ranges	$-13 \le h \le 18$	$-16 \le h \le 16$
	$-18 \le k \le 18$	$-16 \le k \le 15$
	$-31 \le l \le 21$	$-18 \le l \le 9$
No. of measured reflections	13557	8873
No. of unique reflections	1204	960
No. of observed reflections I > 2σ (I)	1047	931
Structure refinement		
No. of parameters used in the refinement	103	87
R(int)	0.0389	0.0369
R(σ)	0.0223	0.0256
GooF	1.13	1.181
*R*1, *I*>2σ (*I*)	0.0549	0.0618
*R*1, all data	0.0615	0.0633
*wR*2 (on F^2)	0.1697	0.1635
$\Delta\rho_{min}$ (-eÅ^{-3}) close to	-0.73 Ag1A	-1.12 W5
$\Delta\rho_{max}$ (eÅ^{-3}) close to	0.72 W3	1.42 C3A
BASF	0.0569(4)	-

Table S2 Atom coordinates, atomic displacement parameters and occupancy of Ag-levyne structure at RT.

Site	*Scattering factor*	*x*	*y*	*z*	*Occ.*	*Ueq*
T1	Si	0.00016(8)	0.23024(8)	0.07077(4)	1	0.0154(3)*
T2	Si	0.23836(9)	0	0.5	1	0.0134(3)*
O1	O	0.0360(3)	0.3498(2)	0.10710(12)	1	0.0295(6)*
O2	O	0.09045(18)	0.1809(4)	0.08574(18)	1	0.0270(8)*
O3	O	0.12823(19)	0.2565(4)	-0.09330(17)	1	0.0280(9)*
O4	O	0.2584(3)	0	0	1	0.0297(9)*
O5	O	0.2226(2)	0.4452(4)	0.18005(19)	1	0.0309(9)*
Ag1	Ag	0	0	0.1431(3)	0.429(19)	0.0316(13)*
Ag1A	Ag	0	0	0.125(5)	0.050(18)	0.067(16)
Ag2	Ag	0.3333	0.6667	0.1667	0.099(7)	0.047(7)*
Ag2A	Ag	0.3333	0.6667	0.2135(7)	0.067(5)	0.035(5)
Ag2B	Ag	0.3333	0.6667	0.2600(12)	0.139(9)	0.150(12)
Ag3	Ag	0.3333	0.6667	-0.0519(16)	0.036(6)	0.064(14)
Ag4	Ag	-0.035(3)	0.4826(13)	0.0621(11)	0.023(9)	0.019(14)
Ag4A	Ag	-0.0754(9)	0.4623(4)	0.0778(4)	0.100(6)	0.048(3)
Ag4B	Ag	0.016(3)	0.5080(16)	0.0496(10)	0.038(7)	0.059(11)
Ag4C	Ag	0.083(4)	0.541(2)	0.0387(14)	0.081(5)	0.18
Ag4D	Ag	0	0.551(3)	0	0.056(4)	0.18
Ag4E	Ag	-0.048(3)	0.447(4)	0.0521(18)	0.050(6)	0.124(14)
W1	O	0.2577(3)	0.5155(6)	-0.1197(3)	1	0.077(2)*
W11	O	0.220(3)	0.440(5)	-0.131(2)	0.15(3)	0.08(2)
W3	O	0.2113(19)	0.499(2)	0.0003(9)	0.485(15)	0.18

*U anisotropic

Table S3 Atom coordinates, atomic displacement parameters and occupancy of Ag-erionite structure at RT.

Site	Scattering factor	x	y	z	Occ.	Ueq
T1	Si	0.23427(11)	-0.00042(11)	0.10401(8)	1	0.0196(4)*
T2	Si	0.09164(16)	0.42382(16)	0.25	1	0.0182(5)*
O1	O	0.0990(3)	0.1981(5)	0.1278(4)	1	0.0330(13)*
O2	O	0.2657(5)	0	0	1	0.0340(13)*
O3	O	0.0878(8)	0.5439(4)	0.25	1	0.038(2)*
O4	O	0.0237(4)	0.3499(4)	0.1611(3)	1	0.0355(10)*
O5	O	0.2287(4)	0.4574(9)	0.25	1	0.041(2)*
O6	O	0.2534(5)	0.1267(3)	0.1355(4)	1	0.0334(13)*
K1	K	0	0	0.25	0.98(4)	0.033(2)*
K1A	K	0	0	0.303(17)	0.030(16)	0.05
C1	Ag	0.40940(19)	0.20470(9)	0.25	0.679(14)	0.0417(11)*
C1A	Ag	0.435(6)	0.218(3)	0.290(6)	0.020(8)	0.047(17)
C2	Ag	0.3333	0.6667	0.2906(13)	0.158(17)	0.018(4)
C2A	Ag	0.3333	0.6667	0.25	0.159(11)	0.019(3)
C2B	Ag	0.3333	0.6667	0.3209(15)	0.208(16)	0.049(3)
C3	Ag	0.6150(13)	0.3850(13)	0.25	0.140(9)	0.167(13)
C3A	Ag	0.6667	0.3333	0.25	0.036(10)	0.1
C3B	Ag	0.6667	0.3333	0.313(5)	0.035(6)	0.1
W2A	O	0.078(3)	0.5389(15)	0.0584(18)	0.36(4)	0.074(11)
W2	O	0.006(3)	0.5030(13)	0.0776(12)	0.28(4)	0.016(8)
W4	O	-0.0493(14)	0.4753(7)	0.0917(8)	0.97(6)	0.030(3)
W4B	O	-0.054(5)	0.473(2)	0.027(4)	0.36(3)	0.15
W4A	O	-0.0869(14)	0.4566(7)	0.1155(9)	0.68(5)	0.028(3)
W5	O	0.3333	0.6667	1.028(3)	0.58(5)	0.15
W5A	O	0.3333	0.6667	0.929(5)	0.29(4)	0.1

*U anisotropic

Table S4 Crystal data and refinement parameters of Ag-levyne data obtained by Cu micro-focus source. The data were refined as 2-component twin

Crystal data	**Ag-levyne**
a (Å)	13.4002(3)
c (Å)	22.5567(5)
V (Å^3)	3507.76(17)
Z	1
Space Group	*R*-3*m*
Refined Chemical formula	$Ag_{5.21}(Si, Al)_{18}O_{36}\cdot 11.15\ H_2O$
Crystal size (mm)	0.100 × 0.080 × 0.075
Intensity measurement	
Diffractometer	Synergy-S
X-ray radiation	Cu$K\alpha$ λ = 1.54184 Å
X-ray power	50 kV, 1mA
Monochromator	Mirror Optics
Temperature (K)	296(2)
Time per frame (s)	
Max. 2θ (°)	154.93
Index ranges	$-14 \le h \le 13$
	$0 \le k \le 16$
	$-27 \le l \le 28$
No. of measured reflections	944
No. of unique reflections	944
No. of observed reflections I > 2σ (I)	924
Structure refinement	
No. of parameters used in the refinement	97
R(σ)	0.039
GooF	1.101
*R*1, *I*>2σ (*I*)	0.0909
*R*1, all data	0.0914
*wR*2 (on F^2)	0.2678
$\Delta\rho_{min}$ (-eÅ^{-3}) close to	-0.72 Ag1B
$\Delta\rho_{max}$ (eÅ^{-3}) close to	0.74 O3
BASF	0.199(9)

Table S5 Atom coordinates, atomic displacement parameters and, occupancy of Ag-levyne structure at RT.

Site	*Scattering factor*	*x*	*y*	*z*	*Occ.*	*Ueq*
T1	Si	0.00022(13)	0.23105(13)	0.07071(7)	1	0.0459(7)
T2	Si	0.23846(16)	0	0.5	1	0.0440(7)
O1	O	0.0347(5)	0.3509(4)	0.1071(2)	1	0.0620(13)
O2	O	0.0916(3)	0.1831(7)	0.0853(3)	1	0.0589(16)
O3	O	0.1291(3)	0.2583(7)	-0.0933(3)	1	0.0576(16)
O4	O	0.2612(6)	0	0	1	0.0615(17)
O5	O	0.2206(4)	0.4413(7)	0.1788(4)	1	0.0654(19)
Ag1	Ag	0	0	0.1425(2)	0.468(19)	0.063(2)
Ag1A	Ag	0	0	0.116(2)	0.165(18)	0.136(12)
Ag1B	Ag	-0.034(4)	-0.067(8)	0.165(4)	0.035(8)	0.16(3)
Ag2	Ag	0.3333	0.6667	0.1667	0.132(18)	0.089(11)
Ag2A	Ag	0.3333	0.6667	0.2034(12)	0.139(13)	0.115(10)
Ag2C	Ag	0.3333	0.6667	0.2569(18)	0.165(19)	0.21(2)
Ag4	Ag	-0.156(10)	0.422(5)	0.019(5)	0.031(6)	0.2
Ag4A	Ag	-0.0757(11)	0.4621(5)	0.0768(5)	0.120(7)	0.088(5)
Ag4B	Ag	-0.016(3)	0.4919(13)	0.0525(9)	0.140(12)	0.144(9)
Ag4C	Ag	0.057(3)	0.5287(16)	0.0458(10)	0.143(8)	0.18
Ag4D	Ag	0	0.553(3)	0	0.066(5)	0.18
W1	O	0.2566(6)	0.5133(12)	-0.1176(6)	1	0.117(5)
W11	O	0.2176(16)	0.435(3)	-0.1366(15)	0.60(6)	0.151(16)
W3	O	0.220(10)	0.509(11)	0.001(5)	0.13(3)	0.18

Figure S1

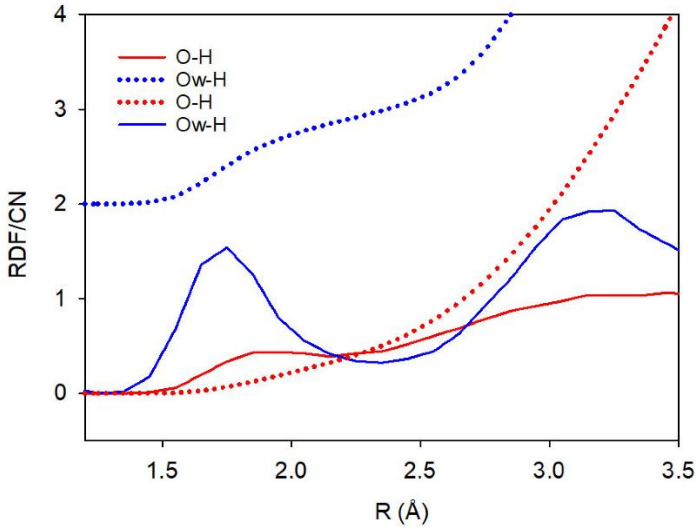

Figure S1 Radial distribution function (RDF) (continuous line) and coordination number (CN) (dottet line) of framework oxygen-hydrogen (O-H) and water oxygen-hydrogen (Ow-H) contacts in Ag-levyne structure as obtained from MD simulation (model with 3 H_2O per Ag ion).

Figure S2

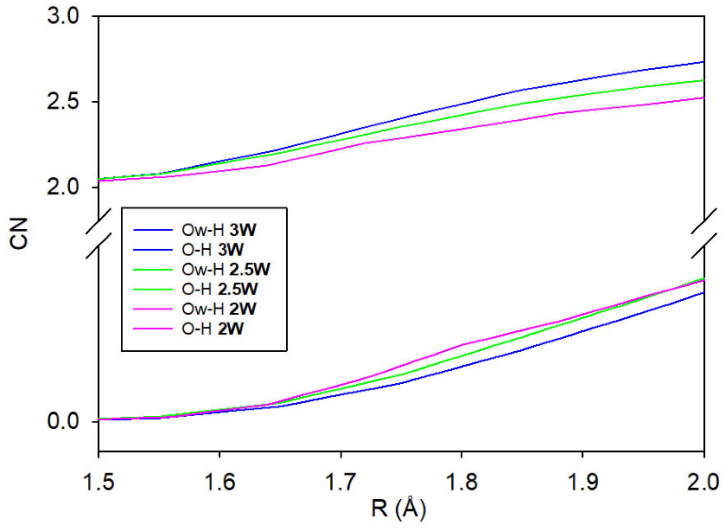

Figure S2 Coordination number (CN) of framework oxygen-hydrogen (O-H) and water oxygen-hydrogen (Ow-H) contacts in Ag-levyne structure as obtained from MD simulation. Results for three simulated structures with different water content are reported: (i) 3W, $3H_2O$ per Ag ion; (ii) 2.5W, $2.5H_2O$ per Ag ion; (iii) 2W, $2H_2O$ per Ag ion.