Improving proton conductivity via crystallinity reduction and sulfonate ligand modification based on UiO-66

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Table S1. Element Content of UiO-66-X and MOG-UiO-66-X (X = -BSA, -pSA)

UiO-66-X	Element Content/%(Experimental/Theoretical)				
	Zr	C	H	N	S
UiO-66	25.71/27.64	36.96/33.96	4.195/3.26	5.09/2.83	0/0
UiO-66-BSA	32.51/38.25	27.68/28.18	3.735/3.46	4.195/2.94	0.195/0.22
UiO-66-pSA	26.87/30.58	30.125/30.20	3.805/3.49	3.89/3.91	0.515/0.537
MOG-UiO-66	21.95/25.6	36.005/33.7	4.1/3.56	3.46/2.62	0/0
MOG-UiO-66-BSA	23.88/27.2	31.35/31.2	4.105/3.0	4.97/4.88	0.33/0.32
MOG-UiO-66-pSA	22.70/25.60	27.975/26.40	4.085/4.90	4.86/5.24	1.32/1.20

Table S2. Empirical Formula and Molecular Formulas of UiO-66-X and MOG-UiO-66-X (X = -BSA, -pASA, -pSA)

UiO-66-X	Empirical Formula	Molecular Formula
UiO-66	$Zr_6C_{56}H_{72}N_4O_{42}$	$Zr_6O_4(OH)_4(BDC)_5(OH)_2\cdot4DMF\cdot4H_2O$
UiO-66-BSA	$Zr_6C_{34}H_{50}N_3O_{32}S_{0.1}$	$Zr_6O_4(OH)_4(BDC)_3(BSA)_{0.1}(OH)_6\cdot3DMF\cdot3H_2O$
UiO-66-pASA	$Zr_6C_{52}H_{47}N_3SO_{39}$	$Zr_6O_4(OH)_4(BDC)_5(pASA)\cdot2DMF\cdot2H_2O$
UiO-66-pSA	$Zr_6C_{51}H_{77}N_6O_{44}S_{0.33}$	$Zr_6O_4(OH)_4(BDC)_{3.5}(pSA)_{0.3}(OH)_4\cdot5DMF\cdot2H_2O$
MOG-UiO-66	$Zr_6C_{60}H_{76}N_4O_{46}$	/
MOG-UiO-66-BSA	$Zr_6C_{52}H_{99}N_7O_{48}S_{0.2}$	/
MOG-UiO-66-pASA	$Zr_6C_{56}H_{73}N_7SO_{35}$	/
MOG-UiO-66-pSA	$Zr_6C_{47}H_{104}N_8S_{0.8}O_{49}$	/

Note: The results of UiO-66-pASA and MOG-UiO-66-pASA are derived by analogy from other materials.

Table S3. T-Plot External Surface Area and Micropore Volume of UiO-66-X and MOG-UiO-66-X (X = -BSA, -pASA, -pSA)

UiO-66-X	T-Plot External Surface Area(cm^2/g)	T-Plot Micropore Volume(cm^3/g)
UiO-66	341.15	0.045381
UiO-66-BSA	215.76	0
UiO-66-pASA	364.74	0
UiO-66-pSA	162.05	0.001861
MOG-UiO-66	461.69	0
MOG-UiO-66-BSA	569.48	0
MOG-UiO-66-pASA	346.83	0
MOG-UiO-66-pSA	489.31	0

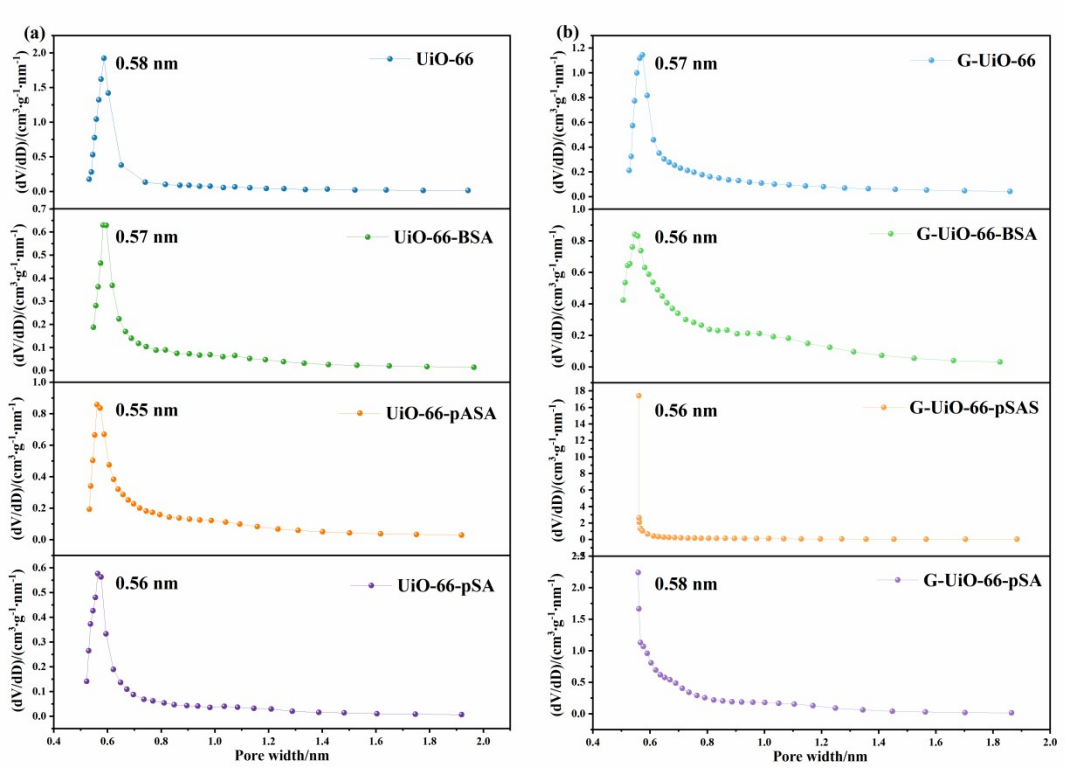

Fig. S1. The most available pore size distribution: (a) UiO-66-X, (b) MOG-UiO-66-X

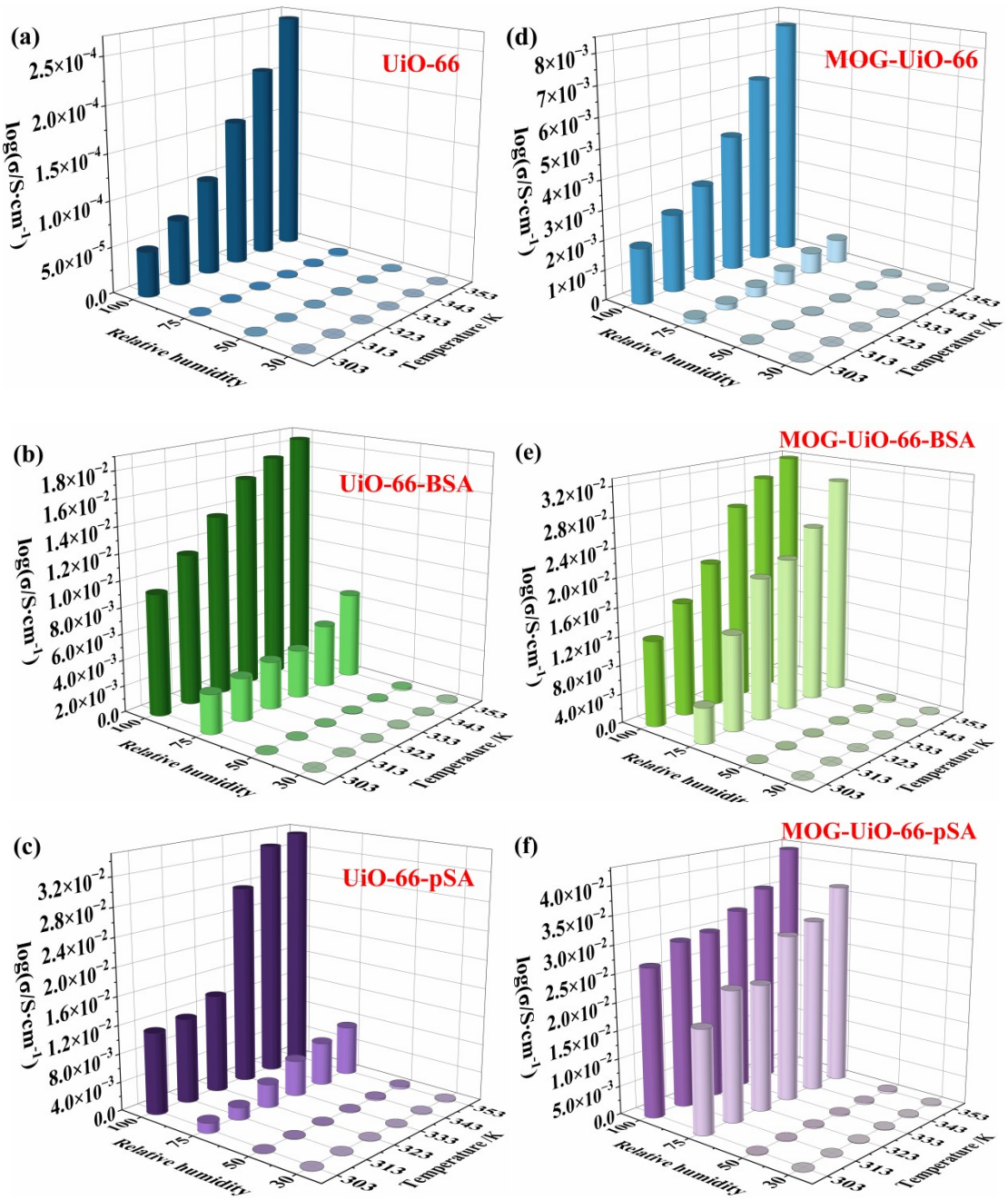

Fig. S2. Conductivity of (a-c) UiO-66-X and (d-f) MOG-UiO-66-X.

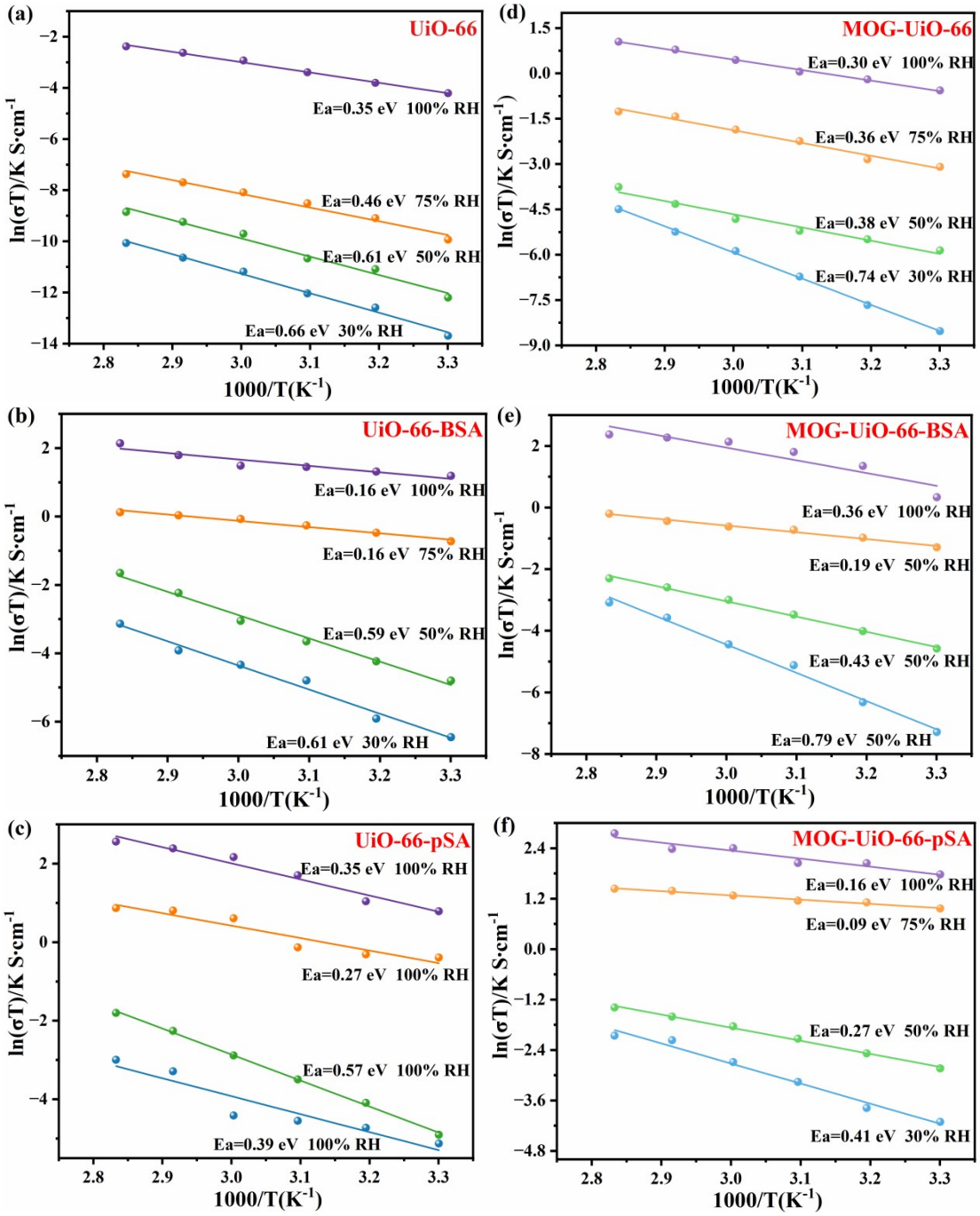

Fig. S3. Activation energies for (a-c) UiO-66-X and (d-f) MOG-UiO-66-X.

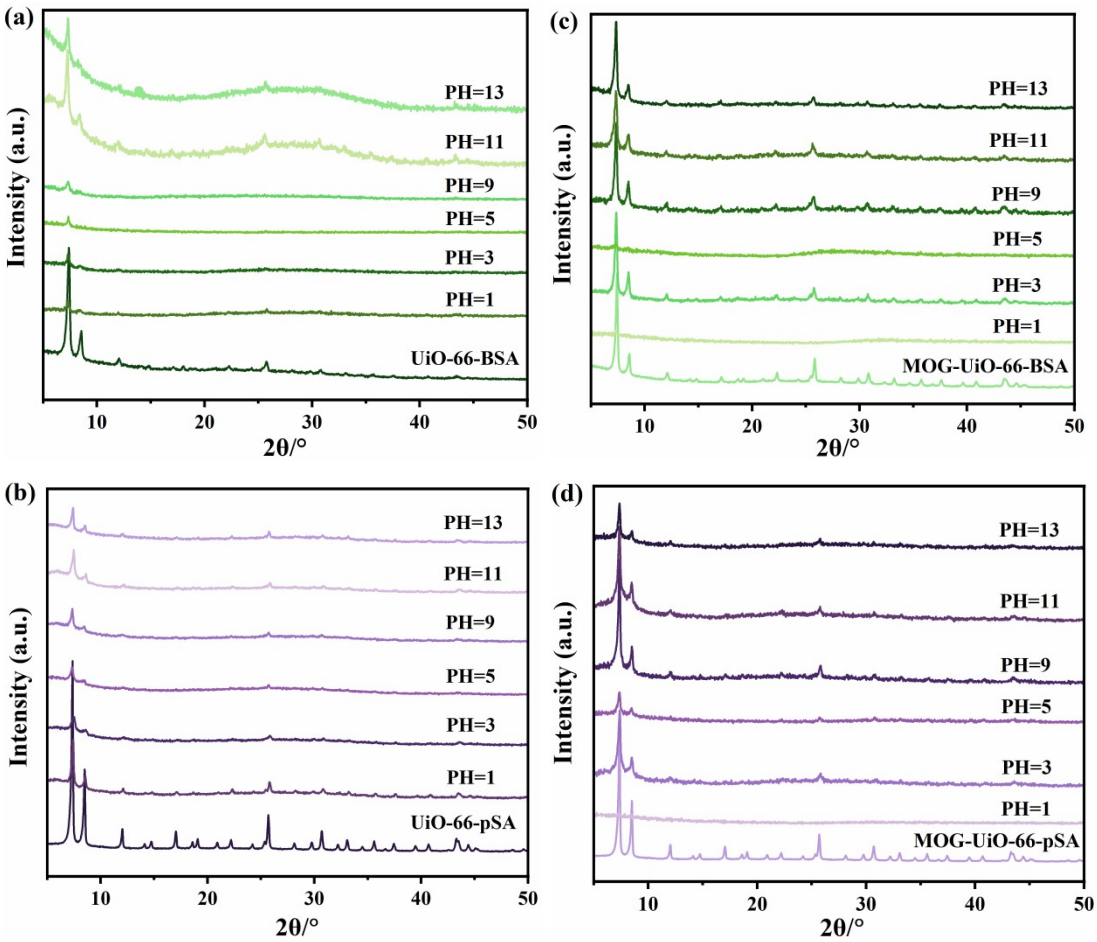

Fig. S4. Stability study for (a, b) UiO-66-X and (c, d) MOG-UiO-66-X at different pH values.

Table S4 σ values ($S \cdot cm^{-1}$) of UiO-66-X and MOG-UiO-66-X at 353 K.

Materials	30% RH	50% RH	75% RH	100% RH
UiO-66	1.21×10^{-7}	4.04×10^{-7}	1.78×10^{-6}	2.62×10^{-4}
UiO-66-BSA	1.23×10^{-4}	1.46×10^{-4}	6.67×10^{-3}	1.85×10^{-2}
UiO-66-pASA	2.69×10^{-4}	3.21×10^{-3}	2.57×10^{-2}	4.56×10^{-2}
UiO-66-pSA	1.42×10^{-4}	3.49×10^{-4}	7.07×10^{-3}	3.44×10^{-2}
MOG-UiO-66	3.16×10^{-5}	6.57×10^{-5}	8.01×10^{-4}	8.06×10^{-3}
MOG-UiO-66-BSA	1.30×10^{-4}	2.84×10^{-4}	3.04×10^{-2}	3.27×10^{-2}
MOG-UiO-66-pASA	2.96×10^{-3}	7.29×10^{-3}	6.48×10^{-2}	9.38×10^{-2}
MOG-UiO-66-pSA	1.83×10^{-4}	3.57×10^{-4}	3.65×10^{-2}	4.22×10^{-2}

Table S5. Activation energies (E_a) of UiO-66-X.

	UiO-66	UiO-66-BSA	UiO-66-pASA	UiO-66-pSA
RHs		E_a/（eV）		
30%	0.66	0.61	0.30	0.39
50%	0.61	0.59	0.29	0.57
75%	0.46	016	0.15	0.27
100%	0.35	0.16	0.20	0.35

Table S6. Activation energies (E_a) of MOG-UiO-66-X.

	MOG-UiO-66	MOG-UiO-66-BSA	MOG-UiO-66-pASA	MOG-UiO-66-pSA
RHs		E_a/（eV）		
30%	0.74	0.79	0.63	0.41
50%	0.38	0.43	0.35	0.27
75%	0.36	0.19	0.11	0.09
100%	0.30	0.36	0.18	0.16