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Structural Disorder of Mechanically Activated δ-$MgCl_2$ Studied by Synchrotron X-Ray Total Scattering and Vibrational Spectroscopy

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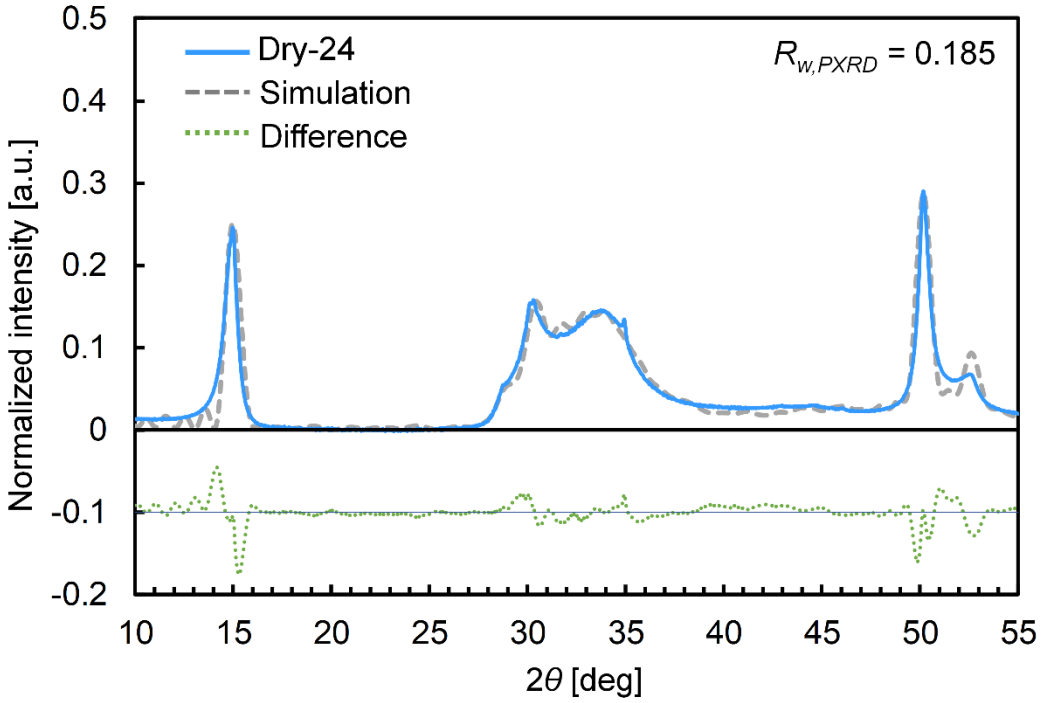

Figure S1. Typical PXRD fitting result.

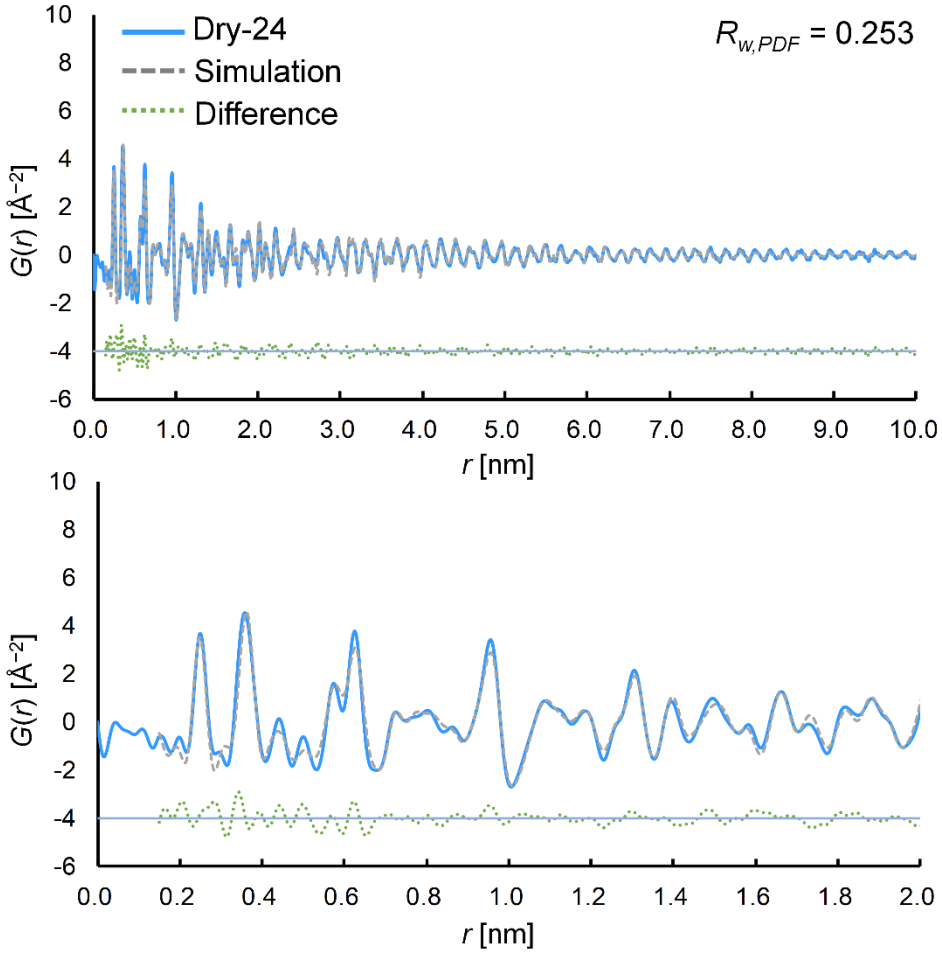

Figure S2. Typical PDF fitting result.

Table S1. Results of PDF fitting with PDFgui [1].

Parameter	Dry-6	Dry-12	Dry-24	Dry-48	EB-24	DBP-24	Tol-24
$R_{w,PDF}$	0.2417	0.2398	0.2527	0.2510	0.2540	0.2669	0.2294
ADP:							
$U_{11,Mg}$, $U_{22,Mg}$ [nm²]	0.000166	0.000178	0.000204	0.000201	0.000185	0.000202	0.000197
$U_{33,Mg}$ [nm²]	0.000731	0.000695	0.000094	0.000102	0.000150	0.000276	0.000107
$U_{11,Cl}$, $U_{22,Cl}$ [nm²]	0.000171	0.000934	0.000182	0.000175	0.000175	0.000205	0.000160
$U_{33,Cl}$ [nm²]	0.000892	0.000167	0.001314	0.001287	0.001080	0.001481	0.001325
Scale factor	1.1956	1.1918	1.2357	1.2374	1.5078	1.8826	1.6941
Delta 1 [nm]	0.2074	0.2087	0.2044	0.2038	0.2015	0.2109	0.2073
Lattice parameter:							
$l_a = l_b$ [nm]	0.3637	0.3637	0.3636	0.3637	0.3636	0.3628	0.3637
l_c [nm] [2]	0.5927	0.5924	0.5926	0.5922	0.5927	0.5956	0.5918
D [nm] [3]	12.5415	12.8884	12.7533	12.9557	10.9180	6.1129	12.6525

[1] Q_{damp} is an instrument-dependent parameter. It was determined as 0.1160 nm^{-1} using a standard sample and fixed as constant in the fitting.

[2] l_c was defined by the separation of neighboring Cl-Mg-Cl layers. See the main text for details.

[3] D is a fittable parameter to express the diameter of the model. This is a built-in function of PDFgui and widely applied for isotropic nanomaterials.