Electronic Supplementary Material for CrystEngComm
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Supplementary data

1) Crystallographic data of the ice structure used in the force field calculations (after optimisation by the developed force field)

Unit Cell $a = 4.7117$ Å $b = 8.5422$ Å $c = 7.7329$ Å $\alpha = 90°$ $\beta = 90°$ $\gamma = 94.9218°$

Space group $P\ 1\ 1\ 2_1$

Symmetry operations x, y, z -x, -y, z +0.5

Atomic coordinates

Name	x	y	z
O1	0.73068	0.40455	0.26505
O2	0.24918	0.91036	0.25491
O3	0.25848	0.58161	0.14471
O4	0.77622	0.08439	0.13485
H5	0.73222	0.40532	0.39220
H6	0.42535	0.97021	0.21652
H7	0.07935	0.52471	0.18341
H8	0.93547	0.02713	0.17598
H9	0.73990	0.29634	0.22327
H10	0.25093	0.80060	0.21678
H11	0.41995	0.52470	0.18356
H12	0.77556	0.08591	0.00767

2) Acetone-acetone interaction energies between molecules in neighbouring boxes (caused by long-range dipole-dipole interactions)

	distance of acetone molecules in different boxes ([uvw] directions in the monoclinic lattice)	interaction energy /kJ mol^{-1}
surface		
3x2	10 Å in [100]; 14 Å in [010]	0.1
10x10	40 Å in [100]; 80 Å in [010]	0.01
bulk ice		
3x2x2	13 Å in [100]; 14 Å in [010]; 12 Å in [001]	0.2
6x4x4	26 Å in [100]; 31 Å in [010]; 27 Å in [001]	0.02
9x8x8	42 Å in [100]; 65 Å in [010]; 59 Å in [001]	10^{-4}
small-angle grain boundary		
Structure A	11 Å in [100]; 30 Å in [010]; 47 Å in [001]	0.1
Structure A’	20 Å in [100]; 48 Å in [010]; 88 Å in [001]	0.04
Structure B	11 Å in [100]; 30 Å in [010]; 48 Å in [001]	0.1