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MDPI

Supporting Information

High-Throughput Computational Screening of Two-Dimensional Covalent Organic Frameworks (2D COFs) for Capturing Radon in Moist Air

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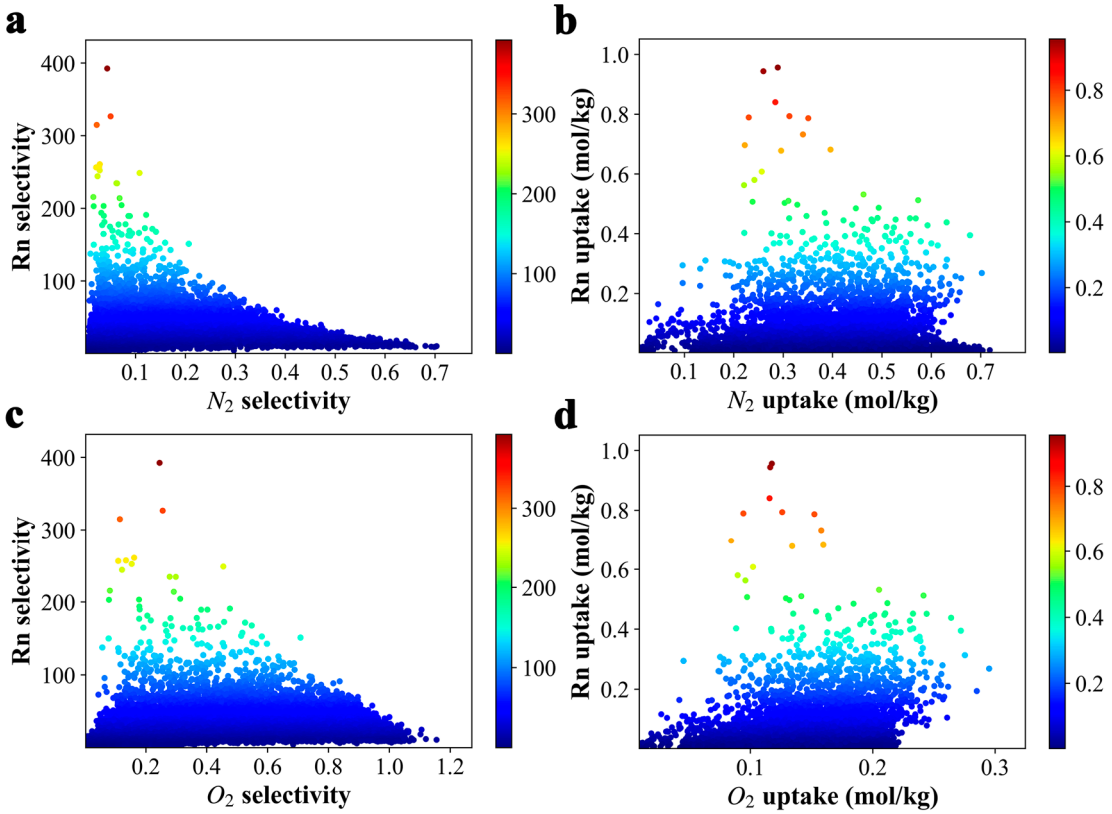


Figure S1. (**a**,**b**) Relationship between radon selectivity/uptake and nitrogen selectivity/uptake of COFs. (**c**,**d**) Relationship betwen radon selectivity/uptake and oxygen selectivity/uptake of COFs.

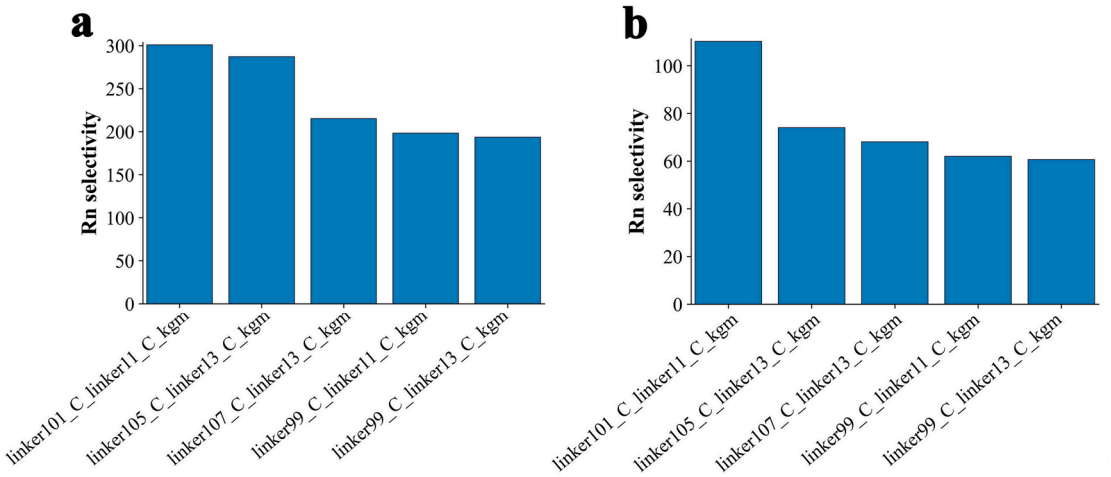


Figure S2. Rn selectivity order of the top five candidates obtained from two different force fields, **(a)** developed by Sanjon et al. [1] and **(b)** developed by Mick et al. [2].

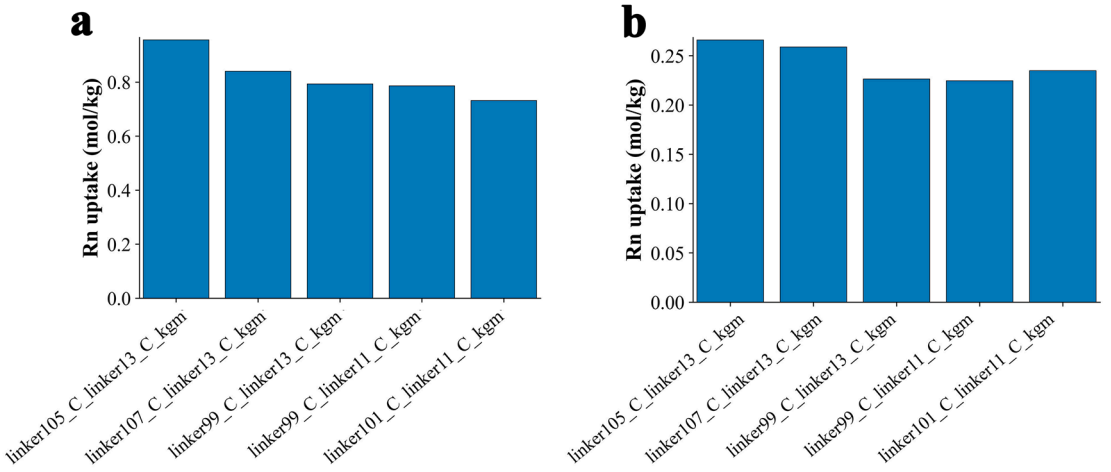


Figure S3. Rn uptake capacity order of the top five candidates obtained from two different force fields, **(a)** developed by Sanjon et al. [1] and **(b)** developed by Mick et al. [2].

Table S1. The IUPAC names and structures of the linker groups in top five COFs. Carbon atoms are shown in gray, nitrogen in light blue, hydrogen in white and Dummy atoms in green.

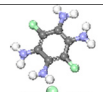
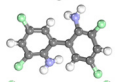
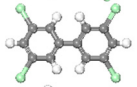
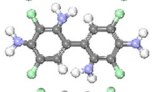
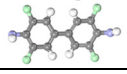
Linker #	IUPAC Name	Structure
11	3,6-dibromobenzene-1,2,4,5-tetraamine	
13	1,4-dibromo-2,3,5,6-tetramethylbenzene	
101	3,3’,5,5’-tetrabromo-2,2’-biphenyldiamine	
99	3,3,5,5-tetrabromo-1,1-biphenyl	
107	3,3’,5,5’-tetrabromo-4,4’-biphenyldiamine	
105	3,3’,5,5’-tetrabromo-4,4’-biphenyldiol	

Table S2. Lennard-Jones Parameters of Rn atom in different force fields.

Model	σ (Å)	ε/k_b (K)
Sanjon et al. [1]	4.53	272.24
Mick et al. [2]	4.15	292.00

References

1. Sanjon, E.P.; Maier, A.; Hinrichs, A.; Kraft, G.; Drossel, B.; Fournier, C. A combined experimental and theoretical study of radon solubility in fat and water. *Sci. Rep.* **2019**, *9*, 10768. https://doi.org/10.1038/s41598-019-47236-y.
2. Mick, J.R.; Barhaghi, M.S.; Potoff, J.J. Prediction of radon-222 phase behavior by Monte Carlo simulation. *J. Chem. Eng. Data* **2016**, *61*, 1625–1631. https://doi.org/10.1021/acs.jced.5b01002.