

— Electronic Supplementary Information —

Tuning the ion conductivity of Zr-based metal organic framework ionogels by linker functionalization

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Table S1: The list of chemicals and solvents used for the experiments

Name	Supplier	CAS-Number
Zirconium(IV) chloride $\geq 99.5\%$ trace metals basis	Sigma-Aldrich	10026-11-6
Terephthalic acid 98%	Sigma-Aldrich	100-21-0
2-Aminoterephthalic acid 99%	Sigma-Aldrich	10312-55-7
2,5-Dihydroxyterephthalic acid 97%	abcr GmbH	610-92-4
Hydrochloric acid fuming 37 %	Merck KGaA	7647-01-0
N,N-Dimethylformamide $\geq 99.5\%$	Carl Roth	68-12-2
Selectipur [®] Dimethylcarbonate, anhydrous	Merck KGaA	616-38-6
1-Ethyl-3-methylimidazolium bis(fluorosulfonyl)imide	proionic	235789-75-0
Tetrahydrofuran, anhydrous, 99.8+%, unstab.	Alfa Aesar	109-99-9
Methanol	Merck KGaA	67-56-1
3-Methyl-3-pentanol	Sigma-Aldrich	77-74-7

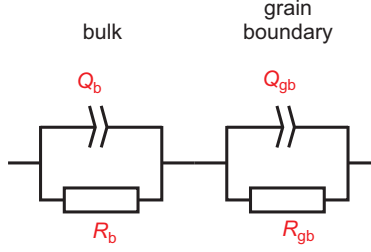


Figure S1: Equivalent circuit used to fit the impedance data at of IL@UiO-66-Li, IL@UiO-66-NH₂-Li, IL@UiO-66-(OH)₂-Li. In addition, for the IL@UiO-66-Li samples a simpler equivalent circuit consisting of only a single RQ unit was used. Q denotes constant phase element.

Table S2: Lattice parameter a obtained from Rietveld refinement and average crystallite size r estimated by using the Scherrer equation, assuming spherical crystallites, for the three MOF materials used in this study.

	UiO-66	UiO-66-NH ₂	UiO-66-(OH) ₂
$a / \text{\AA}$	20.725	20.778	20.820
r / nm	45	50	20

Table S3: Measured BET specific surface area and comparison with values from literature (Katz *et al.*, *Chemical Communications*, **2013**, 49, 9449, DOI: 10.1039/C3CC46105J).

$S_{\text{BET}} / \text{m}^2\text{g}^{-1}$	Literature	Obtained
UiO-66	1580	1520
UiO-66-NH ₂	1200	1297
UiO-66-(OH) ₂	560	441

Table S4: Measured average pore size according to the BJH model. Pore size distribution plots are shown in Figure S5 b) – d).

Diameter / \AA	Tetrahedral pore	Octahedral pore
UiO-66	6.3	17.7
UiO-66-NH ₂	6.3	16.7
UiO-66-(OH) ₂	6.3	17.7

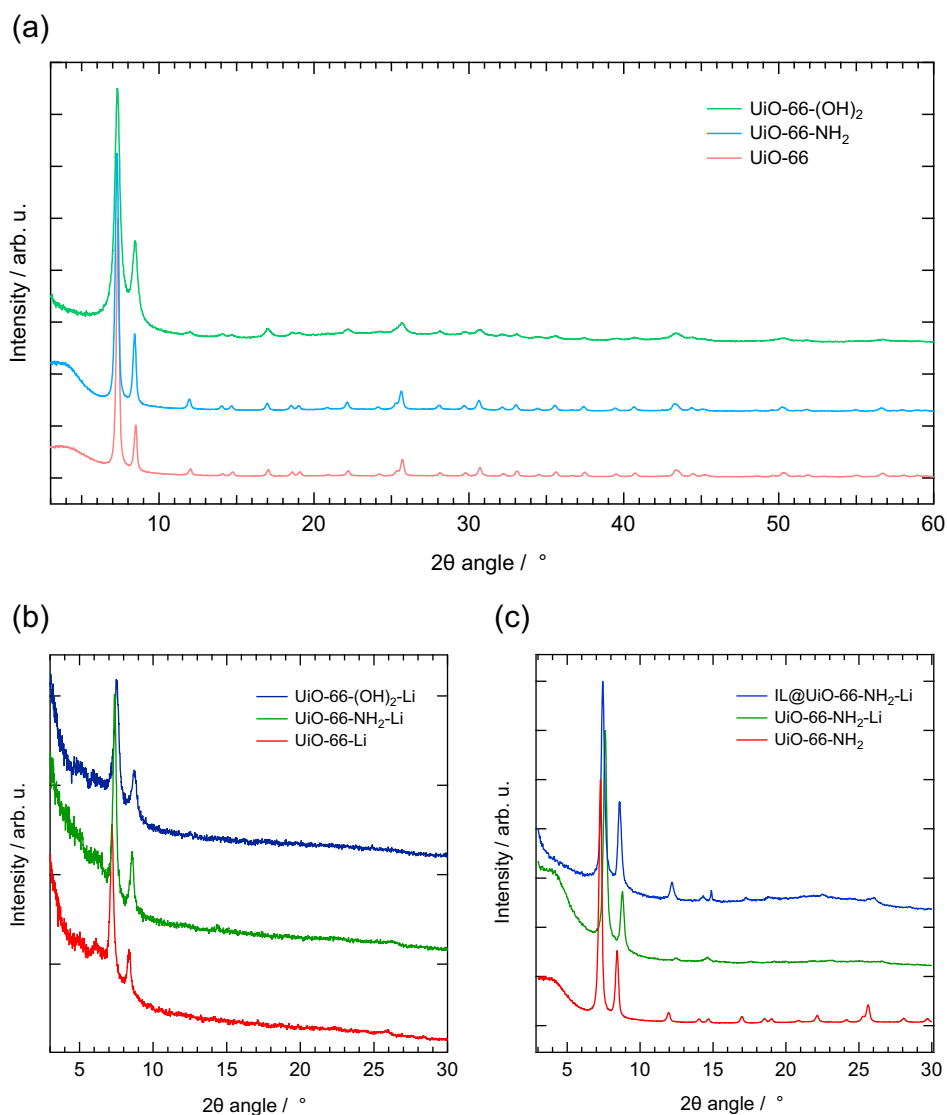


Figure S2: (a) X-ray diffraction patterns of UiO-66, UiO-66-NH₂, UiO-66-(OH)₂ after activation. The three MOF variants are iso-structural, crystallize with the cubic $Fm\text{-}3m$ symmetry and show only very small differences of lattice parameters. (b) X-ray diffraction patterns of UiO-66, UiO-66-NH₂, UiO-66-(OH)₂ after alkoxide grafting. (c) X-ray diffraction patterns of the amine-functionalized MOF measured at successive preparation steps: activated MOF (UiO-66-NH₂), alkoxide-grafted MOF (UiO-66-NH₂-Li) and alkoxide-grafted MOF soaked with ionic liquid (IL@UiO-66-NH₂-Li).

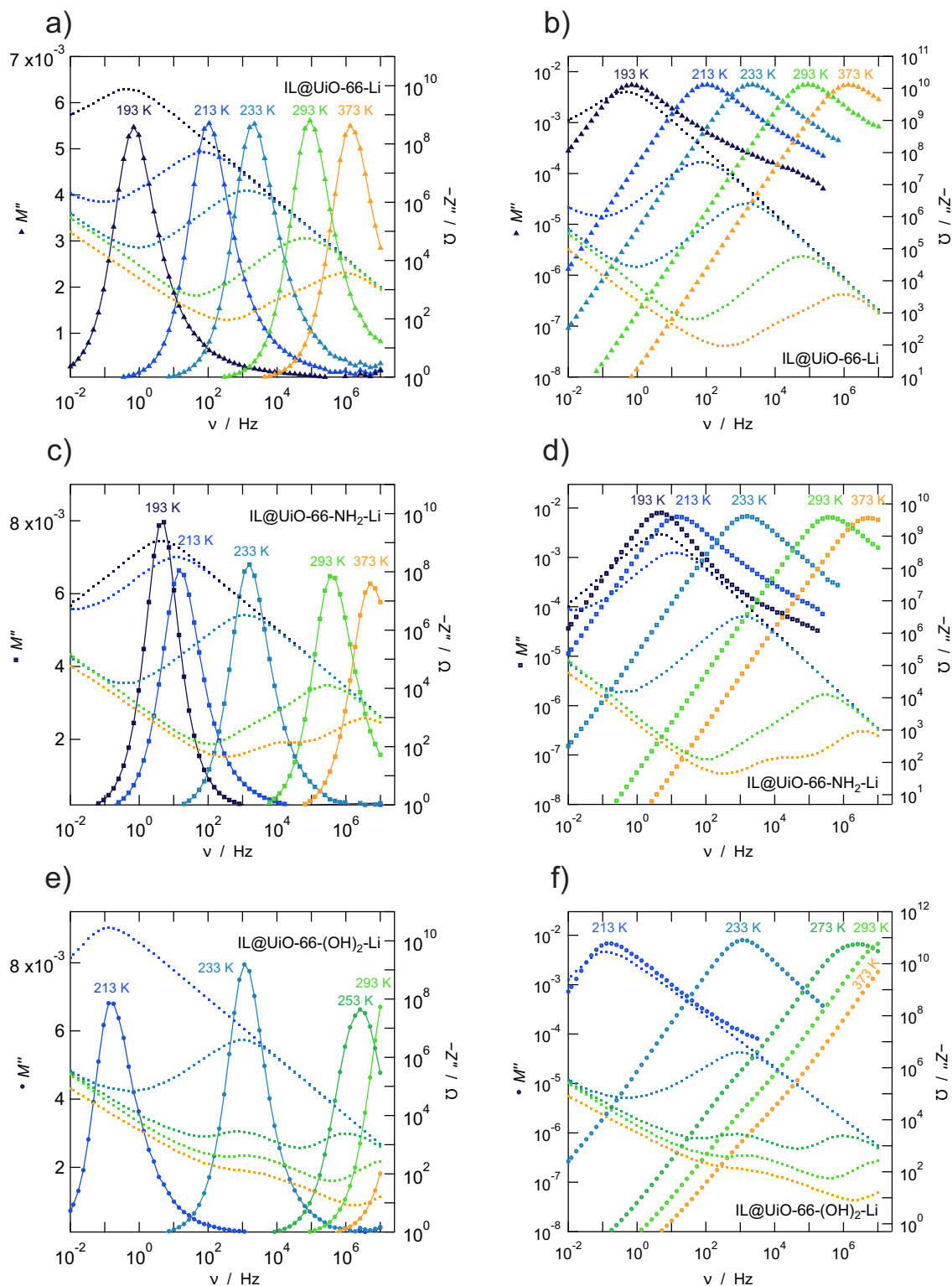


Figure S3: The imaginary part of the electric modulus M'' plotted on both linear and logarithmic scales for the three lithium containing samples. On the right axis the imaginary part of the impedance $-Z''$ is shown. While IL@UiO-66-Li and IL@UiO-66-NH₂-Li show a similar behavior, IL@UiO-66-(OH)₂-Li reveals a distinct electric relaxation behavior, very likely the mobile charged species are different from the other two samples.

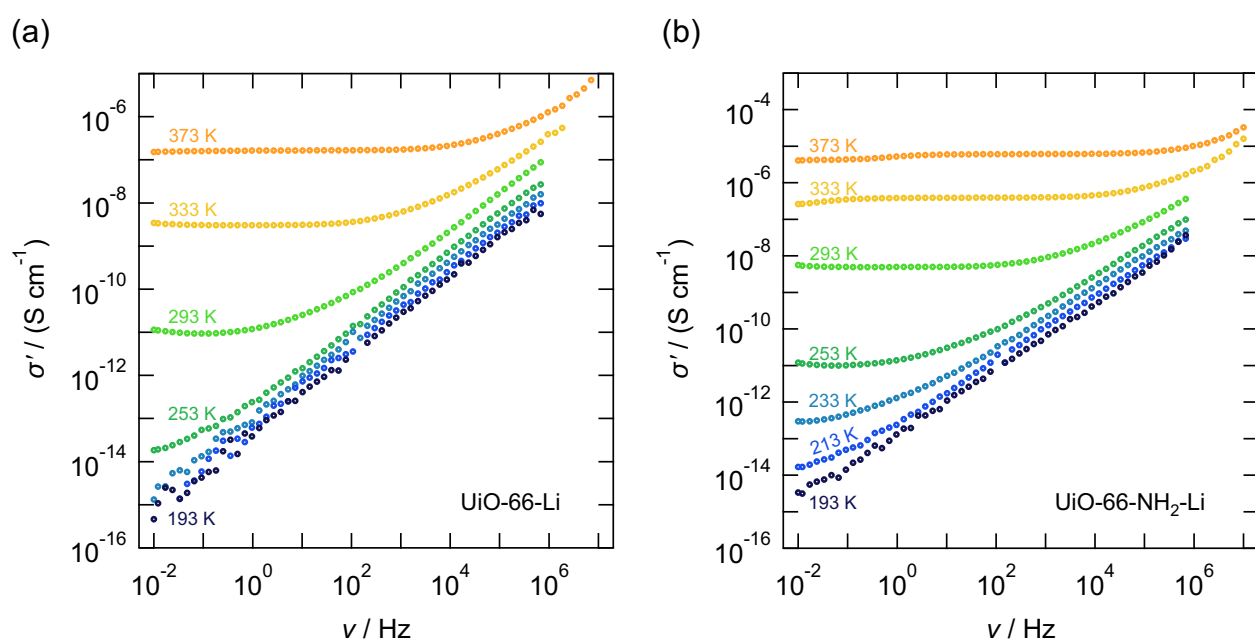


Figure S4: Conductivity isotherms of a) UiO-66-Li and b) UiO-66-NH₂-Li. The figure shows lithium alkoxide samples grafted samples without any ionic liquid added.

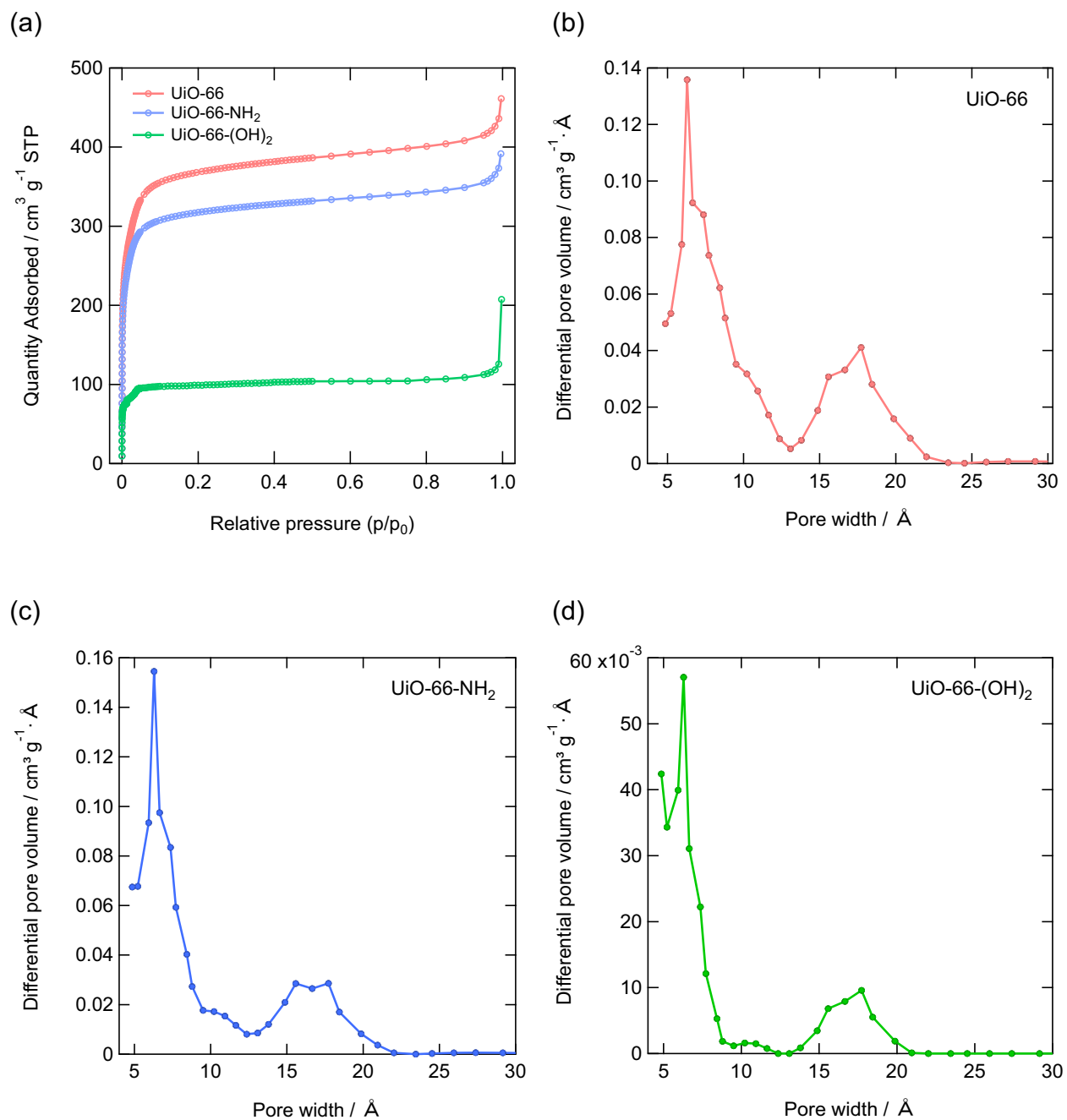


Figure S5: (a) N₂ adsorption isotherms at 77 K of the activated MOFs used for the determination of the specific surface area according to the Brunauer-Emmet-Teller (BET) method. b), c), and d) Pore size distribution plots according to the Barrett–Joyner–Halenda (BJH) model.