Supporting information of:

Characterization and modeling of CO_2 transport through fluorinated thermoplastics

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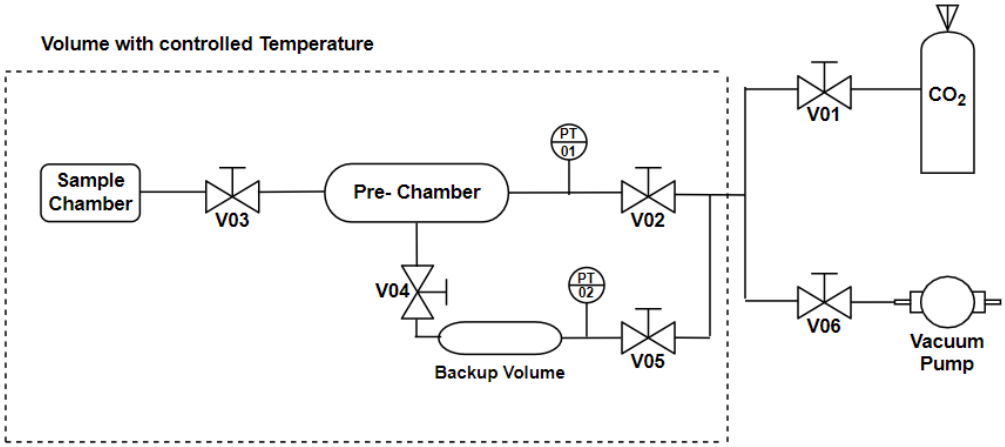

Figure S1: Layout of the Pressure Decay apparatus for CO_2 sorption tests.

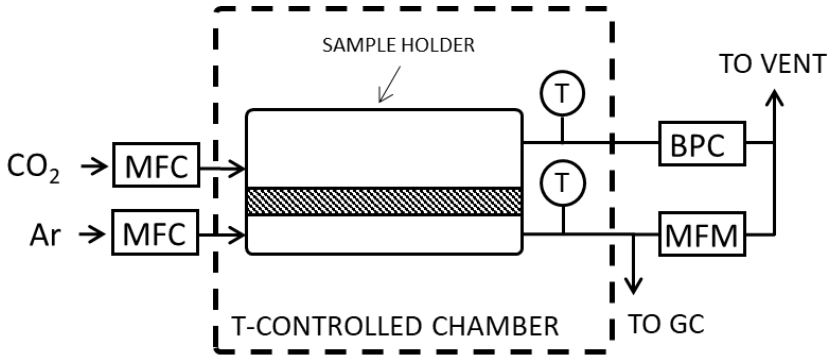

Figure S2: Layout of the permeation setup used in the characterization.

Table S1: Sanchez-Lacombe and non-equilibrium SL equations of state.

	Pure component *i*	
M_i	Molar mass of component *i*	
ρ_i	Density of component *i*	
v_i^*	Molar volume of a lattice cell of component *i*	$v_i^* = \frac{RT_I^*}{p_i^*}$
r_i^0	Number of lattice cells occupied by a molecule of pure component *i*	$r_i^0 = \frac{M_i}{\rho_i^* v_i^*}$
ω_i	Mass fraction of i	
φ_i	Volume fraction of component *i* at close packed conditions	$\varphi_i = \frac{\omega_i/\rho_i^*}{\sum_i^N \omega_i/\rho_i^*}$
ε_i	Non-bonded interaction energy between two lattice cells occupied by component *i*	
L	Mobility coefficient	
L_0	Infinite dilution mobility coefficient	
β	Plasticization factor	
α	Thermodynamic factor	
$\tilde{T}_i$	Reduced temperature of component *i*	$\tilde{T}_i = \frac{T}{T_i^*}$
$\tilde{p}_i$	Reduced pressure of component *i*	$\tilde{p}_i = \frac{p}{p_i^*}$
$\tilde{\rho}_i$	Reduced density of component *i*	$\tilde{\rho}_i = \frac{\rho_i}{\rho_i^*}$
	Multicomponent mixtures	
k_{ij}	Binary interaction parameter between components *i* and *j*	
ρ^*	Characteristic density of the mixture	$\frac{1}{\rho^*} = \sum_i^N \frac{\omega_i}{\rho_i^*}$
p^*	Characteristic pressure of the mixture	$p^* = \sum_i^N \varphi_i p_i^* - \sum_i^{N-1} \sum_{j>i}^N \varphi_i \varphi_j \Delta p_{ij}^*$
Δp_{ij}^*	Binary parameter	$\Delta p_{ij}^* = p_i^* + p_j^* - 2(1-k_{ij})\sqrt{p_i^* p_j^*}$
T^*	Characteristic temperature of the mixture	$T^* = \frac{p^*}{r} \sum_i^N x_i r_i^0 \frac{T_i^*}{p_i^*}$
v^*	Average close-packed molar volume in the mixture	$v^* = \frac{T^* R}{p^*}$
r_i	Number of lattice cells occupied by a molecule in the mixture	$r_i = \frac{r_i^0 v_i^*}{v^*}$
$\tilde{T}$	Reduced temperature of the mixture	$\tilde{T} = \frac{T}{T^*}$
$\tilde{p}$	Reduced pressure of the mixture	$\tilde{p} = \frac{p}{p^*}$

$\tilde{\rho}$	Reduced density of the mixture	$\tilde{\rho} = \frac{\rho}{\rho^*}$

Table S2: Temperature dependence parameters of solubility and diffusion coefficients.

Mat.	S_0				ΔH_S (kJ/mol)	D_0				E_D (kJ/mol)
	6°C	25°C	35°C	45°C		6°C	25°C	35°C	45°C	
PVF	5.9E-03	4.7E-03	2.3E-03	1.9E-03	-22.8	3.1E-09	8.0E-09	1.7E-08	2.4E-08	40.1
PVDF	6.3E-03	3.2E-03	2.4E-03	2.2E-03	-20.7	1.0E-9	5.7E-09	1.4E-08	2.8E-08	62.8
PTFE	2.7E-03	2.5E-03	2.3E-03	9.6E-04	-20.4	2.8E-08	5.9E-08	7.4E-08	1.3E-07	27.5
FEP	2.7E-03	1.2E-03	9.4E-04	8.2E-04	-23.2	2.4E-08	6.5E-08	1.3E-07	2.0E-07	40.5
ETFE	4.3E-03	2.7E-03	2.0E-03	1.7E-03	-17.6	2.4E-08	6.2E-08	8.6E-08	1.4E-07	34.7

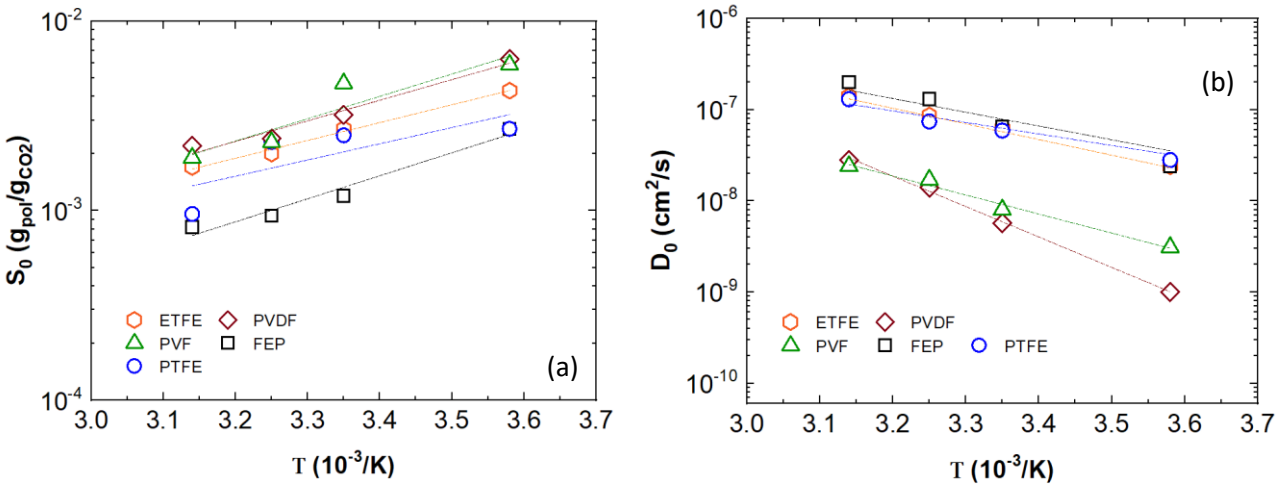

Figure S3: Temperature dependence of solubility coefficient according to van't Hoff equation (a), and diffusion coefficient following Arrhenius equation (b).

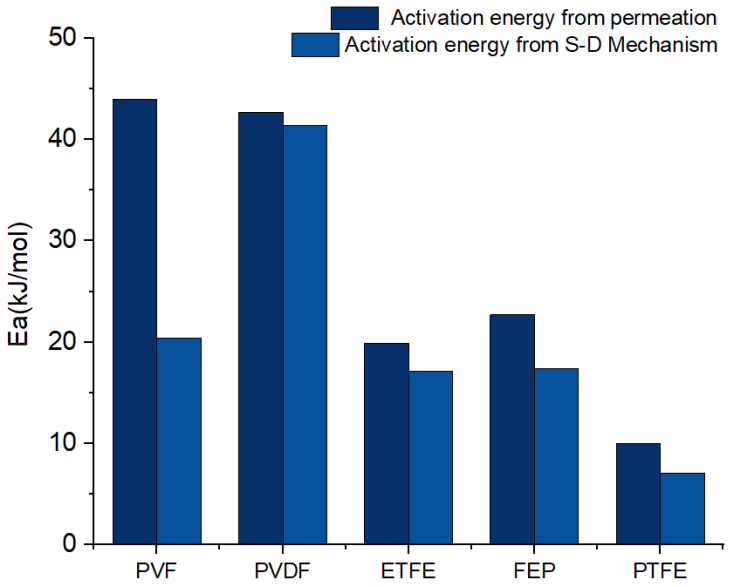

Figure S4: Comparison between activation energy of permeability from permeation experiments and from solution-diffusion mechanism.

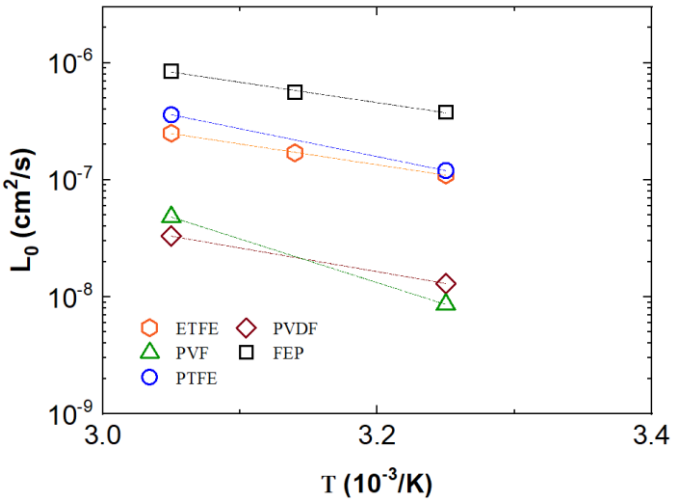

Figure S5: Mobility trend calculated from STM modelling as a function of the inverse of temperature.