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Intercalated supramolecular compounds of kaolinite with ethanolamine and ethyleneglycol: structures and dielectric properties

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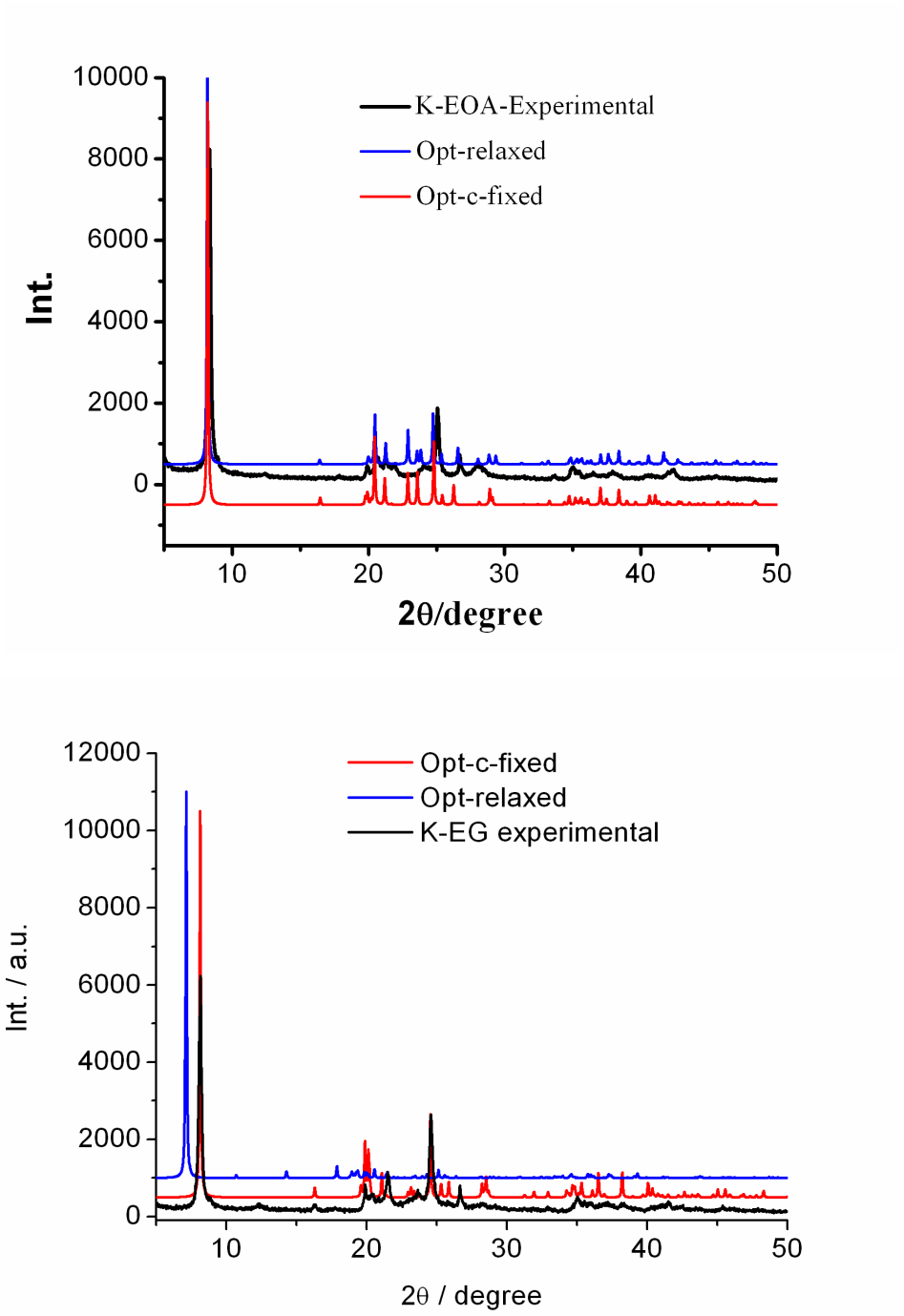

Figure S1 Experimental and calculated PXRD patterns (upper) K-EOA and (down) K-EG (Opt-relaxed: all unit cell parameters are relaxed during the optimization process; Opt-c-fixed: all unit cell parameters, except for c-axis length which was set to be the value obtained from PXRD measurement, are relaxed during the optimization process).

Table S1: Unit cell parameters of kaolinites from single crystal structure analysis at 1.5 K[1] as well as K-EOA and K-EG from the DFT calculation using the second optimization strategy.

	Kaolinite[1]	K-EOA	K-EG
a/Å	5.1535	5.1459	5.1113
b/Å	8.9419	8.8908	8.9443
c/Å	7.3906	11.1673	10.1571
α/°	91.926	92.8062	91.8470
β/°	105.046	104.7271	105.0810
γ/°	89.797	89.1149	88.6808
V/Å^3	328.708	493.5375	448.0751

References

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