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高岭石-水体系中水分子结构的分子动力学模拟

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Molecular Dynamics Simulation on Structure ofWater Molecules in a Kaolinite-Water System

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1. 高岭石-水体系各原子起始坐标如表 1 所示:

表 1 初始晶胞原子坐标（nm）

Table 1 Atom coordinates in initiative cell (nm)

Atom	*x*	*y*	*z*	Atom	*x*	*y*	*z*	Atom	*x*	*y*	*z*
Al	0.06111	0.43279	0.3324	H	0.13653	0.26444	0.51929	H	0.13898	0.8816	0.52215
Al	0.3205	0.28277	0.33169	Al	0.32036	0.87989	0.3324	H	0.39578	0.71153	0.51929
Si	0.49338	0.30139	0.06463	Al	0.57976	0.72987	0.33169	O	−0.0514	0.28007	0.67764
Si	0.24381	0.14662	0.06691	Si	0.75263	0.74848	0.06463	O	0.20482	0.13309	0.67759
O	−0.03443	0.3037	0.22598	Si	0.50307	0.59353	0.06691	O	0.20786	0.72716	0.67764
O	−0.00084	0.58237	0.22741	O	0.22483	0.75079	0.22598	O	−0.05127	0.58018	0.67759
O	0.00158	0.44709	0	O	0.25842	1.02946	0.22741	H	−0.04256	0.3719	0.64597
O	0.1001	0.20413	0.0214	O	0.26084	0.89418	0	H	−0.07622	0.27802	0.76991
O	0.10376	0.68617	0.00071	O	0.35936	0.65123	0.0214	H	0.10077	0.17676	0.72666
O	−0.03351	0.8604	0.23183	O	0.36301	1.13031	0.00071	H	0.28279	0.17676	0.72666
O	0.37881	0.13359	0.43298	O	0.22575	1.30749	0.23183	H	0.21678	0.84314	0.64597
O	−0.09543	0.40799	0.43127	O	0.63806	0.58068	0.43298	H	0.18304	0.72511	0.76991
O	−0.09454	0.75268	0.43441	O	0.16383	0.85508	0.43127	H	−0.16048	0.62385	0.72666
H	0.01239	0.05034	0.23254	O	0.16472	1.19977	0.43441	H	0.54205	0.62385	0.72666
H	−0.1088	0.12861	0.52714	H	0.27165	0.49743	0.23254				
H	−0.12028	0.4345	0.52215	H	0.15046	0.57571	0.52714				

2.CLAYFF 力场各参数如表 2 所示：

表 2 力场参数[10]

Table2 Force field parameters[10]

Nonbonded: $E_{nonbonded} = E_{VDW} + E_{coul} = \sum_{i \neq j} D_{o,ij} \left[\left(\frac{R_{o,ij}}{r_{ij}} \right)^{12} - 2 \left(\frac{R_{o,ij}}{r_{ij}} \right)^{6} \right] + \frac{e^2}{4\pi\varepsilon_0} \sum_{i \neq j} \frac{q_i q_j}{r_{ij}}$

Atom type description	symbol	$D_{0,ii}$(kJ·mol^{-1})	$R_{0,ii}$(nm)	q(e)
water hydrgen	H_W	0	0	0.4100
hydroxyl hydrogen	H_{OH}	0	0	0.4250
water oxygen	O_W	0.6502	0.3553	-0.8200
hydroxyl oxygen	O_{OH}	0.6502	0.3553	-0.9500
bridging oxygen	O_B	0.6502	0.3553	-1.0500
tetrahedral silicon	Si	7.7007×10^{-6}	0.3706	2.1000
octahedral aluminum	Al	5.5639×10^{-6}	0.4794	1.5750

Bond stretching: $E_{bondstretch-ij} = k_1 \left(r_{ij} - r_o \right)^2$

Atom type *i*	Atom type *j*	k_1(kJ·mol^{-1}·nm^{-2})	r_0(nm)
O_W	H_W	231850	0.1000
O_{OH}	H_{OH}	231850	0.1000

Angle bending: $E_{anglebend-ijk} = k_2 \left(\theta_{ijk} - \theta_o \right)^2$

Atom type *i*	Atom type *j*	Atom type *k*	k_2(kJ·mol^{-1}·rad^{-2})	θ_0(°)
H_W	O_W	H_W	191.50	109.47
Al	O_{OH}	H_{OH}	125.52	109.47

$D_{o,ij}$ and $R_{o,ij}$ are empirical parameters between atom *i* and *j* which can be caulculated according to the mean rule: $R_{o,ij}$=1/2($R_{o,ii}$ + $R_{o,jj}$) and $D_{o,ij}$=($D_{o,ii}$ $D_{o,jj}$)$^{1/2}$, where $R_{o,ii}$ and $R_{o,jj}$ are distance parameters of atom *i* and *j*, $D_{o,ii}$ and $D_{o,jj}$ are energy parameters of atom *i* and *j* separately. *e* is the charge of electron, ε_0 is the dielectric permittivity of vacumm. q_i and q_j are partial charge of atom *i* and *j*, r_{ij} is the distance between them. k_1 and k_2 are force constants, r_0 represents the equilibrium bond length, θ_0 represents the equilibrium bond angle and θ_{ijk} is the bond angle among atom *i*, *j* and *k*.