THE UNIVERSITY of EDINBURGH

Edinburgh Research Explorer

Multiscale Screening of Porous Materials: From Molecular Simulation to Process Modelling

Citation for published version:
Hajiahmadi Farmahini, A, Krishnamurthy, S, Gowers, R, Friedrich, D, Brandani, S & Sarkisov, L 2017, 'Multiscale Screening of Porous Materials: From Molecular Simulation to Process Modelling', 11th International Symposium on the Characterization of Porous Solids, Avignon, France, 14/05/17 - 17/05/17.

Link:
Link to publication record in Edinburgh Research Explorer

Document Version:
Publisher's PDF, also known as Version of record

General rights
Copyright for the publications made accessible via the Edinburgh Research Explorer is retained by the author(s) and / or other copyright owners and it is a condition of accessing these publications that users recognise and abide by the legal requirements associated with these rights.

Take down policy
The University of Edinburgh has made every reasonable effort to ensure that Edinburgh Research Explorer content complies with UK legislation. If you believe that the public display of this file breaches copyright please contact openaccess@ed.ac.uk providing details, and we will remove access to the work immediately and investigate your claim.

OPEN ACCESS

Download date: 17. May. 2022

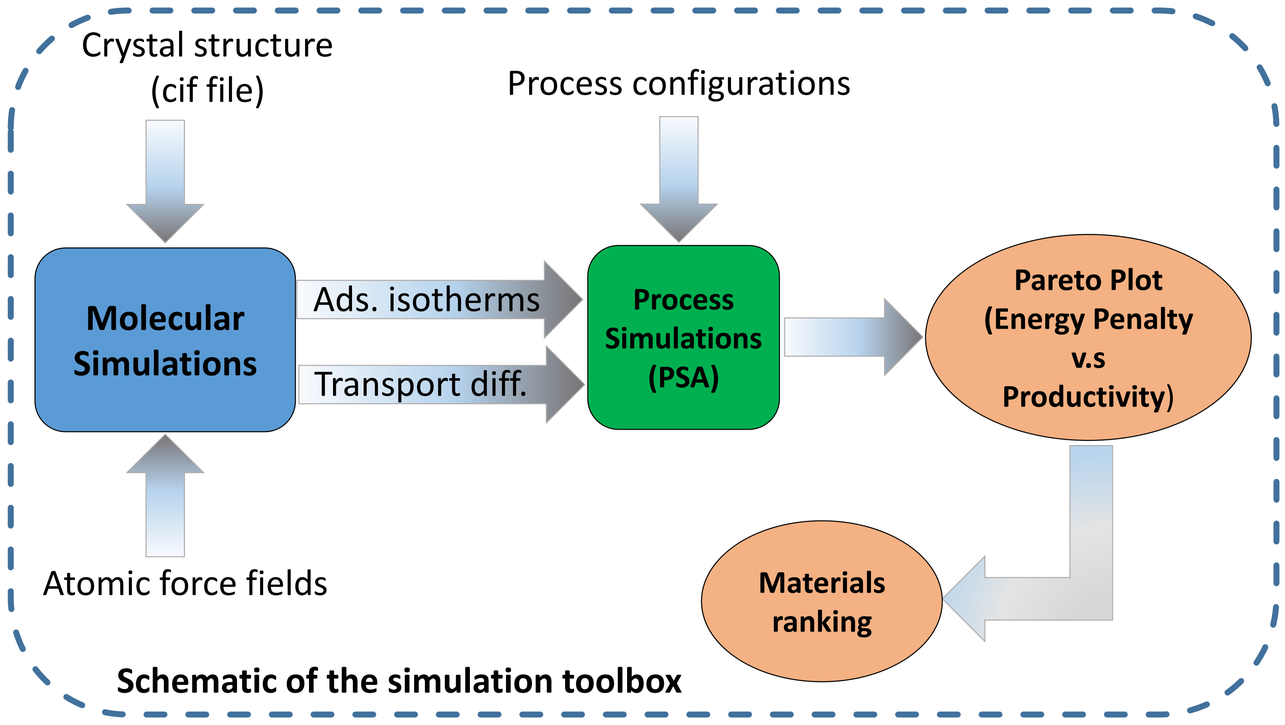
Multiscale Screening of Porous Materials: From Molecular Simulation to Process Modelling

A. H. Farmahini, S. Krishnamurthy, R. Gowers, D. Friedrich, S. Brandani, L. Sarkisov
Institute for Materials and Processes, School of Engineering, The University of Edinburgh
e-mail: a.farmahini@ed.ac.uk

Introduction

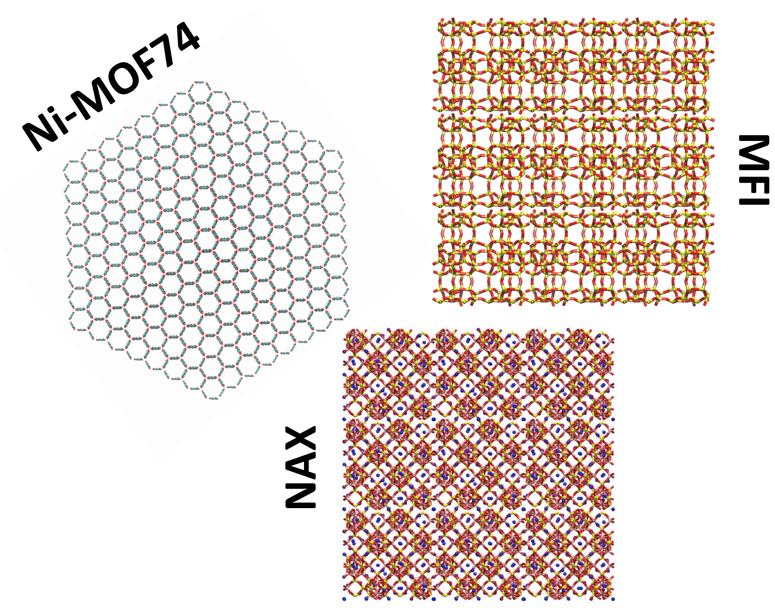
Highlights:

- A multi-scale approach for large-scale screening of porous materials is proposed.
- The key characteristics of the materials are examined in the molecular scales.
- The actual ranking of materials is carried out based on the results obtained from process simulations.
- A process modelling and optimization toolbox is under development in which molecular simulations provide equilibrium and transport data, while the materials ranking is performed in the process scale where effects of process configuration, materials stability and process cycle parameters are taken into account.



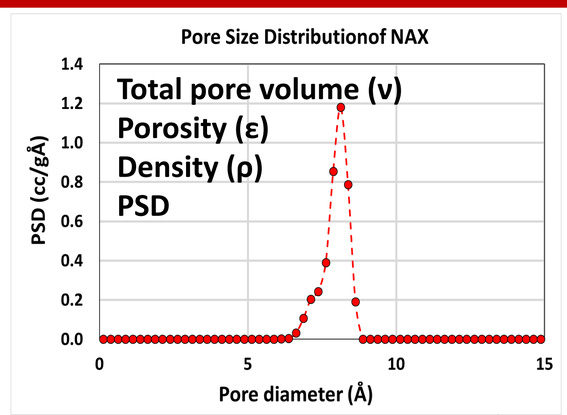
Schematic of the simulation toolbox

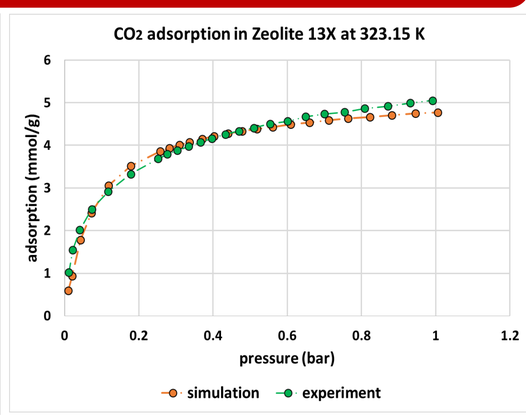
Simulation Modules



Database of Crystal Materials

1. Computational Characterization

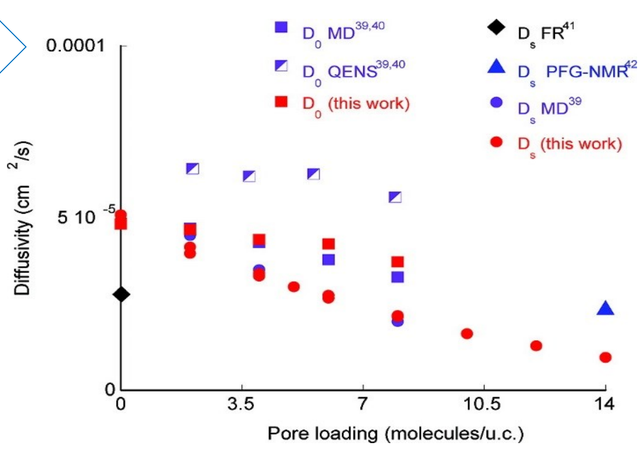




2. Grand Canonical MC Simulations

Dual-site Langmuir model fitted to the GCMC simulated adsorption isotherms

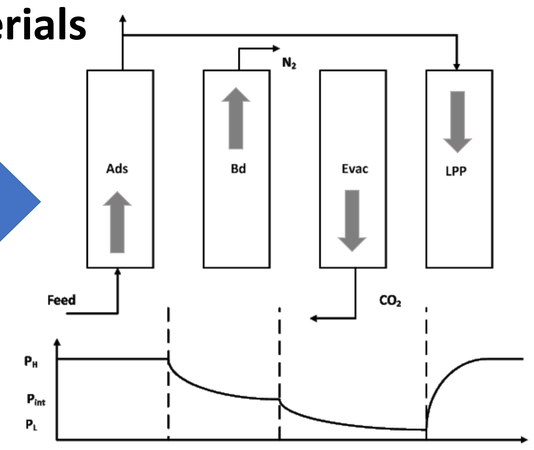
3. Molecular Dynamic Simulations / Classical transport theories



Simulation diffusion of CO_2 and N_2 in Silica Zeolites
(Figure borrowed from J.Phys.Chem.C,2008,112(42),pp16521–16531)

4. Process Simulation

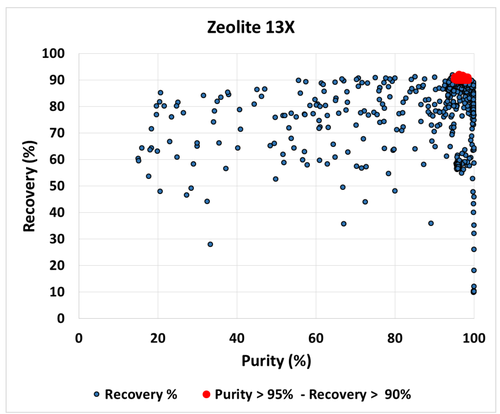
Data obtained from steps 1 to 3

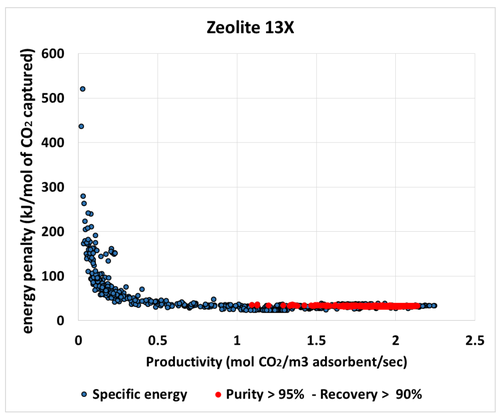


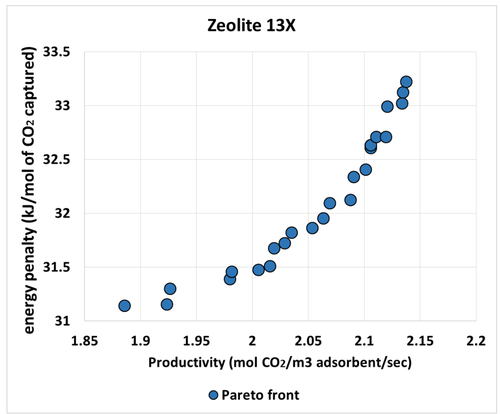
4-step PSA Cycle with LPP:

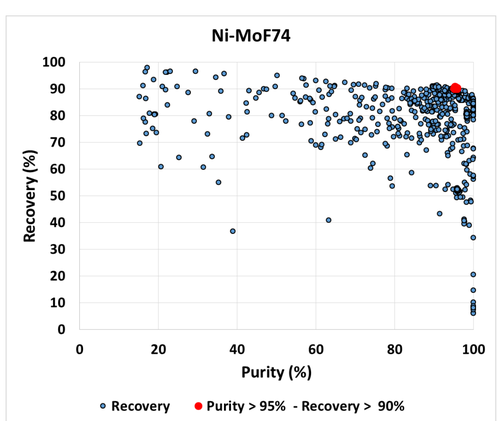
- Adsorption at high pressure with the feed.
- Co-current blowdown to an intermediate pressure to remove nitrogen.
- Counter-current evacuation to remove the product.
- Counter-current pressurizing with the light product to high pressure.

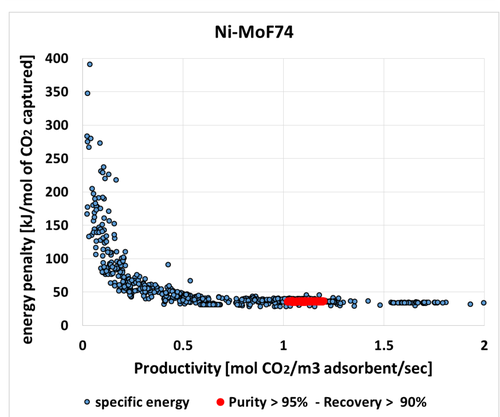
Materials Screening

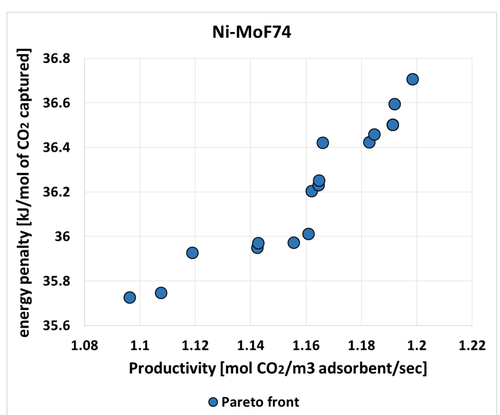












Future work:

- More detailed process study of PSA cycle based on simulation data.
- Improvement of the computational performance of each simulation module (GCMC, MD, Process).
- Modelling gas adsorption for a larger set of crystalline materials to be used in the materials database.
- Materials screening based on the results obtained from process simulation.
- Validation of the results against experiment-based process simulation data.

Acknowledgements:

Edinburgh Compute and Data Facility (ECDF)

EPSRC EP/N007859/1

EPSRC Engineering and Physical Sciences Research Council