The Role of High-throughput Computational Screening in Materials Discovery

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Current advances in materials science has resulted in rapid emergence of thousands of functional adsorbent materials, including metal-organic frameworks (MOFs). This clearly creates multiple opportunities for their potential application, but it also creates the following challenge: *how does one identify the most promising structures, among the thousands of possibilities, for a particular application?* Due to practical constraints, experimental trial-and-error discovery is simply not fast enough and therefore more efficient alternatives must be developed to accelerate the discovery and deployment of new adsorbent materials. To tackle this problem our lab has first generated a curated database containing all the MOFs deposited in Cambridge Structural Database (CSD) – a database that is regularly updated by the Cambridge Crystallographic Database Centre with any new entries.[1] Using computational high-throughput screening (HTS) based on grand canonical Monte Carlo simulations and data mining methods we were capable of analyzing the results interactively and obtaining structure-property relationships through 5D visualisation techniques, thus providing invaluable insights to guide synthetic efforts and to reveal physical limits of performance.

We show key examples of computer-aided material discovery, in which we complete the full cycle from rapid HTS of MOF materials for methane and oxygen storage, to identification, synthesis and measurement of experimental adsorption in top-ranked structures. Our study delimits the relationships between structural properties and gas adsorption performance for up to 70,000 already-synthesized MOFs in dynamic 5D representations (Figure 1), allowing the final user to select the optimal material. We also used recent developments in advanced synthesis, engineering and densification of MOFs to produce pure monolithic structures of up to ca. 1 cm^3 size without using high pressures or additional binders.[2] The resulting materials are able to reach, the DOE target for volumetric storage of methane, with a >50% improvement over any previously reported experimental value. They also report new world-record holding material for oxygen storage, which delivers 22.5% more oxygen than the best known material to date.[3,4]

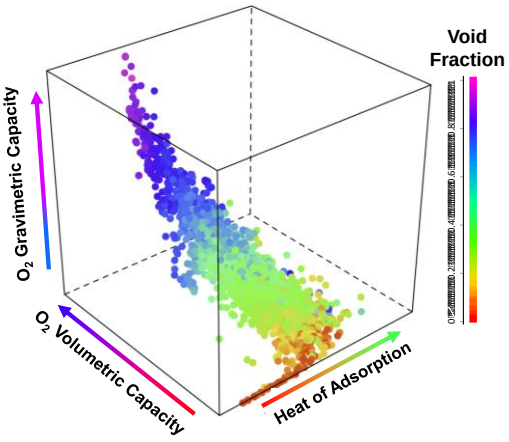

Figure 1. Structure-property relationships between oxygen deliverable capacity, heat of adsorption and void fraction for 2,932 MOF structures at 298 K.

[1] Peyman Z. Moghadam, Aurelia Li, Seth B. Wiggin, Andi Tao, Andrew G. P. Maloney, Peter A. Wood, Suzanna C. Ward, and David Fairen-Jimenez. *Chemistry of Materials* **2017**, 29, 2618–2625.

[2] T. Tian, J. Velazquez-Garcia, T.D. Bennett and D. Fairen-Jimenez. *J. Mat. Chem. A* **2015**, 3, 2999-3005.

[3] T. Tian, Z. Zeng, D. Vulpe, M.E. Casco, G. Divitini, P. A. Midgley, J. Silvestre-Albero, J.-C. Tan, P. Z. Moghadam, and D. Fairen-Jimenez. *Nature Materials* **2018**, 17, 174–179.

[4] P.Z. Moghadam, T. Islamoglu, S. Goswami, J. Exley, M. Fantham, C.F. Kaminski, R.Q. Snurr, O.K. Farha, and D. Fairen-Jimenez. *Nature Communications* **2018**, *Accepted.*