# Supplementary article

# Design of a Nitrogen-Rich Perylene-Triazine Porous Organic Polymer for Iodine and $CO_2$ Adsorption

P. Anupriya[1] and S. Karpagam[1*]

Department of Chemistry, School of Advanced Science, Vellore Institute of Technology, Vellore -14.Tamil Nadu, India

[1*]Email: skarpagam80@yahoo.com, skarpagam@vit.ac.in

Phone: 91-416-2202334, Fax: 91-416-2243092



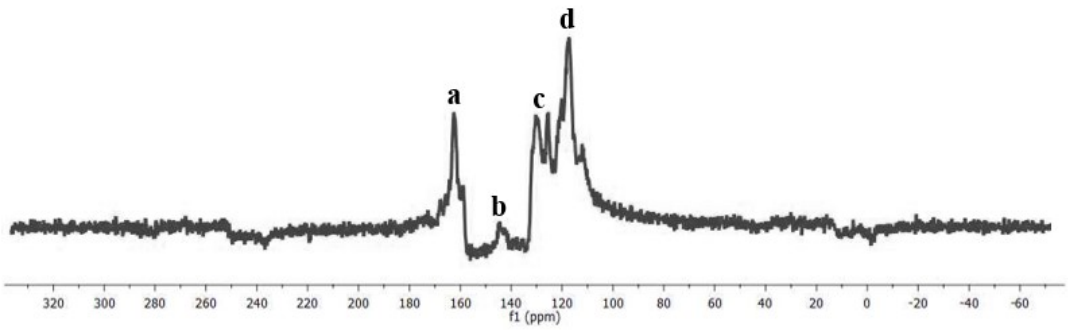

**Fig. S1.** $^{13}$C CP-MAS NMR spectra of **PY-TRI**

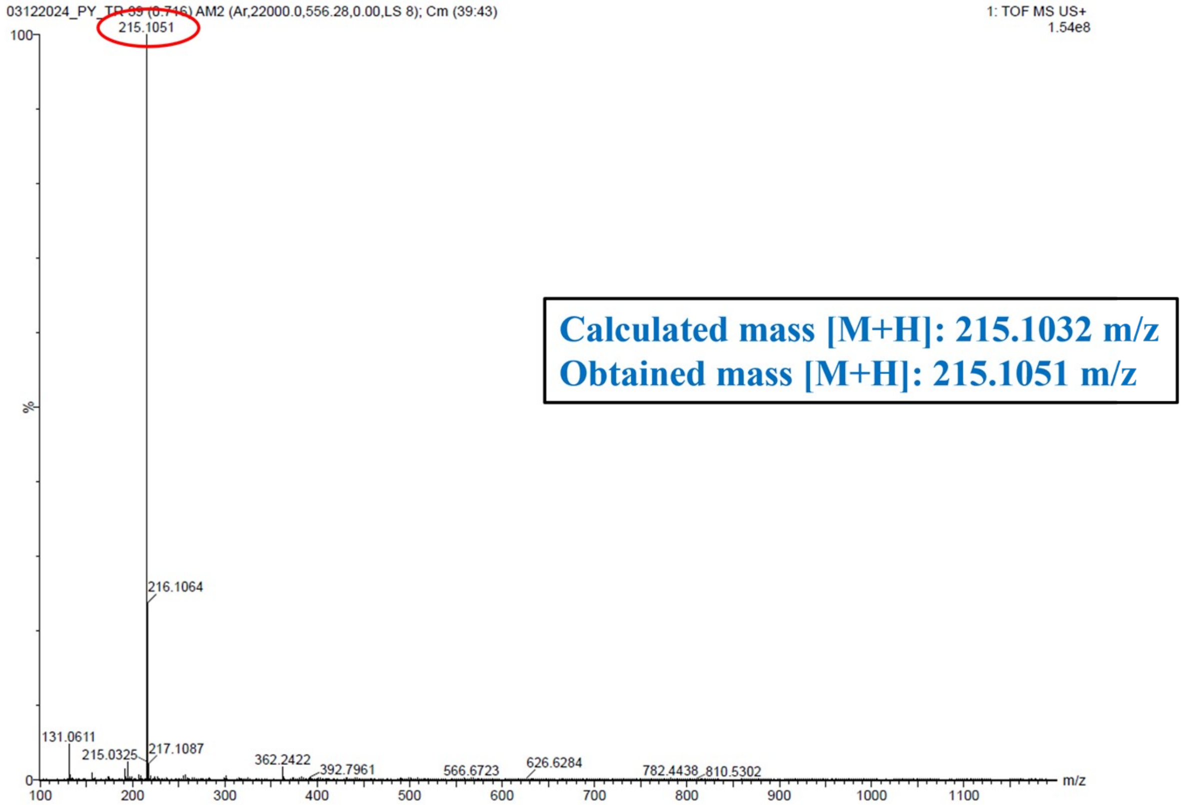


**Fig. S2.** HRMS spectra of compound **PY-TRI**

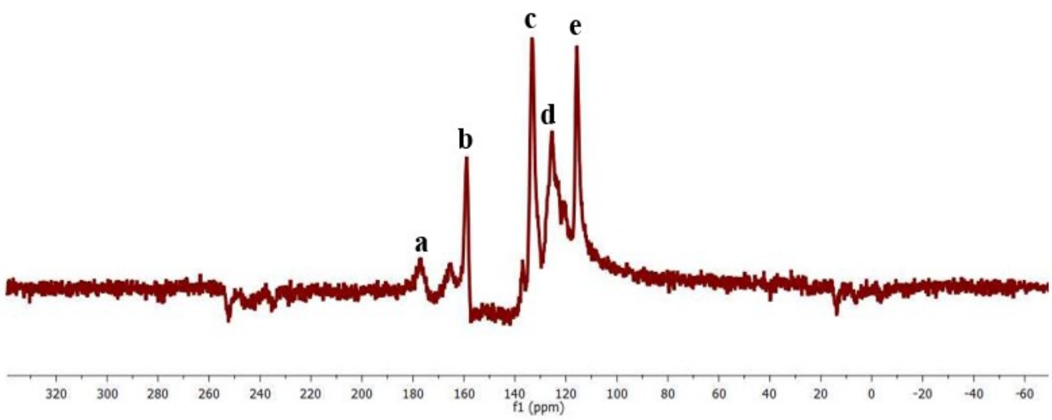


**Fig. S3.** $^{13}$C CP-MAS NMR spectra of **PYTP**

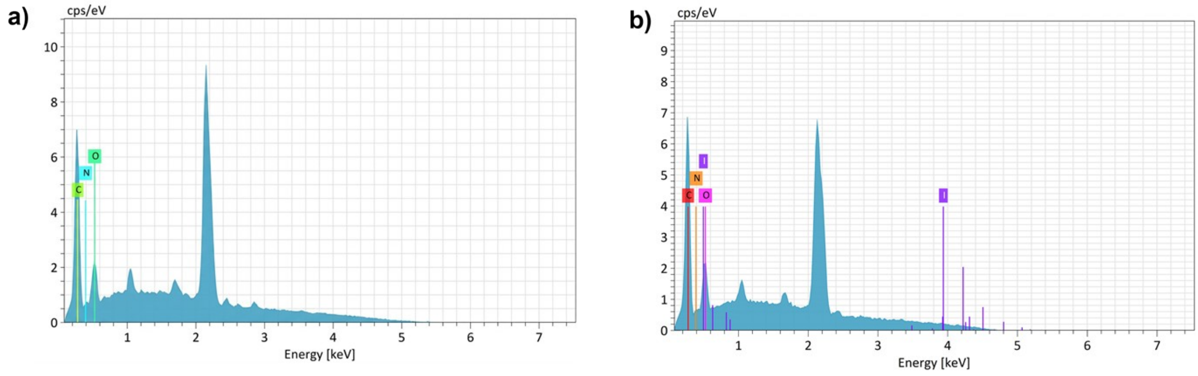


**Fig. S4.** EDX spectra of Polymer a) **PYTP and b) PYTP-$I_2$**

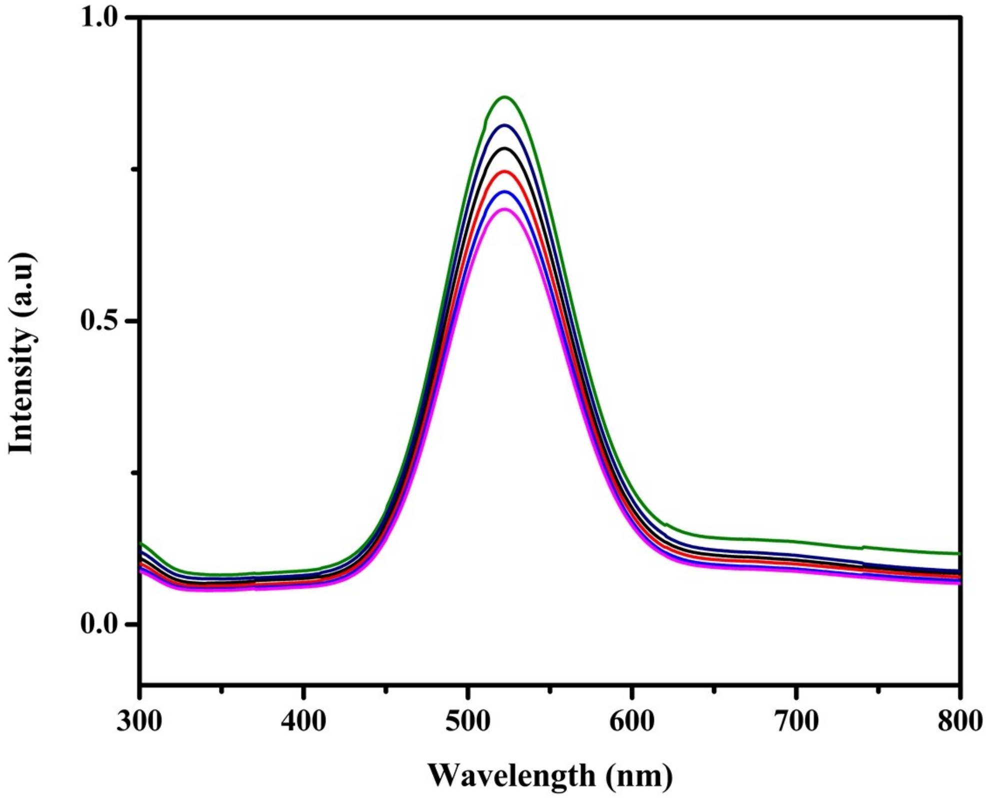


**Fig. S5.** UV-Vis spectra for **PY-TRI**

**Table S1**. Comparison of iodine adsorption performance of PYTP and other reported materials

| S.No. | Compounds | $S_{BET}(m^2g^{-1})$ | Iodine uptake (wt%) | Reference |
|---|---|---|---|---|
| 1 | This work | 135 | 355 | - |
| 2 | Tfp–Td COF | 144.5 | 300 | 1 |
| 3 | PAOP-4 | 209.9 | 108 | 2 |
| 4 | P-TzTz | 137 | 326 | 3 |

| | | | | |
|---|---|---|---|---|
| 5 | CTF-CAR | 277 | 286 | 4 |
| 6 | TTPT | 315.5 | 177 | 5 |
| 7 | NOP-54 | 1178 | 202 | 6 |
| 8 | HCMP-1 | 430 | 159 | 7 |
| 9 | Pha-HCOPs | 217.31 | 131 | 8 |
| 10 | HCP | 584 | 460 | 9 |
| 11 | PT-POP | 475 | 340 | 10 |

**Table S2**. Comparison of $CO_2$ adsorption performance of PYTP and other reported materials

| S.No. | Compounds | Temperature T (K) | $CO_2$ uptake $cm^3$ ($cm^{-3}$) | Reference |
|---|---|---|---|---|
| 1 | This work | 273 | 50 | - |
| 2 | UTSA-30a | 298 | 44.9 | 11 |
| 3 | Cu-F-pymo | 273 | 51.7 | 12 |
| 4 | JUC-199 | 273 | 35 | 13 |
| 5 | NTU-55 | 273 | 63 | 14 |
| 6 | NTU-67 | 298 | 58 | 15 |
| 7 | MOF-808-ARG | 298 | 50.3 | 16 |
| 8 | CD-MOF-1 | 273 | 56 | 17 |
| 9 | CD-MOF-2 | 273 | 68.2 | 17 |
| 10 | Zn-DPNA | 273 | 72 | 18 |

## References

1. S. Song, Y. Shi, N. Liu and F. Liu, RSC Adv., 2021, 11, 10512–10523.

2. Y. T. Wang, L. C. An, Y. Q. Zhang, X. K. Zhang, Z. F. Gao and Y. H. Zhang, J. Appl. Polym. Sci., 2020, 138, 12.

3. X. Pan, C. Ding, Z. Zhang, H. Ke and G. Cheng, Microporous Mesoporous Mater., 2020, 300, 110150.

4. H. Wang, N. Qiu, X. Kong, Z. Hu, F. Zhong, Y. Li and H. Tan, ACS Appl. Mater. Interfaces, 2023, 15, 14846–14853.

5. T. Geng, W. Zhang, Z. Zhu, G. Chen, L. Ma, S. Ye and Q. Niu, Polym. Chem., 2018, 9, 777–784.

6. D. Chen, Y. Fu, W. Yu, G. Yu and C. Pan, Chem. Eng. J., 2018, 334, 900–906.

7. Y. Liao, J. Weber, B. M. Mills, Z. Ren and C. F. J. Faul, Macromolecules, 2016, 49, 6322–6333.

8. L. Lin, H. Guan, D. Zou, Z. Dong, Z. Liu, F. Xu, Z. Xie and Y. Li, RSC Adv., 2017, 7, 54407–54415.

9. X. Li, G. Chen, J. Ma and Q. Jia, Sep. Purif. Technol., 2019, 210, 995–1000.

10. F. K. Esmaeiltarkhani, M. Dinari and N. Mokhtari,New J. Chem., 2024, 48, 1943–1951.

11. Y. He, S. Xiang, Z. Zhang, S. Xiong, F. R. Fronczek, R. Krishna, M. OKeeffe and B. Chen, Chem. Commun., 2012, 48, 10856–10858.

12. Y. Shi, Y. Xie, H. Cui, Y. Ye, H. Wu, W. Zhou, H. Arman, R. B. Lin and B. Chen, Adv. Mater., 2021, 33, 2105880.

13. H. He, F. Sun, B. Aguila, J. A. Perman, S. Ma and G. Zhu, J. Mater. Chem. A, 2016, 4, 15240–15246.

14. Q. Dong, Y. Guo, H. Cao, S. Wang, R. Matsuda and J. Duan, ACS Appl. Mater. Interfaces, 2020, 12, 3764–3772.

15. Q. Dong, Y. Huang, K. Hyeon-Deuk, I. Y. Chang, J. Wan, C. Chen, J. Duan, W. Jin and S. Kitagawa, Adv. Funct. Mater., 2022, 32, 2203745.

16. H. Zhu, W. Xue, H. Huang, L. Chen, H. Liu and C. Zhong, Nano Res., 2022, 16, 6113–6119.

17. L. Li, J. Wang, Z. Zhang, Q. Yang, Y. Yang, B. Su, Z. Bao and Q. Ren, ACS Appl. Mater. Interfaces, 2019, 11, 2543–2550.

18. W. Wang, G. D. Wang, B. Zhang, X. Y. Li, L. Hou, Q. Y. Yang and B. Liu, Small, 2023, 2302975.