

## Hub Publications and Presentations

- 1) Beard T, Bragin M, Malalasekera W, Ibrahim S. 2014. "Numerical simulation of hydrogen discharge in a partially enclosed space" at the 12th International Conference on Combustion & Energy Utilisation, Lancaster, 29 Sept – 3 Oct 2014.
- 2) Bharath V, Millichamp J, Neville T, Mason T, Shearing P, Brown R, Manos G, Brett D. 2016. Measurement of Water Uptake in Thin-Film Nafion and Anion Alkaline Exchange Membranes using the Quartz Crystal Microbalance, *Journal of Membrane Science*. (Vol 497, Jan 2016, 229-238).
- 3) Bill R, Reed D, Book D, Anderson PA. 2015. Effect of the calcium halides, CaCl<sub>2</sub> and CaBr<sub>2</sub>, on hydrogen desorption in the Li-Mg-N-H system. *Journal of Alloys and Compounds* (645, pp. S96-S99, 2015).
- 4) Bimbo N., Xu W., Sharpe J. E., Ting V. P. and Mays T. J., 2016. High-pressure adsorptive storage of hydrogen in MIL-101 (Cr) and AX-21 for mobile applications: cryocharging and cryokinetics. *Materials & Design*, 89, pp. 1086-1094.
- 5) Bimbo N., Physick A.J., Noguera-Díaz A., Pugsley A., Holyfield L.T., Ting V.P., and Mays T.J. 2015. High volumetric and energy densities of methane stored in nanoporous materials at ambient temperatures and moderate pressures. *Chemical Engineering Journal* (2015), 272, 38-47.
- 6) Bimbo N, Sharpe J, Ting V, Noguera-Díaz A, Mays T. 2014. Isothermic enthalpies for hydrogen adsorbed on nanoporous materials at high pressures. *Adsorption* 20, 373-384 (2014).
- 7) Bimbo N, Xu W, Sharpe J, Ting V, Holyfield, Ting V, Mays T. Cryocharging and kinetics of high-pressure hydrogen adsorption in MIL-101(Cr) and AX-21. *Proceedings, 9<sup>th</sup> International Symposium on Surface Heterogeneity Effects in Adsorption and Catalysis on Solids*, p.225, Wrocław, Poland (2015).
- 8) Boldrin P, Ruiz-Trejo E, Yu J, Gruar RI, Tighe CJ, Chang K-C, Ilavsky J, Darr JA, Brandon N. 2015. Nanoparticle scaffolds for syngas-fed solid oxide fuel cells, *Journal of Materials Chemistry A*, Vol: 3, Pages: 3011-3018.
- 9) Boldrin P, Millan-Agorio M, Brandon NP. 2015. Effect of Sulfur- and Tar-Contaminated Syngas on Solid Oxide Fuel Cell Anode Materials. *Energy and Fuels*, Vol: 29, Pages: 442-446.
- 10) Burrows A, Fisher L, Mays T, Rigby S, Ashbrook S, Dawson R. 2015. Post-synthetic modification of zinc metal-organic frameworks through palladium catalysed carbon-carbon bond formation. *Journal of Organometallic Chemistry*. 792, 134-138 (2015).
- 11) Dawson R, Burrows A, Mays T. Nanoporous materials for high-pressure gas storage tanks. *Proceedings, 7<sup>th</sup> International Workshop on the Characterization of Porous Materials*, p.45, Delray Beach, FL, USA (2015).
- 12) Dodds P. E., Staffell I, Hawkes, A. D, Li F, Grünewald P, McDowall W, Ekins P. 2015. Hydrogen and fuel cell technologies for heating: a review. *International Journal of Hydrogen Energy*. (40(5):2065-2083).
- 13) Duboviks V, Lomberg M, Maher RC, Cohen LF, Brandon NP, Offer GJ. 2015. Carbon deposition behaviour in metal-infiltrated gadolinia doped ceria electrodes for simulated biogas upgrading in solid oxide electrolysis cells, *Journal of Power Sources*, Vol: 293, Pages: 912-921.
- 14) Dueso C, Thompson C, Metcalfe IS. 2015. High-stability, high-capacity oxygen carriers: iron oxide-perovskite composite materials for hydrogen production by chemical looping. *Applied Energy* (Volume 157, 1 November 2015, Pages 382-390).
- 15) Fahy K, Kucernak A. 2016. Facile synthesis of palladium phosphide electrocatalysts and their activity for the hydrogen oxidation, hydrogen evolutions, oxygen reduction and formic acid oxidation reactions. *Catalysis Today*. (Volume 262, 15 March 2016, Pages 48-56).
- 16) Fecarotti C., Andrews J. 2016. Performance modelling of fuel cell systems through Petri nets. RAMS 2016, the 62<sup>nd</sup> Annual Reliability & Maintainability Symposium, 25-28 January, 2016, Tucson, Arizona.
- 17) Fecarotti C., Andrews J., Chen R. (under review). A Petri net approach for performance modelling of polymer electrolyte fuel cell systems. *International Journal of Hydrogen Energy*.

- 18) Gadipelli S, Guo Z. 2015. Tuning of MOF-derived carbon with high activity, nitrogen functionality and yield – a case for superior CO<sub>2</sub> capture. *ChemSusChem*, 2015, 8, 2123-2132.
- 19) Gadipelli S, Guo Z. 2015. Graphene-based materials: synthesis and gas sorption, storage and separation. *Progress in Materials Science*, 2015, 69, 1-60.
- 20) Giannissi SG, Hoyes JR, Chernyavskiy B, Hooker P, Hall J, Venetsanos AG, Molkov V. 2015. CFD benchmark on hydrogen release and dispersion in a ventilated enclosure: Passive ventilation and the role of an external wind. *International Journal of Hydrogen Energy*, (Volume 40, Issue 19, 25 May 2015, Pages 6465-6477).
- 21) Giannissi SG, Shentsov V, Melideo D, Cariteau B, Baraldi D, Venetsanos AG, Molkov V. 2015. CFD benchmark on hydrogen release and dispersion in confined, naturally ventilated space with one vent. *International Journal of Hydrogen Energy*. (Volume 40, Issue 5, 9 February 2015, Pages 2415-2429).
- 22) Gkanas E, Grant DM, Stuart AD, Book D, Nayebossadri S, Pickering L, Walker GS. 2014. "Numerical Study on a Two - Stage Metal Hydride Hydrogen Compression System", at the 14th International Symposium on Metal-Hydrogen Systems, 2014, 20 -25 July 2014.
- 23) Gkanas E.I., Grant D.M., Stuart A.D., Eastwick C.N., Book D., Nayebossadri S., Pickering L. and Walker G.S. 2015. Numerical study on a two-stage Metal Hydride Hydrogen Compression system. *Journal of Alloys and Compounds*, 645(S1), pp. S18-S22.
- 24) Holyfield L, Dawson R, Noguera-Díaz A, Bennet J, Burrows A, Mays T. PIM-MOF composites for use in hydrogen storage tanks. Proceedings, 9<sup>th</sup> International Symposium on Surface Heterogeneity Effects in Adsorption and Catalysis on Solids, p.223, Wrocław, Poland (2015).
- 25) Holyfield L, Bimbo N, Ting V, Burrows A, Mays T. Evaluation of an activated carbon as an adsorbent in hybrid high-pressure hydrogen storage tanks. Proceedings, 7<sup>th</sup> International Workshop on the Characterization of Porous Materials, p.15, Delray Beach, FL, USA (2015).
- 26) Hossain M, Myung J, Lan R, Cassidy M, Burns I, Tao S and Irvine J. 2015. Study on direct flame solid oxide fuel cell using flat burner and ethylene flame. *ECS Transaction* 68 (2015) 1989-1999; doi:10.1149/06801.1989ecst
- 27) Jones R. J., Massanet-Nicolau J., Guwy A., Premier G. C., Dinsdale R. M., Reilly M. 2015. Removal and recovery of inhibitory volatile fatty acids from mixed acid fermentations by conventional electro dialysis. *Bioresource Technology*, (Vol 189, 279–284).
- 28) Keenan J, Makarov DV, Molkov VV. 2014. Rayleigh–Taylor instability: Modelling and effect on coherent deflagrations. *International Journal of Hydrogen Energy*. (Volume 39, Issue 35, 3 December 2014, Pages 20467-20473).
- 29) Kim Y., Makarov D., Kashkarov S., Joseph P. and Molkov V. 2015. Modelling heat transfer in an intumescent paint and its effect on fire resistance of on-board hydrogen storage. Presented at Int. Conf. Hydrogen Safety, 19-21 October 2015, Yokohama, Japan.
- 30) Lan R and Tao S. 2014. Novel proton conductors in layered oxide material Li<sub>x</sub>Al<sub>0.5</sub>Co<sub>0.5</sub>O<sub>2</sub>, *Advanced Energy Materials*, 4 (2014) 1301683.
- 31) Lan R and Tao S. 2014. New layered proton-conducting oxides Li<sub>x</sub>Al<sub>0.6</sub>Co<sub>0.4</sub>O<sub>2</sub> and Li<sub>x</sub>Al<sub>0.7</sub>Co<sub>0.3</sub>O<sub>2</sub>, *ChemElectroChem*, 1 (2014) 2098-2103.
- 32) Lan R and Tao S. 2015. High ionic conductivity in a LiFeO<sub>2</sub>-LiAlO<sub>2</sub> composite under H<sub>2</sub>/air fuel cell condition, *Chemistry - A European Journal*, 21 (2015) 1350-1358.
- 33) Malalasekera W, Bragin M, Ibrahim S, Beard T. 2015. Numerical Simulation of Hydrogen Discharge in a Partially Enclosed Space, *Energy Procedia*, 66, pp.153-156,
- 34) Malko D, Lopes T, Kucernak A, The intriguing poison tolerance of non-precious metal oxygen reduction reaction (ORR) catalysts. *Journal. Mat. Chem. A*, (2016,4, 142-152).

- 35) Mao L., Jackson L.M., Dunnett S.J., Vasilyev A. 2014. Investigation of an indicator for future on-line diagnosis of PEM fuel cell flooding using model based techniques. Second European Conference of the Prognostics and Health Management Society, 08-10 July, 2014, Nantes, France.
- 36) Mao L., Jackson L.M., Dunnett S.J. 2015. Fault diagnosis of evaporatively cooled fuel cell system under steady state condition. 6<sup>th</sup> International Conference on Fundamentals and Development of Fuel Cells. 03-05 February, 2015, Toulouse.
- 37) Mao L., Jackson L.M., Dunnett S.J. 2015. Fault diagnosis of practical fuel cell system based on polarization curves. Proceedings of the 21st Advances in Risk and Reliability Technology Symposium, 23-25 June, 2015, Loughborough, UK.
- 38) Mao L., Jackson L.M., Dunnett S.J. 2015. Investigation of PEMFC parameter effects on practical fuel cell system performance. Proceedings of the 5th European PEFC and H2 Forum, 30 June-03 July, 2015, Lucerne, Switzerland.
- 39) Mao L., Jackson L.M., Dunnett S.J. 2015. Investigation of PEMFC parameter effects on practical fuel cell system performance. 5<sup>th</sup> European PEFC & H2 FORUM 2015, 30 June-03 July, 2015, Lucerne, Switzerland.
- 40) Mao L., Jackson L., Dunnett S., Robinson P (under review). Fault diagnosis of practical fuel cell system in a data-driven framework. *International Journal of Hydrogen Energy*.
- 41) Markiewicz M., Zalitis C., Kucernak A. 2015. Performance measurements and modelling of the ORR on fuel cell electrocatalysts – the modified double trap model. *Electrochim. Acta* 2015.
- 42) Mays T. 2014. Practical hybrid high-pressure / sorbent hydrogen storage systems. Proceedings, 14<sup>th</sup> International Symposium on Metal-hydrogen systems: Fundamentals and Applications, p.154, Salford (2014).
- 43) McDowall W. 2014. Exploring possible transition pathways for hydrogen energy: A hybrid approach using socio-technical scenarios and energy system modelling. *Futures*, 63:1-14.
- 44) Metcalfe, I.S. 2015. Ceramic Permeation Membranes and Membrane Reactors. Solid State Ionics, Colorado, 14-19 June 2015.
- 45) Metcalfe, I.S. 2015. The rational design of materials for intensified reaction and separation in energy-related processes. The Society of Chemical Engineers of Japan, Tokyo, 19-21 March 2015.
- 46) Meyer Q, Ashton S, Jervis R, Finegan D, Boillat P, Cochet C, Curnick O, Reisch T, Adcock P, Shearing P, Brett D. 2015. The Hydro-electro-thermal Performance of Air-cooled, Open-cathode Polymer Electrolyte Fuel Cells: Combined Localised Current Density, Temperature and Water Mapping. *Electrochimica Acta*, (Volume 180, 20 October 2015, Pages 307–315).
- 47) Meyer Q., Ronaszegi K., Robinson J.B., Noorkami M., Curnick O., Ashton S., Danelyan A., Reisch T., Adcock P., Kraume R., Shearing P.R., Brett D.J.L. 2015. Combined current and temperature mapping in an air-cooled, open-cathode polymer electrolyte fuel cell under steady-state and dynamic conditions. *Journal of Power Sources*. (Volume 297, 30 November 2015, Article number 21510, Pages 315-322).
- 48) Meyer Q, Ronaszegi K, Pei-June G, Curnick O, Ashton S, Reisch T, Adcock P, Shearing P, Brett D. 2015. Optimisation of air cooled, open-cathode fuel cells: Current of lowest resistance and electro-thermal performance mapping. *Journal of Power Sources*; (Volume 291, 30 September 2015, Pages 261–269).
- 49) Millichamp J, Mason T, Neville T, Rajalakshmi N, Jervis R, Shearing P, Brett D. 2015. Mechanisms and effects of mechanical compression and dimensional change in polymer electrolyte fuel cells – A review. *Journal of Power Sources*, (Volume 284, 15 June 2015, Pages 305–320.)
- 50) Molkov V, Bragin M. Hydrogen–air deflagrations: Vent sizing correlation for low-strength equipment and buildings. *International Journal of Hydrogen Energy*. (Volume 40, Issue 2, 12 January 2015, Pages 1256-1266).

- 51) Molkov V, Shentsov V, Quintiere J. 2014 Passive ventilation of a sustained gaseous release in an enclosure with one vent. *International Journal of Hydrogen Energy*, Volume 39, Issue 15, 15 May 2014, Pages 8158-8168.
- 52) Molkov V, Shentsov V, Brennan S, Makarov D. 2014. Hydrogen non-premixed combustion in enclosure with one vent and sustained release: Numerical experiments. *International Journal of Hydrogen Energy*. (Volume 39, Issue 20, 3 July 2014, Pages 10788-10801).
- 53) Molkov V, Shentsov V. Numerical and physical requirements to simulation of gas release and dispersion in an enclosure with one vent. *International Journal of Hydrogen Energy*. (Volume 39, Issue 25, 22 August 2014, Pages 13328-13345).
- 54) Morris L, Trudeau ML, Reed D, Book D, Antonelli DM. 2015. Thermodynamically neutral Kubas-type hydrogen storage using amorphous Cr (iii) alkyl hydride gels. *Physical Chemistry Chemical Physics* (**17**, pp.9480-9487, 2015).
- 55) Myung J, Shin T, Huang X, Carins G and Irvine J. 2015. Enhancement of Redox Stability and Electrical Conductivity by Doping Various Metals on Ceria,  $Ce_{1-x}M_xO_{2-\delta}$  (M=Ni, Cu, Co, Mn, Ti, Zr), *International Journal of Hydrogen Energy*, 40(35), 12003-12008.
- 56) Myung J, Neagu D, Tham M and Irvine J. 2015. In situ tailored nickel nano-catalyst layer for internal reforming hydrocarbon fueled SOFCs, *ECS Transactions* 68(1):1121-1128, 2015.
- 57) Noguera-Díaz A, Bimbo N, Sharpe, Ting V, Mays T. Characterizing structure-property relationships in nanoporous materials for hydrogen storage. Proceedings, 7<sup>th</sup> International Workshop on the Characterization of Porous Materials, p.43, Delray Beach, FL, USA (2015).
- 58) Noguera-Díaz A, Bimbo N, Holyfield L, Ting V, Mays T. 2015. Structure-property relationships in metal-organic frameworks for hydrogen storage. Proceedings, 9<sup>th</sup> International Symposium on Surface Heterogeneity Effects in Adsorption and Catalysis on Solids, p.51, Wrocław, Poland (2015).
- 59) Parkes MA, Refson K, d'Ayezac M, Offer GJ, Brandon NP, Harrison NM. 2015. Chemical Descriptors of Yttria-Stabilized Zirconia at Low Defect Concentration: An ab Initio Study, *Journal of Physical Chemistry A*, Vol: 119, Pages: 6412-6420.
- 60) Patel H, Mansor N, Gadipelli S, Brett D, Guo Z. 2015. Superacidity in Nafion/MOF Hybrid Membranes Retains Water even under Low Humidity to Enhance Proton Conduction for Fuel Cells, Under Preparation, 2015
- 61) Popov A, Michie I, Kim J-R, Dinsdale RM, Guwy AJ, Esteves SR. Premier GC Enrichment strategy for Enhanced Electrochemically Assisted Microbial Production of Hydrogen. *International Journal of Hydrogen Energy*. (accepted)
- 62) Rhazaoui K, Cai Q, Kishimoto M, Tariq F, Somalu MR, Adjiman CS, Brandon NP. 2015. Towards the 3D Modelling of the Effective Conductivity of Solid Oxide Fuel Cell Electrodes - Validation against experimental measurements and prediction of electrochemical performance, *Electrochimica Acta*, Vol: 168, Pages: 139-147
- 63) Ruiz-Trejo E, Zhou Y, Brandon NP. 2015. On the manufacture of silver-BaCe<sub>0.5</sub>Zr<sub>0.3</sub>Y<sub>0.16</sub>Zn<sub>0.04</sub>O<sub>3- $\delta$</sub>  composites for hydrogen separation membranes. *International Journal of Hydrogen Energy*, Vol: 40, Pages: 4146-4153.
- 64) Ruiz-Trejo E, Boldrin P, Medley-Hallam JL, Darr J, Atkinson A, Brandon NP. 2015. Partial oxidation of methane using silver/gadolinia-doped ceria composite membranes, *Chemical Engineering Science*, Vol: 127, Pages: 269-275.
- 65) Ruiz-Trejo E, Atkinson A, Brandon NP. 2015. Metallizing porous scaffolds as an alternative fabrication method for solid oxide fuel cell anodes, *Journal of Power Sources*, Vol: 280, Pages: 81-89.

- 66) Saldi Z.S., Wen J.X. 2015. Modeling Thermal Response of Polymer Composite Hydrogen Cylinders under Fire Attack. Presented at the 1<sup>st</sup> International Conference on Structural Safety under Fire and Blast, 2-4 September 2015, Glasgow, UK.
- 67) Sharpe J.E., Bimbo N., Ting V.P., Rechain B., Joubert E. and Mays T.J. 2015. Modelling the potential of adsorbed hydrogen for use in aviation. *Microporous and Mesoporous Materials* (2015), 209,135-140.
- 68) Stockford C, Brandon N, Irvine J, Mays T, Metcalfe I, Book D, Ekins P, Kucernak A, Molkov V, Steinberger-Wilckens R, Shah N, Dodds P, Dueso C, Samsatli S, Thompson C. 2015. H2FC SUPERGEN: An overview of the Hydrogen and Fuel Cell research across the UK. *International Journal of Hydrogen Energy*. (Volume 40, Issue 15, 27 April 2015, Pages 5534-5543.)
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- 71) Trang TT, Reed D, Book D, Anderson PA. 2015. Hydrogen release and uptake in the Li-Zn-N system. *Journal of Alloys and Compounds* (645), pp. S295-S298, (2015).
- 72) Urasinska-Wojcik B, Vincent T, Chowdhury M, Gardner J. Ultrasensitive WO<sub>3</sub> gas sensors for NO<sub>2</sub> detection in air and low oxygen environment, *Sensors and Actuators B*, in preparation.
- 73) Vasilyev A, Dunnett S, Jackson L. 2015. Model-based Fault Detection and Isolation of Polymer Electrolyte Membrane Fuel Cells Using Bond Graph Approach. Proceedings of the 21st Advances in Risk and Reliability Technology Symposium, 23-25 June, 2015, Loughborough, UK.
- 74) Vasilyev A, Jackson L, Dunnett S, Mao L. 2015. Fault Detection and Isolation of Polymer Electrolyte Membrane Fuel Cells Using Bond Graphs. Proceedings of the 5th European PEFC and H<sub>2</sub> Forum, 30 June-03 July, 2015, Lucerne, Switzerland.
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- 78) Wu W, Bucknall R. 2014. "Downsizing Fuel Cell Capacity In A Hybrid Hydrogen Vehicle By Regenerative Energy Capture With Super Capacitor", presented at UPEC 2014 International Universities' Power Engineering Conference, Cluj- napoca, Romania.
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