

## SYNSORB: SYNergistic SORBents. Gas Separation Technology

#### Overview

Technologies related to separating acetylene and other contaminants from an ethylene gas mixture using novel stable hybrid porous materials.

Industrial separations and purification processes account for 15% of global energy. Physisorption has been touted as an energy-efficient alternative to traditional separation technologies, i.e. distillation. UL researchers have developed:

- Advanced porous materials for gas separation. Hybrid Ultramicroporous Materials (HUMs) and Azolate Ultramicroporous Materials (AUMs) have shown excellent performance over CO2 and C2H2 capture, especially at trace-level concentrations. UL researchers adopt a systematic Crystal Engineering strategy to develop nextgeneration physisorbent materials via precise control over pore size/chemistry and synergistic sorbent separation for the purification of industrially relevant gases. These advanced materials can be used in SSST.
- 2. A one-step method, Synergistic Sorbent Separation Technology (SSST) for the production of polymer-grade ethylene through the removal of acetylene, ethane, and CO2 impurities (CO2/C2H2/C2H6/C2H4).

### Technology

These UL technologies are based on novel stable hybrid porous materials for separating acetylene (C2H4) and other contaminants from a gas mixture. In particular, the invention relates to separating acetylene from a gas mixture containing acetylene and ethylene and/or a gas mixture comprising acetylene and carbon dioxide and/or a gas mixture comprising acetylene, ethylene, and carbon dioxide, yielding polymer grade (.99.9% purity) ethylene.

The materials, TIFSIX-2-Cu-i and SIFSIX-3-Ni belong to a family of hybrid ultramicroporous materials (HUMs) of general formula M'FSIX-L-M (M = divalent transition metal center; L = dipyridyl organic linker; M' = Si, Ti, Ge, Zr, Sn). These materials display excellent water stability and unusual pore chemistry.

In addition to HUM platforms, the UL research team has developed a new platform of AUMs for synergistic sorbent (SYNSORB) separation. SYNSORB addresses the purification of two commodity gases each of which contains  $\geq 2$  impurities: i.e. methane; ethylene.

Stage of Development: Given that the team has lead materials for several carbon capture applications, it is considered that this technology has reached Technology Readiness Level (TRL): 4.

#### **Benefits**

Researchers at the UL have reached several milestones using HUMs for the separation of industrially relevant gases. In 2019, they reported new benchmark selectivities for C2H2 over CO2 and CO2 over CH4. The team have also demonstrated for the first time the selective removal of trace CO2 from humid air, in concentrations as low as 1000 ppm. These novel materials can be used in "Synergistic Sorbent Separation Technology", SSST. This allows the one-step production of polymer-grade ethylene through the removal of acetylene, ethane, and CO2 impurities (CO2/C2H2/C2H6/C2H4).

#### Societal relevance:

• High-volume gas and vapor separations currently account for ca. 15% of global energy consumption. Energyefficient separation of gases from the multicomponent mixtures targeted by SYNSORB and implemented at a scale suited for industrial chemical processes will significantly improve the global energy consumption landscape. This improvement, in turn, will reduce industrial CO2 emissions. EU member states are committed to a 40% reduction in greenhouse gas emissions as part of the 2030 climate and energy framework, which



also calls for a 27% improvement in energy efficiency. There is therefore a strong societal need for disruptive and ambitious technologies such as those proposed by SYNSORB.

#### Applications

HUMs have shown potential for trace (≤1%) removal of CO2 and C2H2 from many gas mixtures of industrial interest. Synergistic Sorbent Separation Technology (SSST), developed by UL researchers, is a new one-step technique for the purification of industrially relevant gases, allowing the production of polymer-grade (> 99.9%) C2H4 from ternary and quaternary gas mixtures. This work was published in Science and patented.

Overall, SYNSORB reduces the energy footprint of purification processes through crystal engineering (design), characterisation (structure/function) and modelling (binding interactions) studies that enable understanding of how pore size/chemistry impact the properties and performance of physisorbents.

Industrial relevance:

- The development of next-generation sorbents with improved gas/vapour sorption selectivities and working capacities can significantly reduce the energy footprint (by up to 90%) of key commodity purification processes.
- Thanks to the use of physisorbents, SYNSORB will facilitate the commercialisation of adsorptive separation for a number of targeted gases, each of high commercial importance.
- SYNSORB could promote waste minimization by enabling commercially viable separation and utilization of pure gases from waste gas mixtures.

#### **Commercial Opportunity**

UL researchers adopt a systematic Crystal Engineering strategy to:

1. Develop next-generation physisorbent materials via precise control over pore size/chemistry and synergistic sorbent separation for the purification of industrially relevant gases.

2. Develop a new one-step technique for the purification of industrially relevant gases, allowing the production of polymer-grade (> 99.9%) C2H4 (ethylene) from ternary and quaternary gas mixtures.

They are looking for development and commercial partners or licensees to collaborate on scale-up work, and the performance of pilot studies to bring these technologies to market. The University of Limerick is interested in seeking partners to exploit the commercial potential of these technologies by entering into licensing agreements.

Target Market for Innovation: Pharmaceutical companies

Development partner

□Commercial partner

⊠Licensing

□University spin-out

□Seeking investment

1. Patent Title: IMPROVEMENTS RELATING TO GAS SEPARATION

Type: Regional

Country: EPO, USA patents filed

Status: Filed

Priority Date: 13-Sep-2019

Application numbers: EP4010105A2; 20768064.6 (EPO); EP19197407A (EPO); PCT/EP2020/075584W (PCT); EP2020075584W; 17/753,705 (USA)



Link: https://worldwide.espacenet.com/patent/search/family/067956634/publication/EP4010105A2?q=20768064.6%20

2. Patent Title: Methods for Gas Separation

Priority Date: 02-Feb-2016

Application number: CN2016/073137 (PCT, China, Filed); 16888642.2 (Regional, Europe, Granted); 318589791 (Regional, China, Granted); 16/074,903 (Regional, USA, Granted)

Link:

https://worldwide.espacenet.com/patent/search/family/059499247/publication/US11058985B2?q=pn%3DUS11058985 B2

Further details. Papers:

 K.-J. Chen et al., Benchmark C<sub>2</sub>H<sub>2</sub>/CO<sub>2</sub> and CO<sub>2</sub>/C<sub>2</sub>H<sub>2</sub> Separation by Two Closely Related Hybrid Ultramicroporous Materials, *Chem* 1, 753–765 (2016) DOI: https://doi.org/10.1016/j.chempr.2016.10.009

Link: https://www.sciencedirect.com/science/article/pii/S2451929416301966

 K.-J. Chen et al., Synergistic sorbent separation for one-step ethylene purification from a four-component mixture, *Science* 366, 241–246 (2019) DOI: 10.1126/science.aax8666 Link: <u>https://pubmed.ncbi.nlm.nih.gov/31601769/</u>

Other published journals from the research team are available upon request.

#### Contact

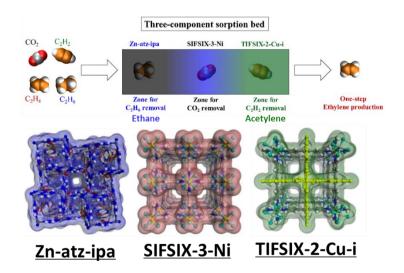
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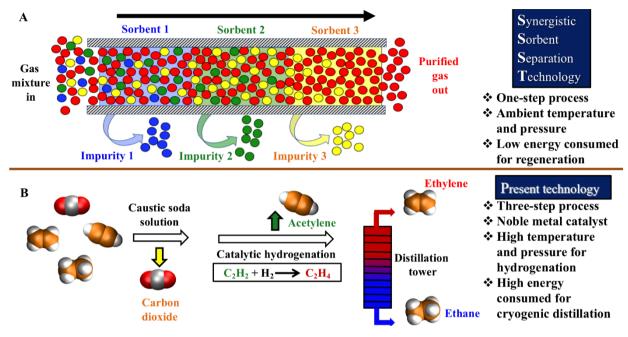
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#### Figures





**Figure 1**: SYNSORB addresses the purification of multi-component gas mixtures that mimic real-world gas mixtures by using bespoke sorbents for each trace impurity, enabling 1-step removal of multiple impurities for the first time. Onestep separation of Ethylene, C2H4. Three bespoke physisorbents remove three trace impurities obtaining polymer grade C2H4 (> 99.9%). Ref. K.-J. Chen et al., Science 2019, 366, 241.



**Figure 2**: Synergistic sorbent separation technology (SSST) vs. present technologies for purification of C2H4: (A) SSST involves an adsorption bed with three bespoke physisorbents to purify the commodity (red) with specific binding sites for each trace impurity (blue, green, yellow); (B) The present process for producing polymer grade C2H4 involves three energy-intensive separation steps. Ref. K.-J. Chen et al., Science 2019, 366, 241.