

Supporting Information

**The crystal morphology of 3,4-bis(3-nitrofurazan-4-yl)furoxan
(DNTF) in the solvent system: Molecular dynamics simulation and
sensitivity study**

Ning Liu,* Ya-nan Li, Svatopluk Zeman, Yuan-jie Shu, Bo-zhou Wang, Yan-shui
Zhou, Qiang-li Zhao and Wen-liang Wang

Email: flackliu@sina.com

Table S1 The predicted crystal habit parameters of DNTF crystal in vacuum by AE model^a

$(h\ k\ l)$	Multiplicity	d_{hkl}	E_{att} (total)	E_{att} (vdW)	E_{att} (elec)	D	R_{hkl}	Total facet area/%
(0 1 1)	4	8.75	-48.71	-44.47	-4.25	48.71	1.24	42.62
(0 0 2)	2	7.55	-39.14	-41.03	1.89	39.14	1.00	30.24
(1 0 1)	4	6.09	-81.54	-63.93	-17.61	81.54	2.08	13.76
(1 1 0)	4	5.66	-83.31	-66.42	-16.89	83.31	2.13	9.22
(1 1 1)	8	5.30	-84.42	-64.10	-20.33	84.42	2.16	4.16

^a All energies are in kcal mol⁻¹, distances are in Å.

Table S2 The diffusion coefficient of solvent molecules on different DNTF surfaces

Solvent	$(h\ k\ l)$	$D/\times 10^{-10}\ \text{m}^2\ \text{s}^{-1}$
H ₂ O/AcOH	(0 0 1)	6.66
	(0 1 1)	6.35
	(1 0 1)	5.36
	(1 1 0)	5.51
	(1 1 1)	5.21
H ₂ O/EtOH	(0 0 1)	7.49
	(0 1 1)	6.13
	(1 0 1)	5.72
	(1 1 0)	5.06
	(1 1 1)	5.37

Table S3 Results of sensitivity for crystallized DNTF

Samples	Impact sensitivity, $P/\%$	Friction sensitivity, $P/\%$
DNTF 1 ^a	90	18
DNTF 2 ^b	92	60

^a DNTF crystal cultivating from the solvent of H₂O/AcOH.

^b DNTF crystal cultivating from the solvent of H₂O/EtOH.

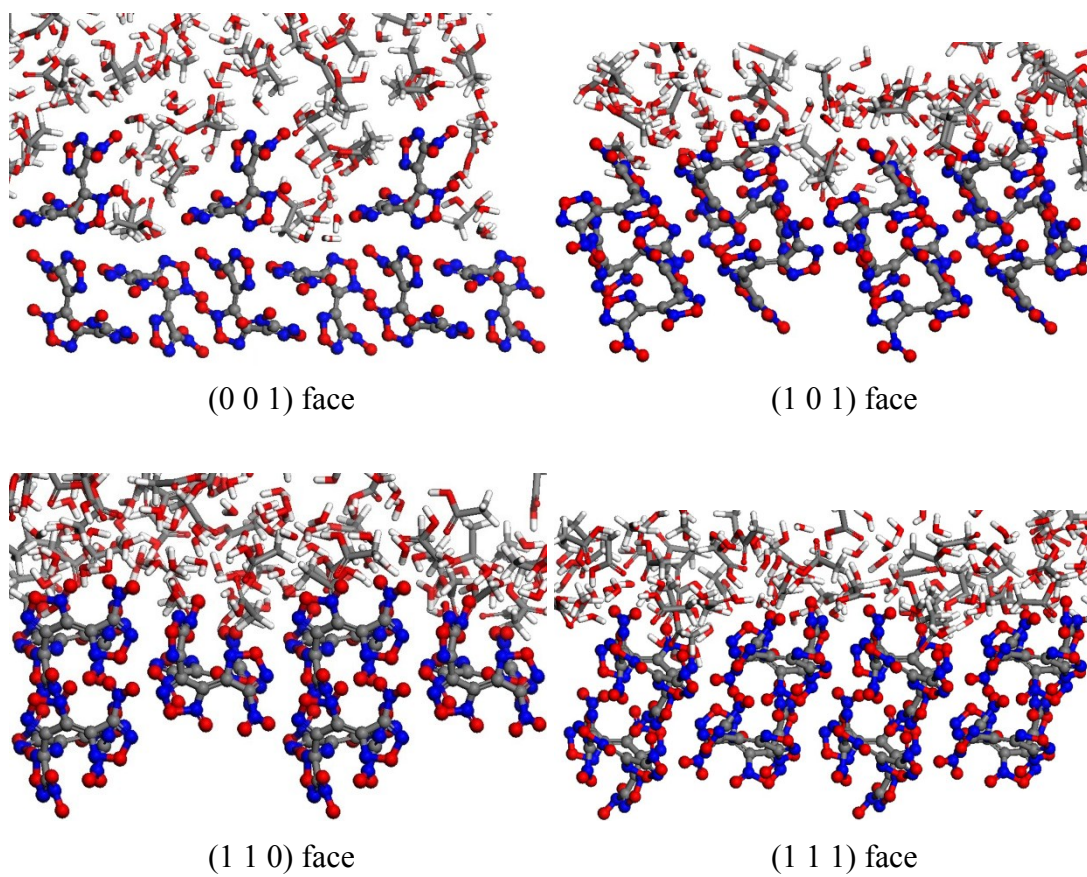


Fig. S1 The configurations of DNTF surface-H₂O/AcOH interfaces from the MD equilibrium.

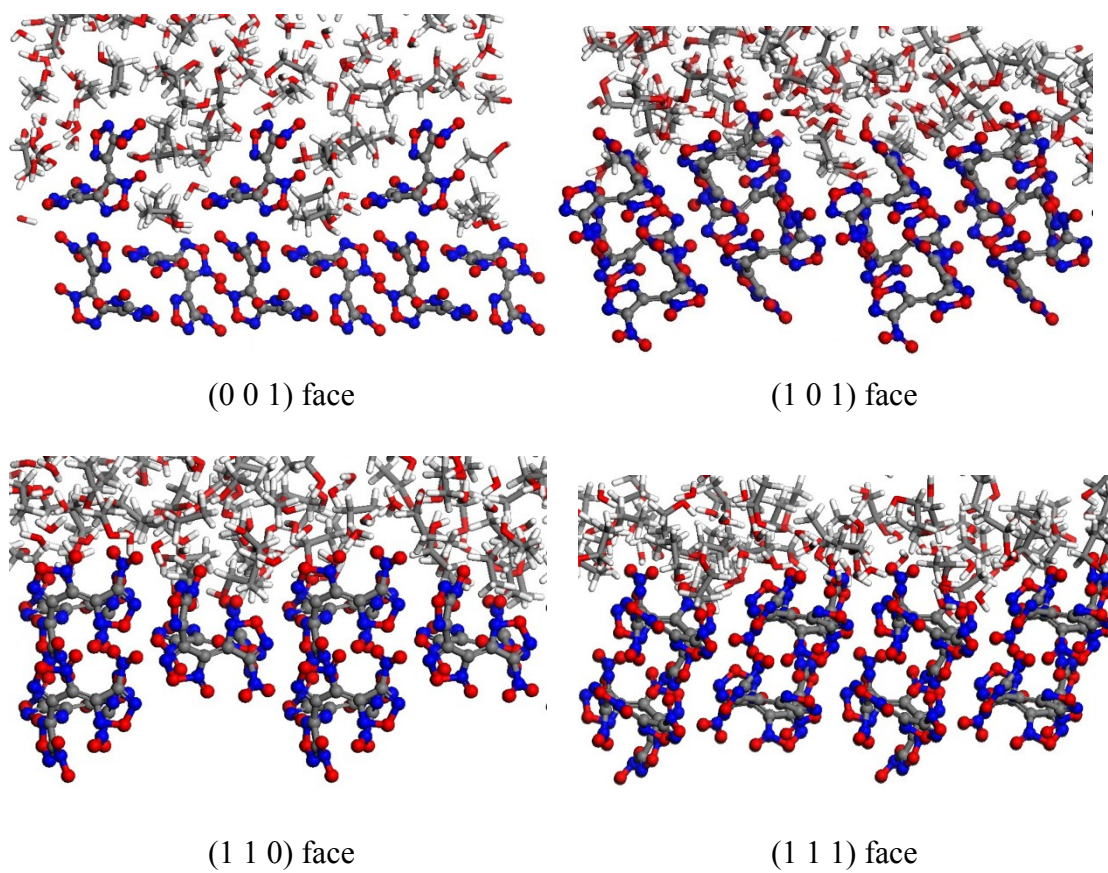


Fig. S2 The configurations of DNTF surface-H₂O/EtOH interfaces from the MD equilibrium.