Supporting Information

DFT Simulations of the Structure and Cation Order of Norsethite, $BaMg(CO_3)_2$

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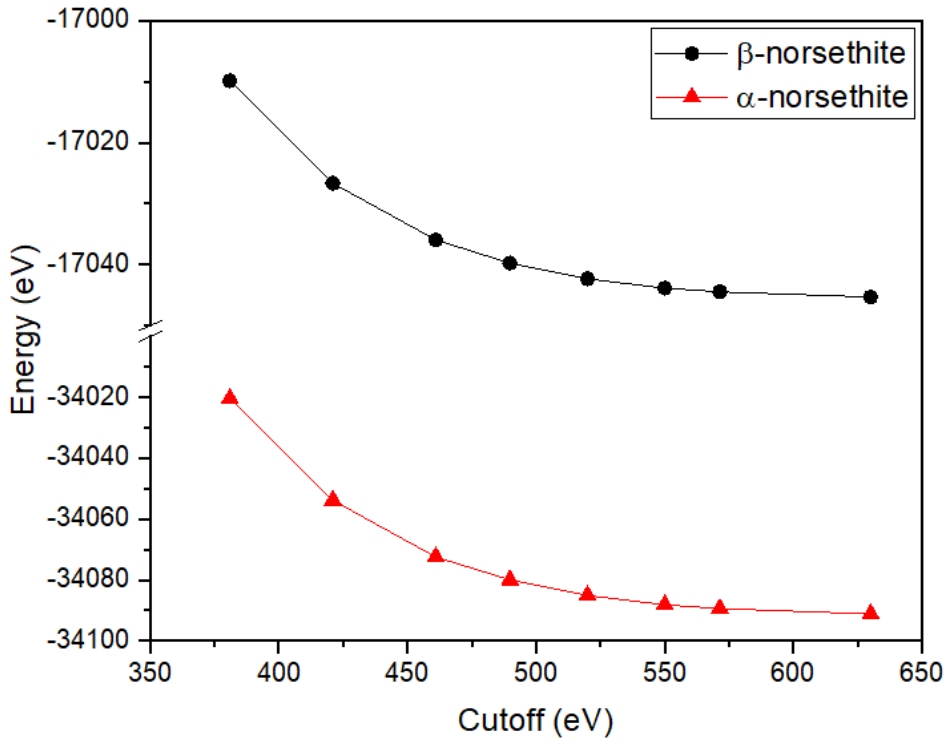

Figure S1. Cut-off values versus calculated energy of α-norsethite (red triangles) and β-norsethite (black circles).

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Table S1. Crystal cell parameters of the stoichiometric ordered α-norsethite, comparison of experimental with calculated parameters in this work, using different functionals and pseudopotentials.

	Experimental[a]	Experimental[b]	Theoretical (this work)			
			PBE[c]	RPBE[c]	PBESOL[c]	PBE[d]
a (Å)	5.015	5.010	5.014	4.894	5.026	5.009
b (Å)	5.015	5.010	5.014	4.894	5.026	5.009
c (Å)	33.474	33.400	34.244	30.657	32.806	34.416
α (deg)	90	90	90	90	90	90
β (deg)	90	90	90	90	90	90
γ (deg)	120	120	120	120	120	120

[a] Experimental data at 100 K (Effenberger et al., 2014); [b] Experimental data at 100 K (Ende et al., 2017); [c] With OTFG ultrasoft pseudopotentials. [d] With OTFG norm conserving pseudopotential.

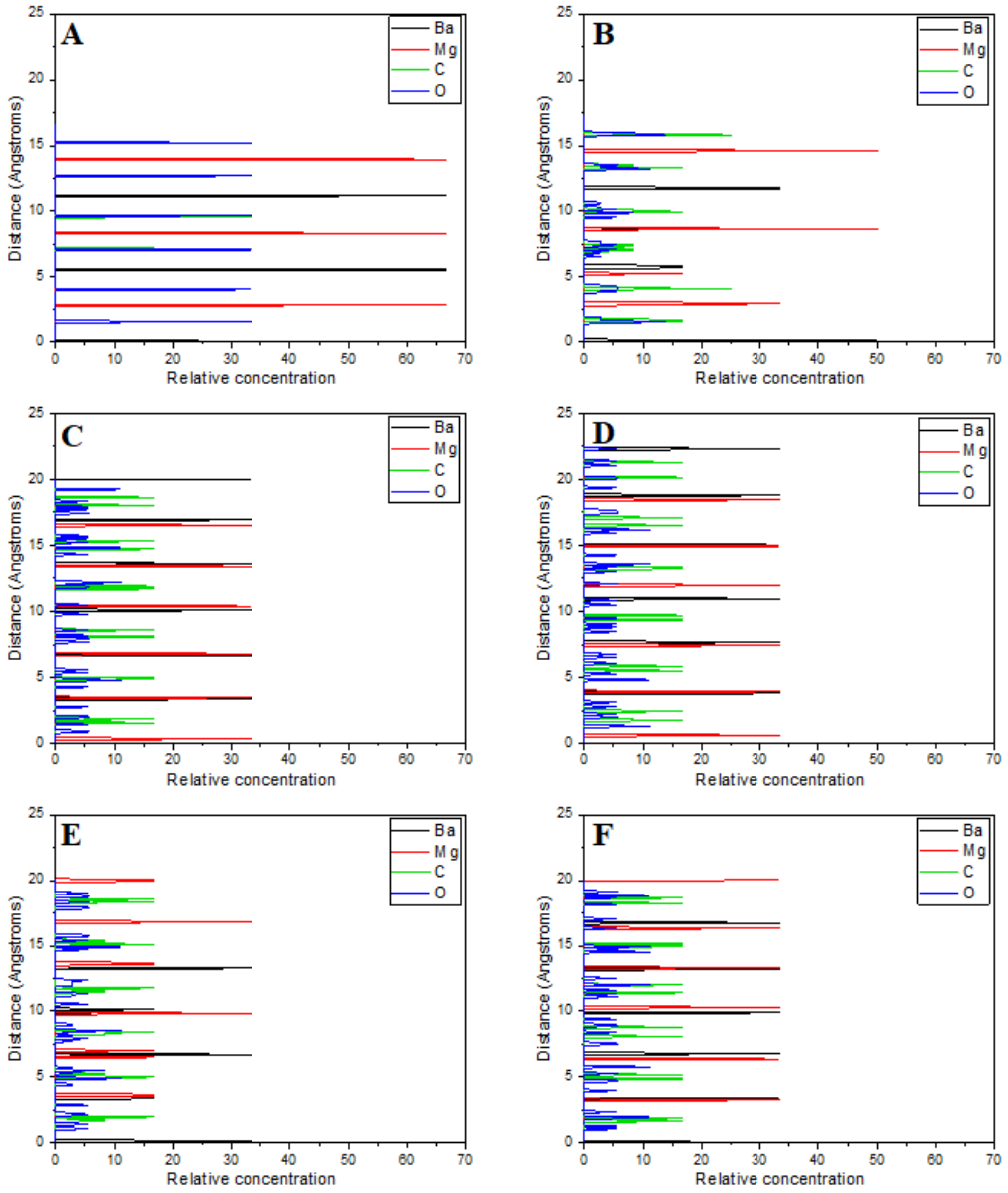

Figure S2. Concentration profile of barium, magnesium, carbon and oxygen atoms projected along [001] direction of Nor1 (A), D1 (B), V1 (C), V2 (D), V3 (E) and V4 (F).