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Johnson Matthey Highlights

A selection of recent publications by Johnson Matthey R&D staff and collaborators

NON-PEER REVIEWED FEATURE

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Simplified Analytic Particulate Filter Backpressure Models, Including the Additive Flow Resistance Model

T. C. Watling, *Emiss. Control Sci. Technol.*, 2022, **8**, (3–4), 138

Different approximations and assumptions were used to develop three simplified analytic models: a 'low-α' model, a 'low-inertia' model and a generalised additive flow resistance (AFR) model. The models were all applicable to asymmetric and symmetric particulate filters. The limitations and validity of the models were examined by comparing their predictions against each other and a detailed numeric model. The AFR model gave good backpressure predictions when under favourable conditions, whereas the low-α model was shown to consistently under-predict backpressure. The low-inertia model demonstrated validity over a wider range of conditions.

Dynamics at Polarized Carbon Dioxide–Iron Oxyhydroxide Interfaces Unveil the Origin of Multicarbon Product Formation

R. Arrigo, R. Blume, V. Streibel, C. Genovese, A. Roldan, M. E. Schuster, C. Ampelli, S. Perathoner, J. J. Velasco Vélez, M. Hävecker, A. Knop-Gericke, R. Schlögl and G. Centi, *ACS Catal.*, 2022, **12**, (1), 411

The gas-phase selective reduction of CO_2 to isopropanol on a nitrogen-doped carbon-supported iron oxyhydroxide electrocatalyst was explored using a combination of techniques. The authors suggest a three-carbon-atom product formation mechanism based on their observations. In this mechanism, atomic carbon is formed intermediately followed by hydrogenation in the presence of hydrogen cations upon cathodic polarisation. The effectiveness of the mechanism was only observed for thin ferrihydrite-like nanostructures. Larger ferrihydrite-like nanoparticles were shown to be inadequate for electron transport.

Gas Adsorption in the Topologically Disordered Fe-BTC Framework

A. F. Sapnik, C. W. Ashling, L. K. Macreadie, S. J. Lee, T. Johnson, S. G. Telfer and T. D. Bennett, *J. Mater. Chem. A*, 2021, **9**, (47), 27019

In this study, gas adsorption in the MIL-100 and Fe-BTC metal organic frameworks was investigated. The sorption behaviour of the two frameworks was very different, despite their comparable structure and chemistry. A greater interaction strength with guest molecules was observed for Fe-BTC, which also demonstrated a twofold increase in the amount of C_3H_6 adsorption over C_3H_8. An ideal adsorbed solution theory was used to explore thermodynamic selectivity towards a range of industrially relevant binary mixtures. The authors suggest that Fe-BTC, which is topologically disordered, has robust separation capabilities.

Structural Chemistry, Flexibility, and CO_2 Adsorption Performance of Alkali Metal Forms of Merlinoite with a Framework Si/Al Ratio of 4.2

E. L. Bruce, V. M. Georgieva, M. C. Verbraeken, C. A. Murray, M.-F. Hsieh, W. J. Casteel, A. Turrina, S. Brandani and P. A. Wright, *J. Phys. Chem. C*, 2021, **125**, (49), 27403

The CO_2 adsorption properties of caesium, potassium and sodium-exchanged forms of a merlinoite (MER) zeolite (**Figure 1**) were measured to investigate their structural response to CO_2 uptake and dehydration. The potassium form stayed in the wide-pore form, whereas the sodium and caesium forms transformed to a narrow-pore form after dehydration. The caesium

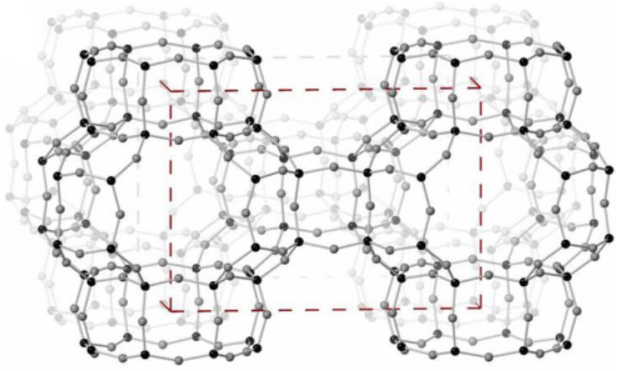

Fig. 1. Open framework structure of MER. Tetrahedral cation sites and oxygen sites are shown in black and grey, respectively. The unit cell is indicated by a dashed red line. From E. L. Bruce *et al*., *J. Phys. Chem. C*, 2021, **125**, (49), 27403

and sodium forms also demonstrated stepped CO_2 adsorption isotherms. A synchrotron PXRD technique was used to explore the effects of CO_2 adsorption on the framework configuration and the cation site distributions. Enhanced adsorption kinetics for argon were shown for all cation forms of MER (4.2).

Combining Quasielastic Neutron Scattering and Molecular Dynamics to Study Methane Motions in ZSM-5

A. P. Hawkins, A. Zachariou, I. P. Silverwood, C. Yong, P. Collier, I. Todorov, R. F. Howe, S. F. Parker and D. Lennon, *J. Chem. Phys*., 2022, **157**, (18), 184702

The dynamics of methane in H-ZSM-5 zeolite catalysts used for methanol-to-hydrocarbon reactions was explored using molecular dynamics (MD) simulations and quasi-elastic neutron scattering (QENS). Measurements were made between 5 K and 373 K, with used and fresh catalysts investigated. High methane mobility was observed in fresh ZSM-5. Moderate levels of coke build up did not significantly affect methane diffusion. However, minimal long-range diffusion was recorded for highly coked samples, where methane was confined to single pores within the zeolite. The MD and QENS measurements demonstrated agreement within 50%.

Machine Learning Accelerated High-Throughput Screening of Zeolites for the Selective Adsorption of Xylene Isomers

D. Hewitt, T. Pope, M. Sarwar, A. Turrina and B. Slater, *Chem. Sci*., 2022, **13**, (44), 13178

With the aim of identifying promising materials for selective adsorption of *meta*-xylene, the authors screened existing zeolite databases using deep neural network and classical simulation methods. Novel anomaly detection techniques were also employed. The results found eight hypothetical zeolite topologies that are several orders of magnitude more selective towards *meta*-xylene than ZSM-5. These hypothetical frameworks would be capable of matching the diffusion seen in existing materials under much lower operating temperatures. These findings could be a driving force for synthetic efforts to realise these promising materials, which could also have significant energy savings.

Optimized Three-Way Catalysts for Emission Control on a Heavy-Duty Stoichiometric Natural Gas Engine

D. Qiao, J. Wang, M. H. Chuma, S. Xu, Q. Li, H. Hu, H. Ji and P. Andersen, SAE Technical Paper 2022-01-0588, SAE International, Warrendale, USA, 29th March, 2022

In this study, the authors optimised catalyst structure, promoters and OSC materials to create a modified gasoline TWC, which was then investigated in a laboratory reactor with a heavy duty stoichiometric natural gas engine. CH_4 light off performance improved with the use of promoters, with T_{50} decreases of 13ºC for the aged catalyst and 20ºC for the fresh catalyst. Natural gas bench testing results demonstrated that NOx and CH_4 emissions reduced when the TWC was modified with an advanced oxygen storage material. NH_3 emissions, a byproduct of TWC operation on a stoichiometric natural gas engine, were shown to be reduced by using NH_3 slip catalyst modifications.

Molybdenum Sulfide Embedded Mesoporous N-Doped Carbon as a Noble Metal-Free Highly Selective Catalyst for Conversion of CO_2 to CO

S. Sameer, G. Singh, J. Gahtori, R. Goyal, I. K. Ghosh, N. Barrabes and A. Bordoloi, *J. Environ. Chem. Eng*., 2022, **10**, (6), 108988

A molybdenum-doped SBA-15 template and a two-step sequential synthesis method were used to incorporate sulfur (in molybdenum sulfide form) into mesoporous nitrogen-doped carbon. The adsorptive CO_2 to CO conversion activity of the MoS_2/CN_X catalyst was investigated and compared to MoO_3/CN_X and MoO_3/SBA15 catalysts. The 2.5 MoS_2/CN_X catalyst had a high number of bridging S_2^{2-} mode and sulfur vacancies, which led to 99% selectivity towards CO and 52% CO_2 conversion with good stability up to 85 h.

Accelerating the Path to Net Zero with Blue Hydrogen: A Route to Achieving Best-In-Class Environmental Performance and Economics

R. Hardy and N. Vijh, Abu Dhabi International Petroleum Exhibition and Conference (ADIPEC), Abu Dhabi, UAE, 31st October–3rd November, 2022,

Paper No. SPE-210888-MS, One Petro, Richardson, USA, 31st October, 2022

Johnson Matthey has developed a novel carbon capture and storage-enabled production process to deliver 'blue' hydrogen. The energy efficient process combines an autothermal reformer (ATR) and gas-heated reformer (GHR). The GHR-ATR technology produces 10% less CO_2, consumes 10% less natural gas and has 75% lower capital cost for the CO_2 capture system in comparison to conventional steam methane reforming. HyNet North-West, the UK's first low carbon hydrogen plant due to be built in 2026, will incorporate Johnson Matthey's GHR-ATR blue hydrogen technology.

nNPipe: a Neural Network Pipeline for Automated Analysis of Morphologically Diverse Catalyst Systems

K. P. Treder, C. Huang, C. G. Bell, T. J. A. Slater, M. E. Schuster, D. Özkaya, J. S. Kim and A. I. Kirkland, *npj Comput. Mater.*, 2023, **9**, 18

In this study, the authors describe a neural network pipeline (nNPipe) for the automated analysis of morphologically diverse catalyst materials. Two standalone convolutional neural networks trained on multiscale image simulations form the nNPipe data-processing method. This method allows quick analysis of 2048 × 2048 pixel images. This is an improvement on previous methods which are slow and have limited workable image sizes. The inference performance of real industrial catalytic samples was compared to that of idealised catalytic samples. These data, along with insights from further analysis, were used in the context of an automated imaging scenario.

Blast Furnace Gas Decarbonisation Through Calcium Assisted Steel-Mill Off-Gas Hydrogen Production. Experimental and Modelling Approach

G. Grasa, M. Díaz, J. R. Fernández, A. Amieiro, J. Brandt and J. C. Abanades, *Chem. Eng. Res. Des.*, 2023, **191**, 507

A laboratory-scale fixed bed reactor and readily available functional materials were used to study the main reaction stages of the calcium assisted steel-mill off-gas hydrogen (CASOH) production process. The CASOH process was sustained by commercial materials such as CuO and CaO and was used to generate a H_2/N_2 stream from blast furnace gases. Sorbent regeneration with a copper-based chemical combustion loop led to the production of a rich CO_2 gas stream. The results from this study will be used to design experimental campaigns at the TRL7 CASOH pilot plant which is currently under construction.