Electronic Supplementary Material (ESI) for CrystEngComm

Supplementary Materials

Evolutionary Metadynamics: a Novel Method to Predict Crystal Structures

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Potential used for Al_2SiO_5 and $MgSiO_3$

We studied Al_2SiO_5 and $MgSiO_3$ with simple classical simulations based on the ionic shell model. The ionic shell model included pairwise interactions described by the following expression:

$$U_{ij}(R_{ij}) = \frac{z_i z_j}{R_{ij}} + b_{ij}\exp(-\frac{R_{ij}}{\rho_{ij}}) - \frac{c_{ij}}{R_{ij}^6} \quad (1)$$

a core-shell term for polarizable oxide ions (only for Al_2SiO_5):

$$U_s = k_s (\Delta r)^2 \quad (2)$$

and three-body angle-bending potentials (only for Al_2SiO_5):

$$U_{ijk} = k_b (\varphi-\varphi_0)^2 \quad (3)$$

The values of the parameters are given in Tables S1 and S2.

Table S1. Parameters of the ionic shell model for Al_2SiO_5

(Z_{Si}=+4.0; Z_{Al}=+3.0; Z_O=-2.0)

Pair Potentials			
Interaction	B_{ij}, eV	ρ_{ij},	C_{ij}, eV* Å^6
O-O 2	023.8	0.2674	12.83
Al-O 1	474.4	0.3006	0
Si-O 1	283.9	0.3205	10.66
Shell parameters			

k_s (O) = 74.9204 eV/Å^2 q(shell) = -2.84819 Q(core) = +0.84819
Three-body potentials
k_b(O-Al-O) = k_b(O-Si-O) = 2.09724 eV/rad^2

Table S2. Parameters of the ionic shell model for $MgSiO_3$

(Z_{Si}=+2.9043; Z_{Al}=+1.9104; Z_O=-1.6049)

Pair Potentials			
Interaction	B_{ij}, eV	ρ_{ij},	C_{ij}, eV* Å^6
O-O 2023	.800	0.2674	12.83
Mg-O 1007	.526	0.2866	0
Si-O 1108	.983	0.2827	0