# nature portfolio

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Last updated by author(s):	Aug 19, 2023

## **Reporting Summary**

Nature Portfolio wishes to improve the reproducibility of the work that we publish. This form provides structure for consistency and transparency in reporting. For further information on Nature Portfolio policies, see our <u>Editorial Policies</u> and the <u>Editorial Policy Checklist</u>.

For all statistical analyses, confirm that the following items are present in the figure legend, table legend, main text, or Methods section.

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n/a	Confirmed		
	$\square$ The exact sample size (n) for each experimental group/condition, given as a discrete number and unit of measurement		
	🔀 A statement on whether measurements were taken from distinct samples or whether the same sample was measured repeatedly		
	The statistical test(s) used AND whether they are one- or two-sided  Only common tests should be described solely by name; describe more complex techniques in the Methods section.		
	A description of all covariates tested		
	A description of any assumptions or corrections, such as tests of normality and adjustment for multiple comparisons		
	A full description of the statistical parameters including central tendency (e.g. means) or other basic estimates (e.g. regression coefficient) AND variation (e.g. standard deviation) or associated estimates of uncertainty (e.g. confidence intervals)		
	For null hypothesis testing, the test statistic (e.g. <i>F</i> , <i>t</i> , <i>r</i> ) with confidence intervals, effect sizes, degrees of freedom and <i>P</i> value noted <i>Give P values as exact values whenever suitable.</i>		
	For Bayesian analysis, information on the choice of priors and Markov chain Monte Carlo settings		
	For hierarchical and complex designs, identification of the appropriate level for tests and full reporting of outcomes		
	Estimates of effect sizes (e.g. Cohen's <i>d</i> , Pearson's <i>r</i> ), indicating how they were calculated		
	Our web collection on <u>statistics for biologists</u> contains articles on many of the points above.		
Software and code			
Poli	cy information about <u>availability of computer code</u>		

Data collection

Gromacs software package was used to conduct the molecule dynamic simulations (Fig. 2d, e, Fig. 4, Supplementary Fig. 6). Gaussian 09 software package was used to evaluate geometries and energetics of molecules (Fig. 6a-d).

Data analysis

Zeo++ software was used to analyse cavity size distributions of QSPIP-TMC and PIP-TMC network (Supplementary Fig.9).

For manuscripts utilizing custom algorithms or software that are central to the research but not yet described in published literature, software must be made available to editors and reviewers. We strongly encourage code deposition in a community repository (e.g. GitHub). See the Nature Portfolio guidelines for submitting code & software for further information.

### Data

Policy information about availability of data

All manuscripts must include a <u>data availability statement</u>. This statement should provide the following information, where applicable:

- Accession codes, unique identifiers, or web links for publicly available datasets
- A description of any restrictions on data availability
- For clinical datasets or third party data, please ensure that the statement adheres to our <u>policy</u>

Data available on request from the corresponding author.

Research	involving	human	participar	nts, their	data, or	biologica	l material
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Policy information about st and sexual orientation and	udies with <u>human participants or human data</u> . See also policy information about <u>sex, gender (identity/presentation),</u> <u>race, ethnicity and racism</u> .		
Reporting on sex and gen	der This work doesn't involve human participants, their data or biological material. Thanks!		
Reporting on race, ethnic other socially relevant groupings	ity, or This work doesn't involve human participants, their data or biological material. Thanks!		
Population characteristics	Please see above. Thanks!		
Recruitment	This work doesn't involve human participants, their data or biological material. Thanks!		
Ethics oversight	This work doesn't involve human participants, their data or biological material. Thanks!		
Note that full information on t	he approval of the study protocol must also be provided in the manuscript.		
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Please select the one below	that is the best fit for your research. If you are not sure, read the appropriate sections before making your selection.		
Life sciences	Behavioural & social sciences		
For a reference copy of the docum	ent with all sections, see <u>nature.com/documents/nr-reporting-summary-flat.pdf</u>		
Ecological, e	volutionary & environmental sciences study design		
	these points even when the disclosure is negative.		
Study description	We designed a quaternized-spiro piperazine (QSPIP) monomer and translated its beneficial properties into large-area membranes (1 × 2 m2) via interfacial polymerization with trimesoyl chloride. The quaternary ammonium and spiral conformation of QSPIP confer more positive charge and free volume to the membrane, leading to one of the highest permeance (~22 L m-2 h-1 bar-1) compared to state-of-the-art Mg2+/Li+ nanofiltration membranes. Meanwhile, membrane structures are chlorine resistant and membranes performance were reproducible at the membrane module level.		
Research sample	We prepared all membrane samples by ourselves in lab and we didn't use biological samples.		
Sampling strategy	The sample of small membrane and large-area membrane was chosen randomly (8 x 8 cm2) for nanofiltration test. Each data (including flux, rejection, roughness, etc) was repeated for at least three times to avoid the accidental error.		
Data collection	H.W. performed the experimental studies with help from X.F. and J.P. K.C. and X.G. carried out the energy calculation and simulations.		
Timing and spatial scale	Separation performance was evaluated by cross-flow (rate: 0.5 L min-1) nanofiltration and membranes were stabilized at 6 bar for 30 min before test. Each data was continually collected for at least 1 h.		
Data exclusions	No data were excluded from the analyses.		
Reproducibility	X.F. and J.P. succeed to reproduce the experimental findings.		
Randomization	All membrane samples were chosen randomly for test.		
Blinding	We did't involve the blinding in this work. All data were collected.		
Did the study involve field	d work? Yes No		

## Reporting for specific materials, systems and methods

We require information from authors about some types of materials, experimental systems and methods used in many studies. Here, indicate whether each material, system or method listed is relevant to your study. If you are not sure if a list item applies to your research, read the appropriate section before selecting a response.

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