Electronic Supporting Information

Insights into understanding water mediated proton conductivity in intercalated hybrid solid of kaolinite at ambient temperature

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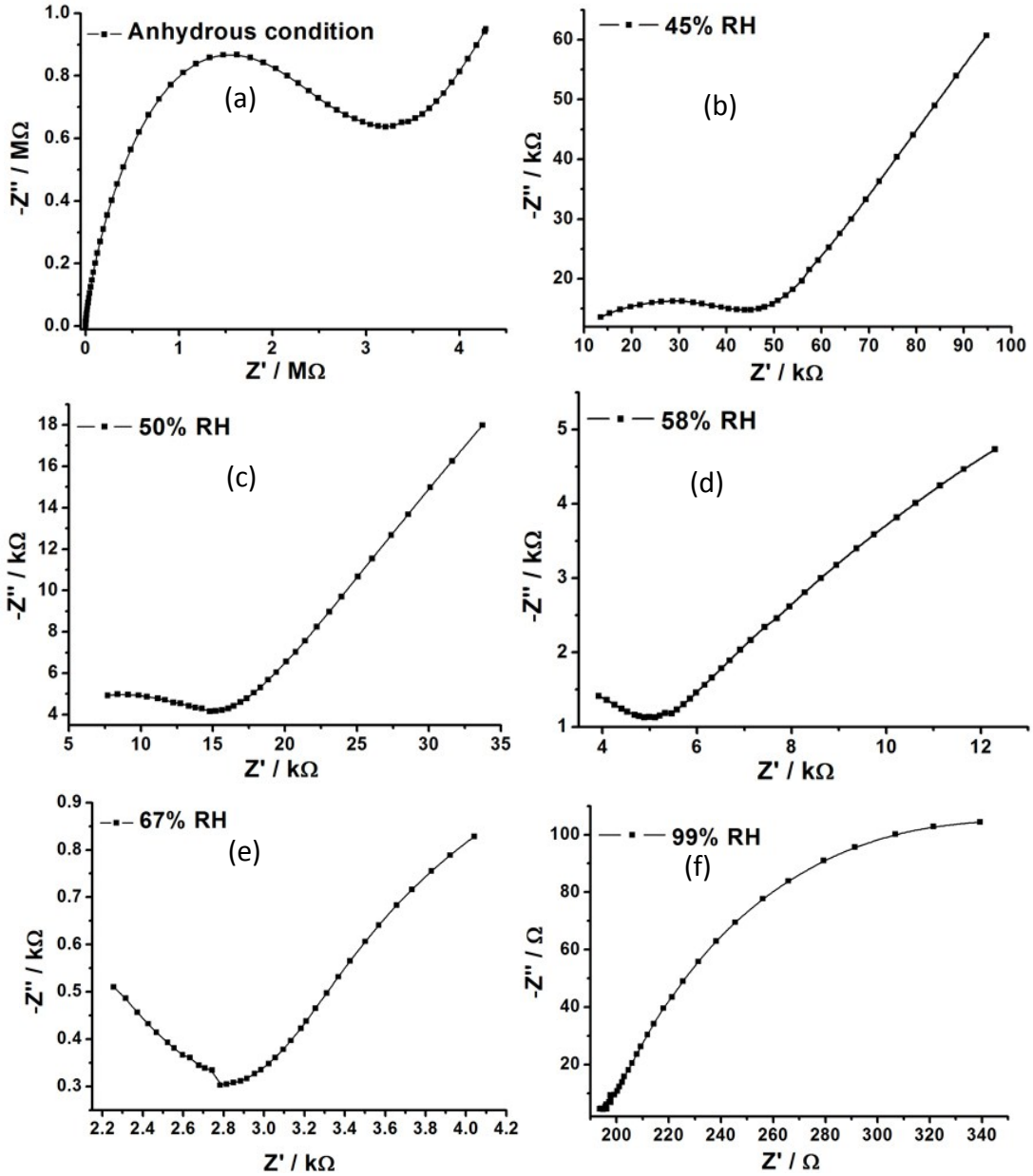


Fig. S1: (a) Nyquist plots of K-Ala at T = 303 K under the selected relative humidity: (a) anhydrous condition, (b) 45% RH, (c) 50% RH, (d) 58% RH, (e) 67% RH, (f) 99% RH.

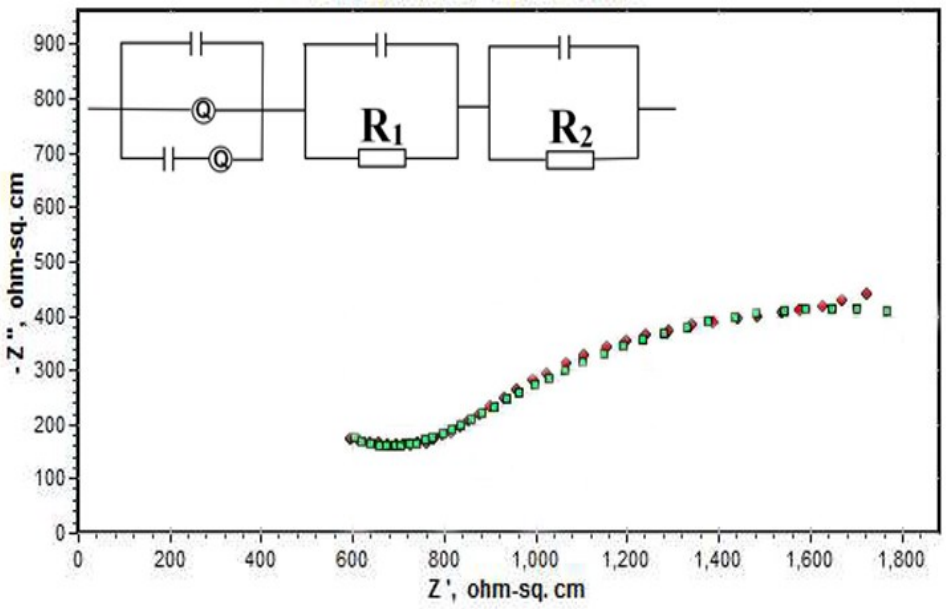
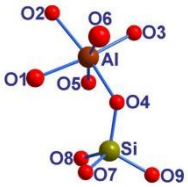


Fig. S2: Nyquist plots with fitted curve (green dots), inset: the equivalent circuit diagram.

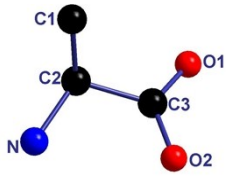
Table S1: Comparison of bond lengths (Å) and bond angles (°) of AlO_6 and SiO_4 species in the optimized structures of raw kaolinite, K-Ala, K-Ala-H_2O and K-Ala-$2H_2O$, respectively



Molecular fragment		Single crystal[1]	Optimized K-Ala	Optimized K-Ala-H_2O	Optimized K-Ala-$2H_2O$
			Bond distances		
	Al-O_1	1.912	1.920	1.932	1.930
	Al-O_2	1.915	1.941	1.876	1.863
AlO_6	Al-O_3	1.868	1.937	1.854	1.847
Octahedron	Al-O_4	1.930	1,946	1.873	1.869
	Al-O_5	1.927	1.943	1.850	1.932
	Al-O_6	1.892	1.963	1.841	1.921
	Si-O_4	1.613	1.629	1.628	1.638
SiO_4	Si-O_7	1.608	1.625	1.589	1.635
Tetrahedron	Si-O_8	1.618	1.638	1.617	1.645
	Si-O_9	1.613	1.624	1.587	1.591
			Bond angles		
	O_1-Al-O_2	76.677	78.194	71.490	69.681
AlO_6	O_1-Al-O_4	93.661	92.733	96.043	96.453
Octahedron	O_3-Al-O_2	93.980	99.799	99.407	100.40

	O_3-Al-O_4	97.004	90.280	94.605	95.112
	O_5-Al-O_1	93.433	88.894	96.659	97.621
	O_5-Al-O_2	96.270	89.236	92.004	93.117
	O_5-Al-O_3	77.752	75.980	72.777	71.611
	O_5-Al-O_4	93.419	95.705	99.538	99.461
	O_6-Al-O_1	94.835	98.616	87.427	87.138
	O_6-Al-O_2	93.743	97.317	95.774	95.933
	O_6-Al-O_3	95.472	96.583	104.21	104.98
	O_6-Al-O_4	77.751	78.873	73.192	72.089
	O_4-Si-O_7	113.43	110.64	104.58	107.44
	O_4-Si-O_8	109.99	108.76	108.72	103.84
SiO_4	O_4-Si-O_9	111.65	111.87	111.84	112.38
Tetrahedron	O_7-Si-O_8	105.81	105.68	112.68	105.92
	O_8-Si-O_9	106.43	107.57	106.58	113.09
	O_9-Si-O_7	109.16	112.04	112.51	114.18

Table S2: Comparison of bond lengths (Å) and bond angles (°) of Ala molecule in the optimized structures of single crystal, K-Ala and K-Ala-H_2O and K-Ala-$2H_2O$, respectively



Molecular fragment		Single crystal[2]	Optimized K-Ala	Optimized K-Ala-H_2O	Optimized K-Ala-$2H_2O$
			Bond distances		
	C_1-C_2	1.520	1.509	1.519	1.525
	C_2-C_3	1.533	1.570	1.554	1.569
	C_3-O_1	1.251	1.281	1.274	1.274
	C_3-O_2	1.251	1.299	1.267	1.266
	C_2-N	1.481	1.525	1.516	1.521
Ala			*Bond angles*		
	C_1-C_2-C_3	110.97	117.32	106.93	108.00
	C_1-C_2-N	109.83	102.84	103.08	104.06
	C_2-C_3-O_1	116.59	114.49	117.00	117.08
	C_2-C_3-O_2	117.51	118.79	113.57	113.69
	O_1-C_3-O_2	125.90	126.46	129.42	129.22
	C_3-C_2-N	110.51	106.48	110.50	109.84

References

1 D. L. Bish, *Clays Clay Miner.,* 1993, **41**, 738.

2 F. Kimura, W. Oshima, H. Matsumoto, H. Uekusa, K. Aburaya, M. Maeyama and T. Kimura, *CrystEngComm.*, 2014, **16**, 6630.