

The post-synthetic modification of porous materials for improving performance in globally relevant gas and liquid separations

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Humanity faces numerous immense, interconnected challenges including climate change, diminishing clean water access, energy provision, and waste management. While solutions to many of these issues exist conceptually, their practical implementation requires advanced separation technologies capable of efficiently removing targeted species from gas, liquid, or solid mixtures. Despite the maturity of the separation field and its many existing technologies, separations remain highly energy intensive, consuming approximately 15% of global energy.[1] Additionally, many current technologies are economically prohibitive for large-scale deployment. Therefore, developing efficient, low-cost separation technologies presents a significant opportunity—offering substantial global benefits through energy and cost savings while improving environmental quality and human well-being.

Our research focuses on pioneering advanced porous adsorbent materials engineered to separate specific compounds from gases or liquids through precisely controlled chemical and physical interactions at the adsorbent interface. Among the diverse landscape of potential adsorbents, metal-organic frameworks (MOFs) emerge as exceptionally promising candidates, distinguished by their extraordinary internal surface areas—reaching up to 7,800 m²/g—remarkable chemical versatility, and capacity for selectively binding a host of diverse guest species.[2] Through strategic selection of MOF building blocks, including metal ions and organic ligands, we can engineer their pore structures with unprecedented precision for targeted applications.

This presentation will illuminate our research dedicated to developing MOFs, MOF-polymer composites, and MOF-derived carbon materials for addressing globally significant separation challenges.[3-9] We will highlight our recent breakthroughs in adsorbent design, with particular emphasis on innovative post-synthetic modification strategies that dramatically enhance performance. Additionally, we will present detailed performance assessments across multiple critical applications, including carbon dioxide capture, water purification, and resource recovery from waste streams—demonstrating the transformative potential of these materials for a more sustainable world.

[1] D. Sholl, R. Lively, R. *Nature* **2016**, 532, 435–437 .

[2] I. M. Hönicke, I. S. V. Bon, I. A. Baburin, N. Bönisch, S. Raschke, J. D. Evans, S. Kaskel, *Angew. Chem. Int. Ed.* **2018**, 57, 13780–13873.

[2] S. Yang, V. V. Karve, A. Justin, I. Kochetygov, J. Espín, M. Asgari, O. Trukhina, D. T. Sun, L. Peng, W. L. Queen, *Coord. Chem. Rev.*, **2021**, 427, 213525. <https://doi.org/10.1016/j.ccr.2020.213525>

[3] D. T. Sun, L. Peng, W. R. Reeder, D. K. Britt, M. Moosavi, D. Tiana, E. Oveisi, W. L. Queen, *ACS Central Sci*, **2018**, 4, 3, 349–356.

- [4] D. T. Sun, S. Yang, E. Oveisi, N. Gasilova, W. L. Queen, *J. Am. Chem. Soc.* **2018**, *140*, 48, 16697–16703.
- [5] A. Justin, J. Espín, M. J. Pougin, D. Stoian, T. Schertenleib, M. Mensi, I. Kochetygov, A. Ortega-Guerrero, W. L. Queen* submitted, *Adv. Funct. Mater.* **2023**, 2307430. <https://doi.org/10.1002/adfm.202307430>
- [6] V. V. Karve, J. Espín, M. Asgari, S. Van Gele, E. Oveisi, W. L. Queen, *Adv. Funct. Mater.*, **2023**, *33*, 2212283. <https://doi.org/10.1002/adfm.202212283>
- [7] T. Schertenleib, V. V. Karve, D. Stoian, M. Asgari, O. Trukhina, E. Oveisi, M. Mensi, W. L. Queen, *Chem. Sci.*, **2024**, *15*, 8323–8333
- [8] J. Roth, O. Trukhina, D. Alouss, D. Stoian, T. Schertenleib, T. Felder, W. L. Queen, *ChemSusChem.*, **2024**, e202401642. <https://doi.org/10.1002/cssc.202401642>
- [9] L. Peng, S. Yang, S. Jawahery, S. M. Moosavi, A. J. Huckaba, M. Asgari, E. Oveisi, Md. K. Nazeeruddin, B. Smit, and W. L. Queen, *J. Am. Chem. Soc.* **2019**, *141*, 31, 12397–12405.