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Supplementary material

Crystallographic insights into the hydrogen barrier mechanism of polyethylene furanoate (PEF) for high-pressure storage applications: comparison with polyamide 6 and polyethylene

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S1. The fitting process of CVFF parameters

The CVFF parameters for furan rings are fitted to the DFT results with basic numerical optimization methods. The 4 equations for the bond length, bond angle, dihedral torsion and out-of-plane (oop) are as follow:

$$E_r = K_r(r - x_r)^2 \tag{1}$$

$$E_\theta = K_\theta(\theta - x_\theta)^2 \tag{2}$$

$$E_\phi = K_\phi[1+\cos(n_\phi\phi - x_\delta)] \tag{3}$$

$$E_\chi = K_\chi[1+cos(n_\chi\chi - x_\chi)] \tag{4}$$

where r, θ, ϕ, χ represent the bond length, bond angle, dihedral angle and improper dihedral angle, respectively. Figure S1 shows the labels of atoms near furan rings and the fitted parameters are shown in Table S1.

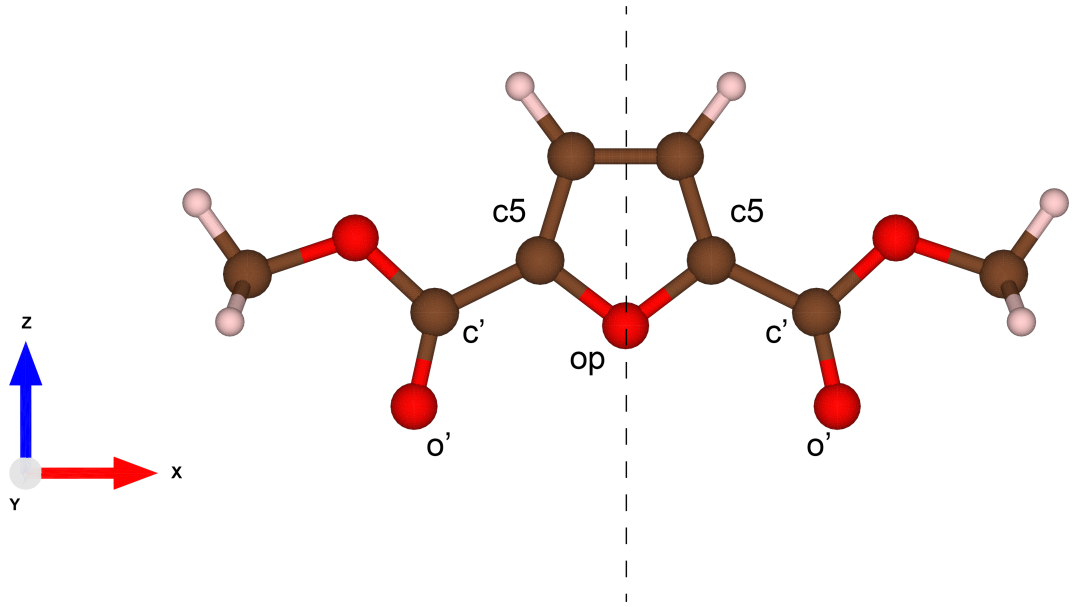

Figure S1. (Color online) Molecular structure of a PEF monomer with atom labels near the furan ring.

Table S1. Fitted results for CVFF parameters.

Order	Label	Equation	K	$x_{\{r,\theta,\delta,\chi\}}$	n
1	c'-c5	A.1	280.9	1.528	–
2	c5-op	A.1	420.0	1.356	–
3	c'-c5-c5	A.2	59.0	127.40	–
4	c5-c5-op	A.2	35.0	110.50	–
5	c'-c5-op	A.2	58.9	125.53	–
6	c5-c'-o'	A.2	79.8	122.11	–
7	o-c'-c5	A.2	106.5	112.56	–
8	c5-op-c5	A.2	75.0	105.28	–
9	c'-c5-op-c5	A.3	8.43	180.0	2
10	c'-c5-c5-op	A.4	12.68	180.0	2