

## ESI

### **Design and preparation of hybrid ferroelectric material through ethyleneglycol covalently grafted to Kaolinite**

Qiao Qiao,<sup>a</sup> Yan-Ni Ding,<sup>a</sup> Shun-Ping Zhao,<sup>\*b</sup> Li Li,<sup>a</sup> Jian-Lan Liu,<sup>a</sup> Xiao-Ming Ren<sup>\*a,c,d</sup>

<sup>a</sup>State Key Laboratory of Materials-Oriented Chemical Engineering and College of Chemistry and Molecular Engineering, Nanjing Tech University, Nanjing 210009, P. R. China

<sup>b</sup>Anhui Provincial Laboratory of Optoelectronic and Magnetism Functional Materials and School of Chemistry and Chemical Engineering, Anqing Normal University, Anqing 246011, P. R. China

<sup>c</sup>College of Materials Science and Engineering, Nanjing Tech University, Nanjing 210009, P. R. China

<sup>d</sup>State Key Laboratory of Coordination Chemistry, Nanjing University 210093, P. R. China

Tel.: +86 25 58139476

Fax: +86 25 58139481

Email: [xmren@njtech.edu.cn](mailto:xmren@njtech.edu.cn)

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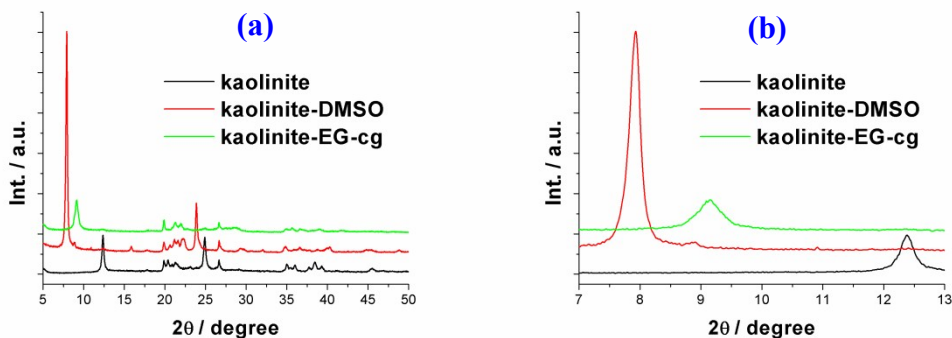


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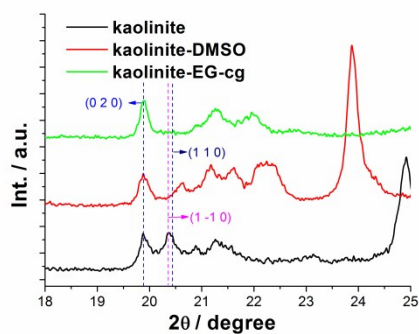


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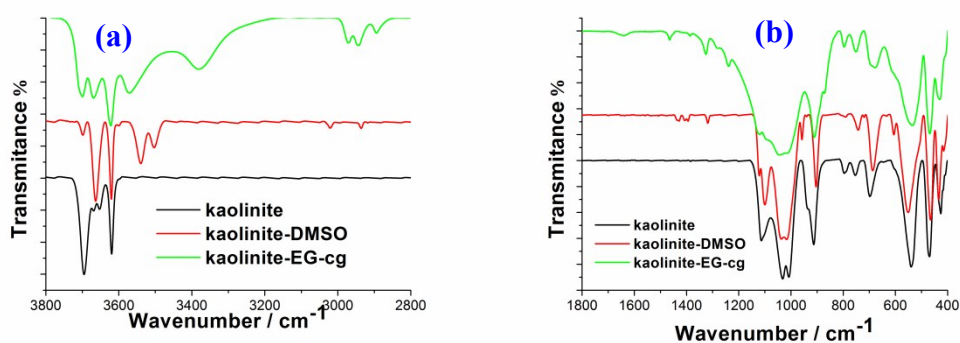


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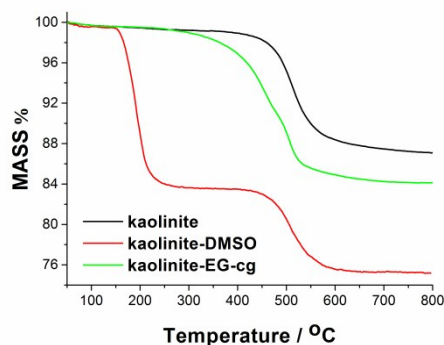


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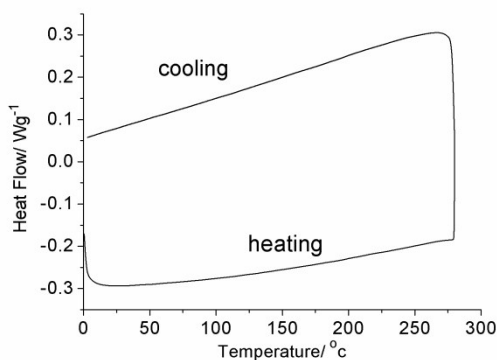


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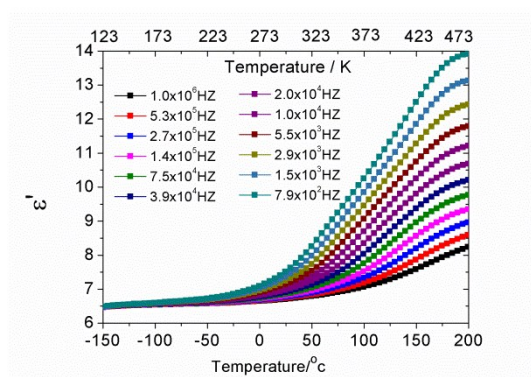


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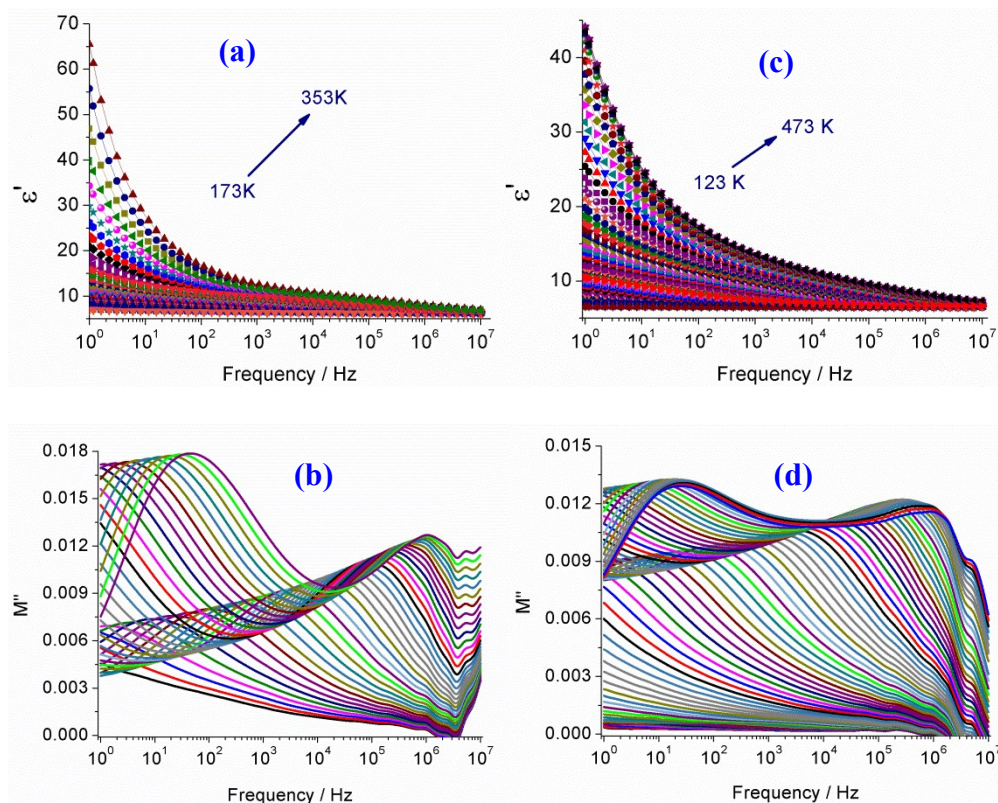


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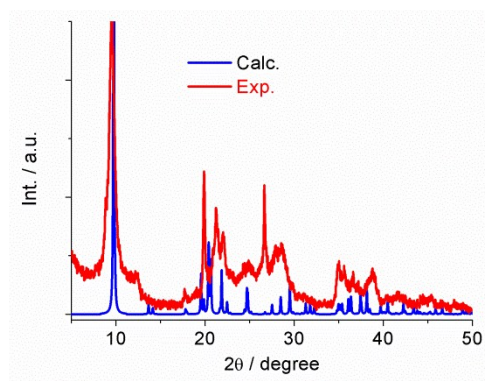


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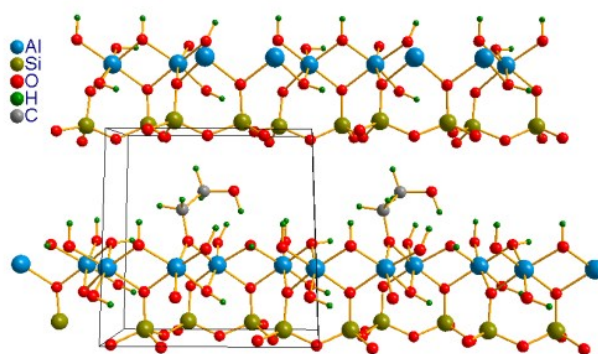


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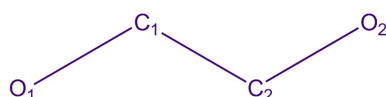
	K-EG-cg	Assignment
Region I	3620	$\nu(\text{OH})$ of inner OH group
	3695,3667	$\nu(\text{OH})$ of inner-surface OH group
Region II	3575,3391	$\nu(\text{R-OH})$
Region III	2970, 2945, 2895	$\nu(\text{C-H})$
	1466	$\nu(\text{C-C}), \delta(\text{CH}_2)$
Region IV	1648, 1330	OH bending vibrations
	1030-1070	Al-O-C linkage

Table S2: Unit cell parameters of K-EG-cg from geometry optimization together with raw Kaolinite obtained from single crystal structure\*

	K-EG-cg	Raw kaolinite*
a/Å	5.1535	5.1535
b/Å	8.9419	8.9419
c/Å	9.4038	7.3906
$\alpha/^\circ$	91.926	91.926
$\beta/^\circ$	105.046	105.046
$\gamma/^\circ$	89.797	89.797
V/Å <sup>3</sup>	418.248	328.708

The c-axis length was fixed during the optimization

Table S3: Bond distances (Å) and bond angle ( $^\circ$ ) in EG\*\*



	Single crystal	Optimization
O1-C1	1.427	1.429
C1-C2	1.514	1.490
C2-O2	1.431	1.427
$\angle\text{O1-C1-C2}$	112.0(3)	111.11
$\angle\text{C1-C2-O2}$	109.5(9)	106.75

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

\*\* R. Boese and H. C. Weiss, *Acta. Cryst.*, 1998, **C54**, IUC9800024.