Supporting Information

Impact of the chemical structure on the dynamics of mass transfer of water in conjugated microporous polymers: A neutron spectroscopy study

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Table S1. Neutron incoherent cross section (cm^{-1}) of the samples studied in this work. The density of the CMPs is taken to be 0.8 $g.cm^{-3}$.

water concentration (wt%)	S-CMP3	S-CMP1	F-CMP3	H_2O	D_2O
0	1.328	1.242	1.944		
100				5.621	0.138
0.16	1.116			0.899	
0.36	0.850			2.024	
0.475	0.697			2.670	
0.48	0.691			2.698	
0.64	0.478			3.597	
0.65	0.465			3.654	
0.685	0.418			3.850	
0.33	0.890				0.046
0.48	0.691				0.066
0.67	0.438				0.092
0.22			1.516	1.237	
0.32			1.322	1.799	
0.40			1.166	2.248	
0.55			0.875	3.092	
0.64			0.700	3.597	
0.40		0.451		3.710	

Table S2. Bessel function contributions to the dynamical structure factor of rotational motions of H_2O.

Q (Å^{-1})	$j_0^2(Qa)$	$3j_1^2(Qa)$	$5j_2^2(Qa)$
0.5	0.89	0.17	0.00
0.8	0.73	0.39	0.03
1.1	0.53	0.65	0.09
1.4	0.34	0.86	0.20
1.7	0.17	0.99	0.37

Table S3. Fitting parameters for H_2O and D_2O.

		0.5 Å^{-1}	**0.8 Å^{-1}**	**1.1 Å^{-1}**	**1.4 Å^{-1}**	**1.7 Å^{-1}**
H_2O	A(Q)	0.016	0.017	0.017	0.017	0.017
	B(Q)	0.097	0.069	0.057	0.037	0.043
D_2O	A(Q)	0.014	0.016	0.017	0.018	
	B(Q)	0.119	0.091	0.062	0.015	

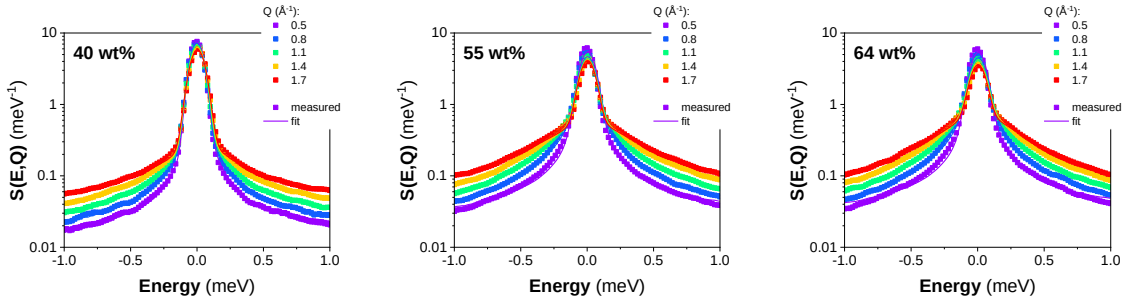

Figure S1. Measured (scatter points), and associated fit (solid line), room temperature Q-dependent QENS spectra of F-CMP3 mixed with different concentrations of H_2O.

Table S4. Fitting parameters for F-CMP3 mixed with different concentrations of H_2O.

	χ^2	B(Q)				
		0.5 Å^{-1}	0.8 Å^{-1}	1.1 Å^{-1}	1.4 Å^{-1}	1.7 Å^{-1}
40 wt%	4.22	0.006	0.004	0.002	0.000	0.000
55 wt%	4.69	0.025	0.019	0.015	0.006	0.006
64 wt%	2.74	0.031	0.023	0.017	0.005	0.001

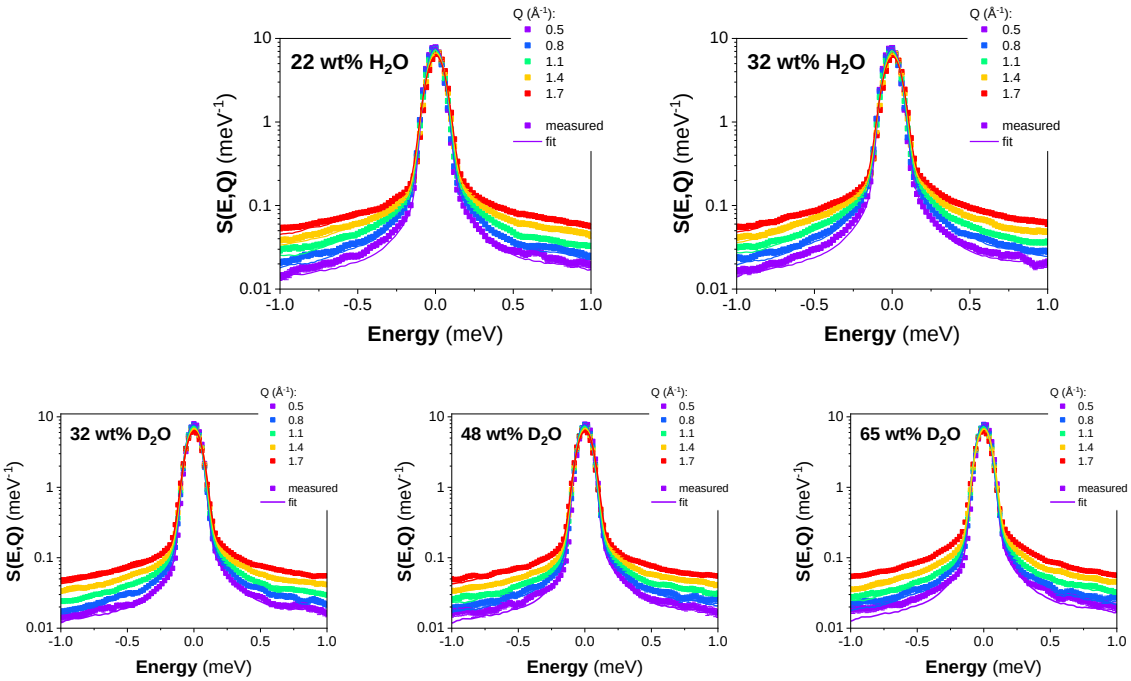

Figure S2. Measured (scatter points), and associated fit (solid lines) using the average model, room temperature Q-dependent QENS spectra of F-CMP3:H_2O at 22 wt% and 32 wt% of H_2O, and F-CMP3:D_2O at 32 wt%, 48 wt% and 65 wt% of D_2O.

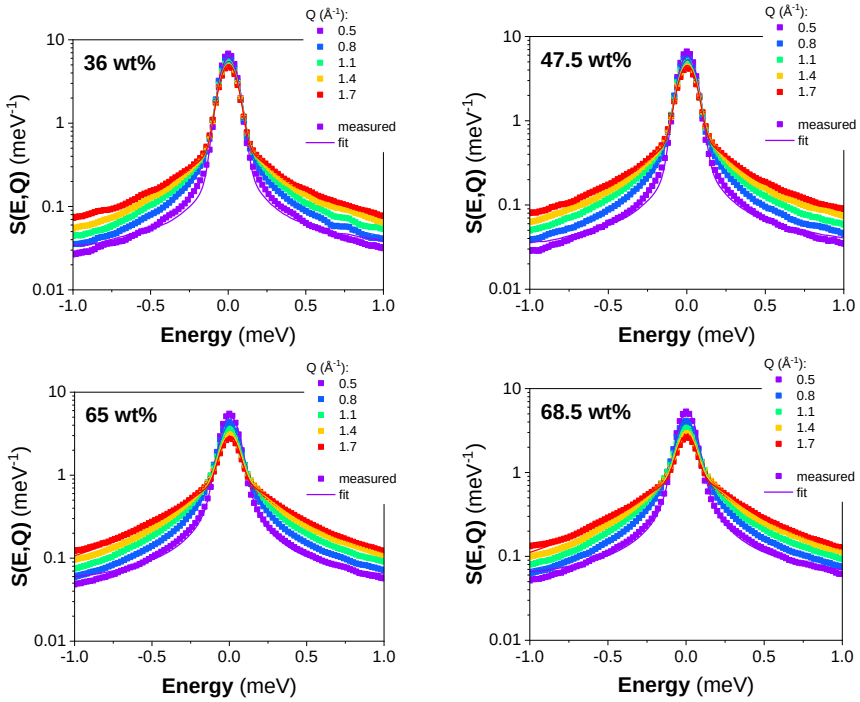

Figure S3. Measured (scatter points), and associated fit (solid line), room temperature Q-dependent QENS spectra of S-CMP3:H_2O with different concentrations of H_2O.

Table S5. Fitting parameters for S-CMP3 mixed with different concentrations of H_2O.

	χ^2	B(Q) 0.5 Å^{-1}	0.8 Å^{-1}	1.1 Å^{-1}	1.4 Å^{-1}	1.7 Å^{-1}
36 wt%	0.85	0.019	0.014	0.011	0.003	0.000
47.5 wt%	0.81	0.023	0.018	0.014	0.005	0.000
65 wt%	2.57	0.047	0.035	0.026	0.012	0.006
68.5 wt%	1.58	0.053	0.038	0.028	0.012	0.007

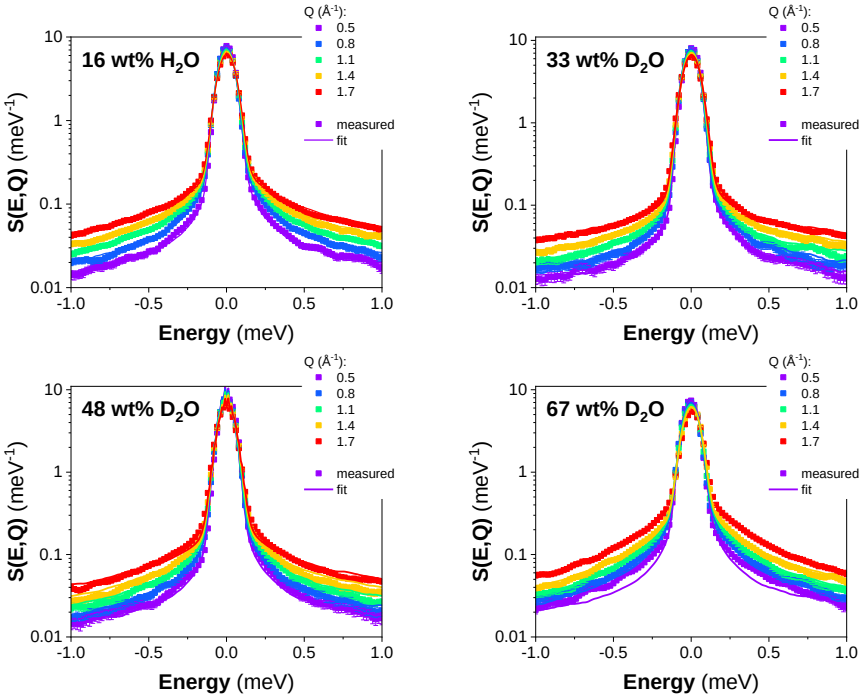

Figure S4. Q-dependent QENS spectra (scatter points) and fit using the average model (solid line) of S-CMP3 mixed at 16 wt% of H_2O, and at 33 wt%, 48 wt% and 67 wt% of D_2O.

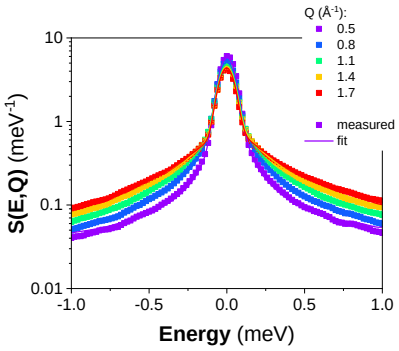

Figure S5. Q-dependent QENS spectra (scatter points) and fit (solid line) of S-CMP1:H_2O (30 wt% of H_2O).

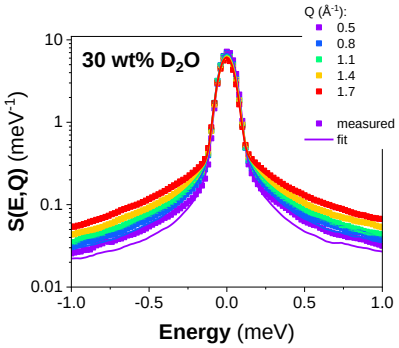

Figure S6. Q-dependent QENS spectra (scatter points) and fit using the average model (solid line) of S-CMP1:D2O (30 wt% of D2O).

Table S6. Fitting parameters for S-CMP1:H2O (30 wt% of H2O)

	χ^2	B(Q)				
		0.5 Å^{-1}	0.8 Å^{-1}	1.1 Å^{-1}	1.4 Å^{-1}	1.7 Å^{-1}
30 wt%	1.02	0.030	0.023	0.018	0.010	0.001

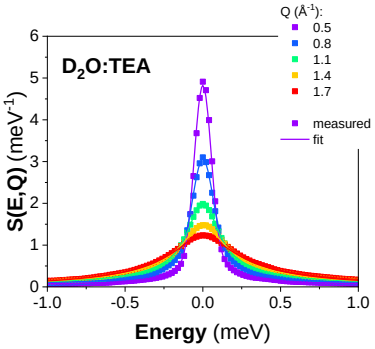

Figure S7. Q-dependent QENS spectra (scatter points) and fit (solid line) of the mixture of solvents D2O:TEA.

Table S7. Fitting parameters for D2O:TEA – χ^2=0.58

	0.5 Å^{-1}	0.8 Å^{-1}	1.1 Å^{-1}	1.4 Å^{-1}	1.7 Å^{-1}
A(Q)	0.017	0.017	0.016	0.016	0.017
B(Q)	0.062	0.065	0.059	0.039	0.010

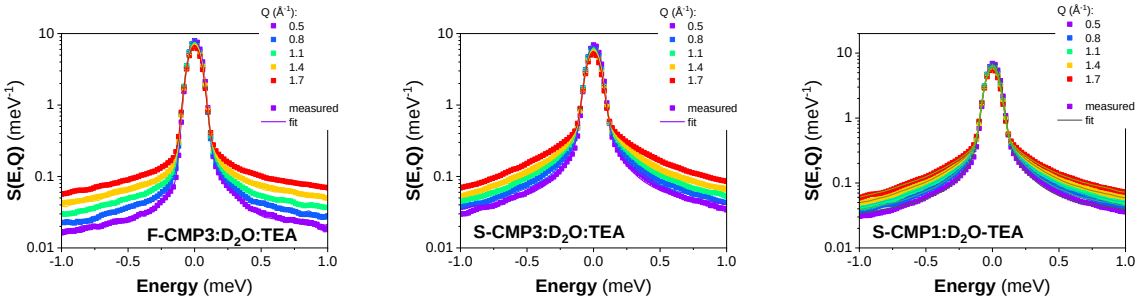

Figure S8. Q-dependent QENS spectra (scatter points) and fit (solid line) of F-CMP3:D2O:TEA (left), S-CMP3:D2O:TEA (middle), and S-CMP1:D2O:TEA (right).

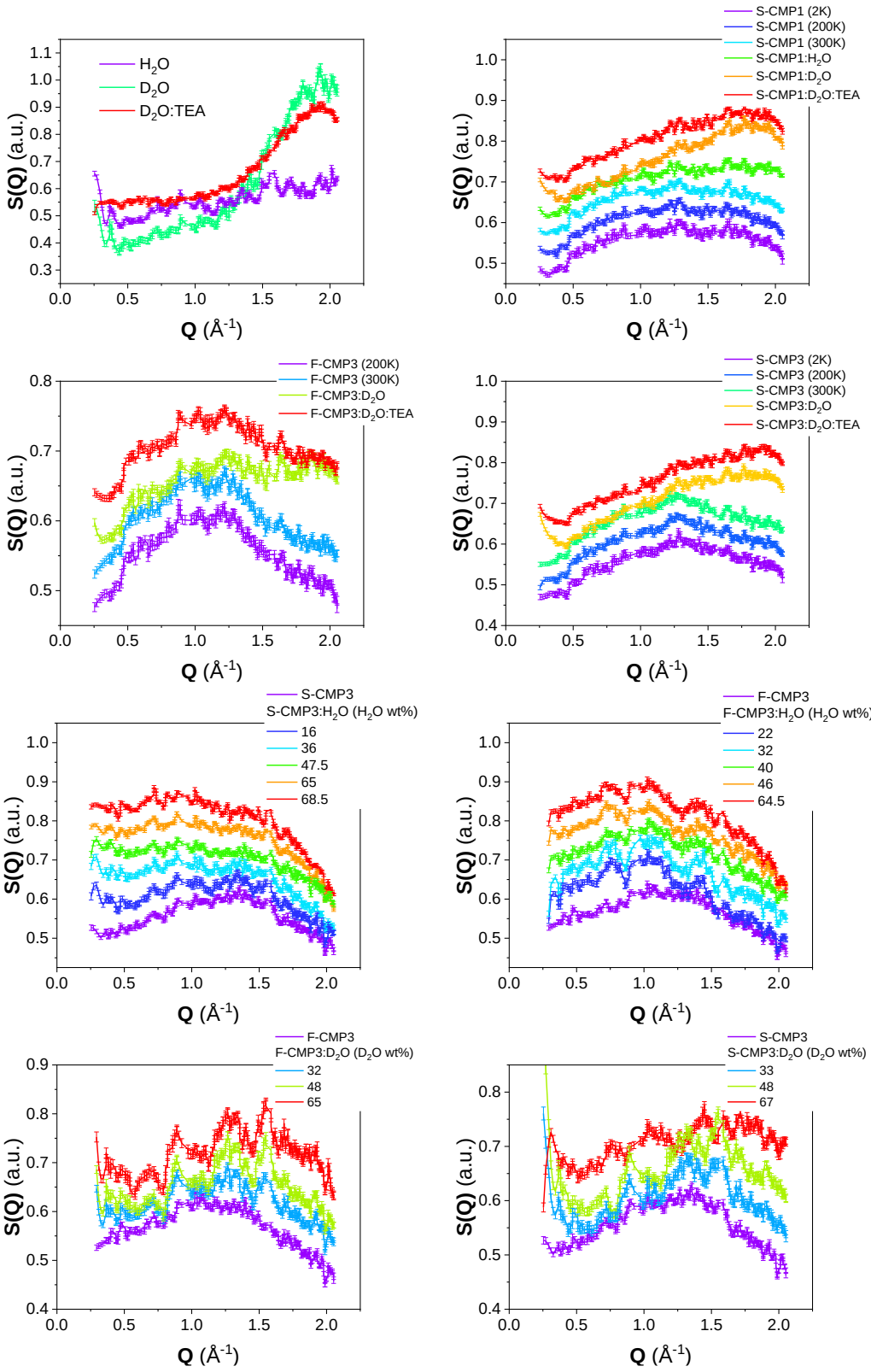

Figure S9. Neutron diffractograms of the studied CMP materials, solvents and their mixtures, from the IN6 measurements.

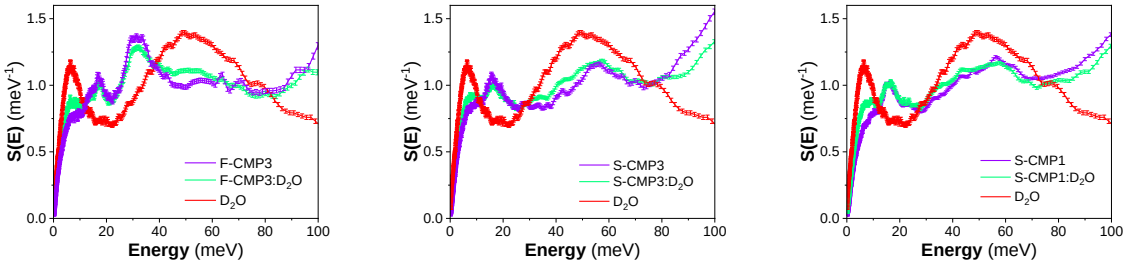

Figure S10. Room temperature generalised density of states (GDOS) of F-CMP3 (left), S-CMP3 (middle) and S-CMP1 (right), bulk D_2O and associated mixture (top).

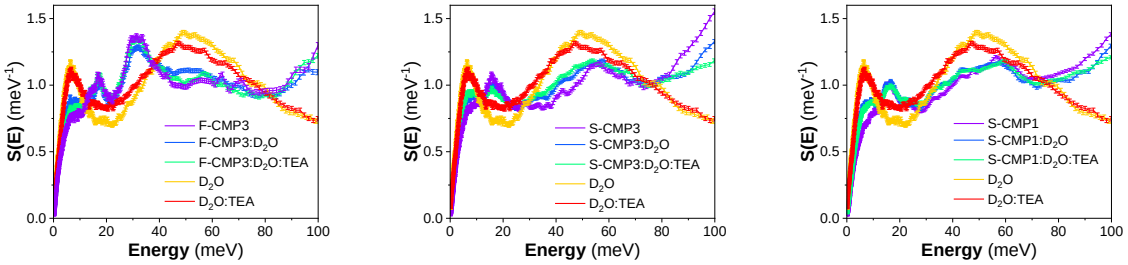

Figure S11. Room temperature generalised density of states (GDOS) of F-CMP3, solvents and associated mixtures (left), S-CMP3, solvents and associated mixtures (middle), and S-CMP1, solvents and associated mixtures (right).

Table S8. Mode frequencies and associated assignments of the CH_2 and SO_2 groups from our DFT-based single-molecule calculations. These modes couple with the vibrational degree-of-freedoms of benzene.[1] The calculated frequencies have been scaled by a factor of 0.97 to better match the measurements.

	Freq (cm^{-1})	**mode**
CH_2	230.569	rocking + out of plane backbone motions
	243.6155	
	693.7828	rocking+E2u
	714.793	wagging+E2g
	741.1382	twisting+E2u
	762.4394	E2g
	796.3894	rocking+A2u
	815.8185	twisting+A2u
	853.2993	rocking+B2g
	869.411	twisting+B2g
SO_2	652.3929	scissor+E2g
	676.3228	E2u
	683.1613	wagging+E2g
	693.6567	E2u
	703.3761	scissor+E2g
	803.6062	A2u
	810.5417	A2u
	846.6839	wagging+E2g
	851.4369	E1g
	851.757	symmetric stretch+E2g

REFERENCES

(1) Preuss, M.; Bechstedt, F. Vibrational Spectra of Ammonia, Benzene, and Benzene Adsorbed on Si (001) by First Principles Calculations with Periodic Boundary Conditions. *Physical Review B - Condensed Matter and Materials Physics* **2006**, *73* (15), 155413. https://doi.org/10.1103/PhysRevB.73.155413.