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氟置换高岭石层间羟基的能量最小化模拟

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Energy Minimization Modeling of Fluorine Substitution for Interlayer Hydroxyl in Kaolinite

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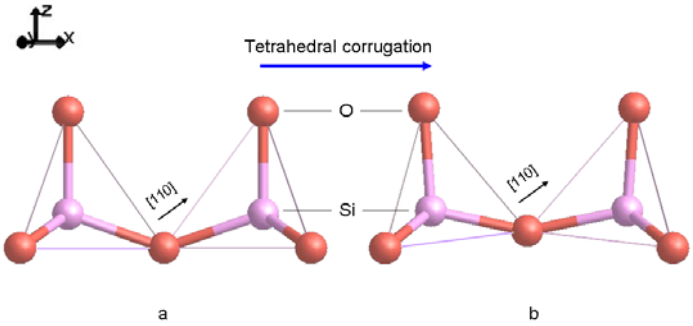

图 s1　四面体起皱示意图

Fig.s1　Schematic diagram of tetrahedral corrugation

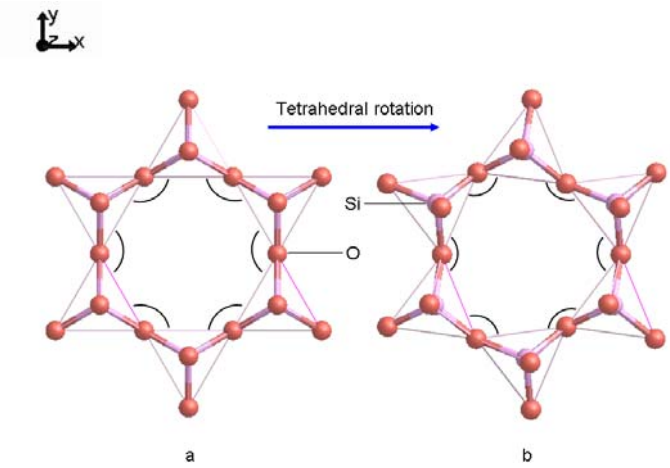

图 s2　四面体旋转示意图

Fig.s2　Schematic diagram of tetrahedral rotation

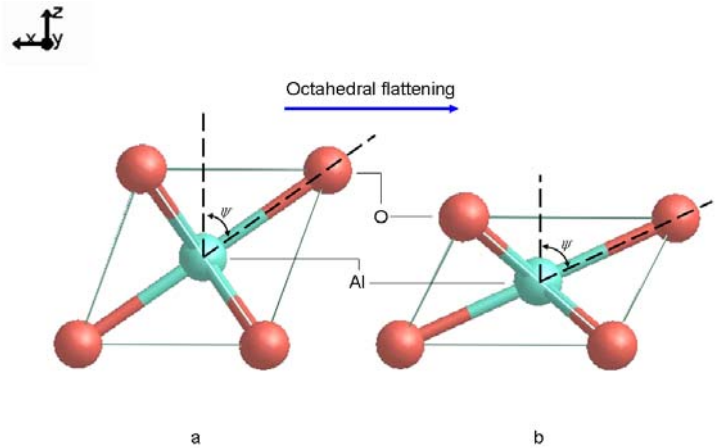

图 s3　八面体展平示意图

Fig.s3　Schematic diagram of octahedral flattening

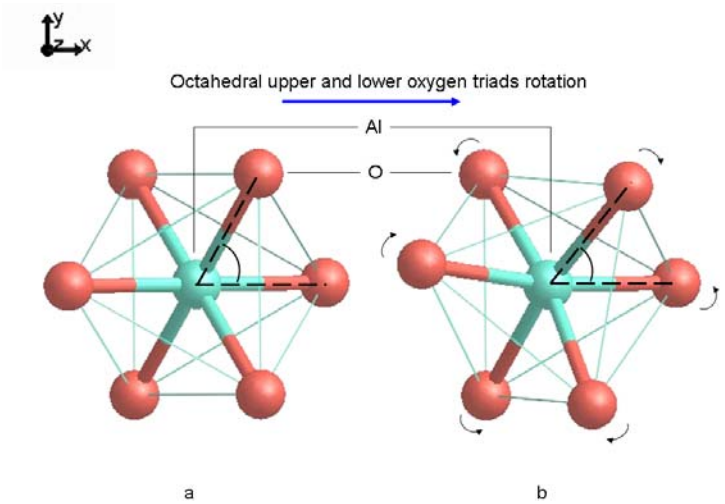

图 s4　八面体上下三原子氧对相对旋转示意图

Fig.s4　Schematic diagram of octahedral upper and lower oxygen triads rotation

表 s1　层间羟基的氟置换对高岭石晶胞参数和结构无序的影响

Table s1 Effect of fluorine substitution for interlayer hydroxyl on cell parameters and structure distortions in kaolinite

Fluorine content in interlayer hydroxyl groups	0.00	0.10	0.20	0.30	0.40	0.50	0.60	0.70	0.80	0.90	1.00
a (nm)	5.1552	5.1524	5.1539	5.1515	5.1494	5.1477	5.1466	5.1461	5.1486	5.1468	5.1480
b (nm)	8.9020	8.9012	8.8859	8.8873	8.8894	8.8923	8.8949	8.8972	8.8990	8.8988	8.8993
c (nm)	7.2878	7.2984	7.2437	7.2551	7.2752	7.3076	7.3545	7.4266	8.0243	7.8142	8.1831
α(deg.)	93.61	93.52	90.67	90.26	89.73	89.24	89.18	89.35	80.67	91.83	96.38
β(deg.)	107.19	107.11	104.52	104.48	104.45	104.40	104.28	104.09	111.68	105.78	107.03
γ(deg.)	90.68	90.59	90.52	90.43	90.35	90.28	90.23	90.20	90.16	90.16	90.15
Interlayer distance	2.65	2.6752	2.7254	2.7564	2.7959	2.8468	2.9143	3.0092	3.1718	3.3634	3.6428
Tetrahedral sheet											
Mean Si-O bond length b_1 (nm)	1.5687	1.5693	1.5667	1.5667	1.5651	1.5646	1.5644	1.5644	1.5644	1.5646	1.5651
Mean O-Si-O bond angle α_1 (deg.)	109.46	109.31	109.45	109.29	109.43	109.42	109.40	109.38	109.35	109.33	109.30
Mean Si-O-Si bond angle α_2 (deg.)	141.71	142.39	142.70	143.52	144.40	145.28	146.15	146.95	147.89	148.44	149.12
Tetrahedral thickness d_1 (nm) [a]	2.1051	2.1057	2.1163	2.1116	2.1062	2.1020	2.0990	2.0974	2.0962	2.0978	2.0991
Tetrahedral rotation angle α(deg.) [b]	4.00	3.7606	3.9183	3.5603	3.1695	2.7599	2.3930	2.0735	1.3191	1.6856	1.7905
Tetrahedral corrugation ΔZ (nm) [c]	0.1011	0.1040	0.1248	0.1321	0.1402	0.1458	0.1489	0.1505	0.1513	0.1511	0.1515
Octahedral sheet											
Mean Al-O/F bond length b_2 (nm)	1.9774	1.9708	1.9652	1.9581	1.9512	1.9308	1.9261	1.9321	1.9150	1.9184	1.9105
Mean OH bond length b_3 (nm)	1.0309	1.0341	1.0386	1.0434	1.0501	1.0587	1.0711	1.0916	1.1279	1.2383	—
Mean body diagonal O-Al-O/F bond angle θ_6 (deg.)	168.35	168.86	168.61	168.73	168.75	168.69	168.56	168.38	168.17	167.82	167.45
Mean co-edge O-Al-O/F bond angle θ_3 (deg.)	81.84	81.54	81.31	80.94	80.56	80.16	79.75	79.30	78.80	78.26	77.61
Octahedral thickness d_2 (nm) [d]	2.1903	2.1786	2.1699	2.1565	2.1429	2.1287	2.1133	2.0961	2.0758	2.0542	2.0286
Octahedral flattening angle ψ (deg.) [e]	56.37	56.45	56.49	56.59	56.69	56.55	56.73	57.15	57.18	57.63	57.93
Octahedral upper and lower oxygen triads rotation angle ω (deg.) [f]	5.16	5.34	5.49	5.70	5.90	6.50	6.62	6.42	6.85	6.70	6.87

a) d_1=mean z coordinate of connected oxygens - mean z coordinate of basal oxygens; b) α = 0.5mean|120-∠O-O-O|, here ∠O-O-O is the angle among three adjacent oxygens in basal oxygen hexagonal ring; c) ΔZ = average deviation between basal oxygens along [110] and other basal oxygens; d) d_2= mean z coordinate of connected and inner hydroxyl oxygens - mean z coordinate of basal oxygens; e) ψ = arcos($0.5d_2 / b_2$); f) ω=0.5 (60-θ), here θ is the projection of θ_3 on (001) plane, and cos($0.5\theta_3$)= cos(0.5θ) · cos(arcsin($0.5d_2/b_2$)).