List of Joint Research Papers (2020-2026)

1) Jonathan Ruiz Esquius, Gerardo Algara-Siller, Ioannis Spanos, Simon J. Freakley, Robert Schlögl, and Graham J. Hutchings, "Preparation of Solid Solution and Layered IrO_x–$Ni(OH)_2$ Oxygen Evolution Catalysts: Toward Optimizing Iridium Efficiency for OER", *ACS Catalysis* **2020** *10* (24), 14640-14648 https://doi.org/10.1021/acscatal.0c03866 (with CCI and CEC).

2) Bowker, M.; DeBeer, S.; Dummer N. F.; Hutchings, G. J.; Scheffler, M.; Schüth, F.; Taylor, S. H.; Tüysüz, H. "Advancing critical chemical processes for a sustainable future: Challenges for industry and the Max Planck-Cardiff Centre on the fundamentals of heterogeneous catalysis (FUNCAT)", *Angew. Chem. Int. Ed.* **2022**, 134, e202209016 https://doi.org/10.1002/anie.202209016 (with FHI, CEC and CCI).

3) Belthle, K.; Beyazay, T.; Ochoa-Hernández, C.; Miyazaki, R.; Martin, F. W.; Tüysüz, H. "Effect of silica modification (Mg, Al, Ca, Ti, and Zr) on supported cobalt catalysts for H_2 dependent CO_2 reduction to metabolic intermediates", *J. Am. Chem. Soc.* **2022**, 144, 21232 https://doi.org/10.1021/jacs.2c08845 (with KoFo and FHI).

4) Yu, M.; Weidenthaler, C.; Wang, Y.; Budiyanto, E.; Şahin E. O.; Chen, M.; DeBeer, S.; Ruediger, O.; Tüysüz, H. "Surface boron modulation on cobalt oxide nanocrystals for electrochemical oxygen evolution reaction", *Angew. Chem. Int. Ed.* **2022**, 61, e202211543 https://doi.org/10.1002/anie.202211543 (with KoFo and CEC).

5) Esquius, J. R., Morgan, D. J., Siller, G. A., Gianolio, D., Aramini, M., Lahn, L., Kasian, O., Kondrat, S. A., Schlögl, R., Hutchings, G. J., Arrigo, R., Freakley, S. J., "Lithium-Directed Transformation of Amorphous Iridium (Oxy)hydroxides To Produce Active Water Oxidation Catalysts", *J. Am. Chem. Soc.* **2023** 145 (11), 6398-6409 https://doi.org/10.1021/jacs.2c13567 (with CCI and CEC).

6) Miyazaki, R.; Belthle, K.; Tüysüz, H.; Foppa, L.; Scheffler, M.; "Materials genes of CO_2 hydrogenation on supported cobalt catalysts: an artificial intelligence approach integrating theoretical and experimental data", *J. Am. Chem. Soc.* **2024**, 146, 543 https://doi.org/10.1021/jacs.3c12984 (with FHI and KoFo).

7) Reichle, S.; Kang, L.; Demirbas, D.; Weidenthaler, C.; Felderhoff, M.; DeBeer, S.; Schüth, F*. Mechanocatalytic Synthesis of Ammonia: State of the Catalyst During Reaction and Deactivation Pathway. *Angew. Chem. Int. Ed.* **2024**, *63*, e202317038. https://doi.org/10.1002/anie.202317038 (with CEC and KoFo).

8) Stefan Bauer, Peter Benner, Tristan Bereau, Volker Blum, Mario Boley, Christian Carbogno, Richard Catlow, Gerhard Dehm, Sebastian Eibl, Ralph Ernstorfer, Ádám Fekete, Lucas Foppa, Peter Fratzl, Christoph Freysoldt, Baptiste Gault, Luca M Ghiringhelli, Sajal K Giri, Anton Gladyshev, Pawan Goyal, Jason Hattrick-Simpers, Lara Kabalan, Petr Karpov, Mohammad S Khorrami, CT Koch, Sebastian Kokott, Thomas Kosch, Igor Kowalec, Kurt Kremer, Andreas Leitherer, Yue Li, Christian H Liebscher, Andrew Logsdail, Zhongwei Lu, Felix Luong, Andreas

Marek, Florian Merz, Jaber Rezaei Mianroodi, Joerg Neugebauer, Zongrui Pei, Thomas AR Purcell, Dierk Raabe, Markus Rampp, Mariana Rossi, Jan M Michael Rost, James E Saal, Ulf Saalmann, Kasturi Narasimha Sasidhar, Alaukik Saxena, Luigi Sbailo, Markus Scheidgen, Marcel Schloz, Daniel Schmidt, Simon Teshuva, Annette Trunschke, Ye Wei, Gerhard Weikum, R Patrick Xian, Yi Yao, Junqi Yin, Meng Zhao, Matthias Scheffler. "Big data map for materials science", *Modelling and Simulation in Materials Science and Engineering*, **2024**, *32,* 063301. https://doi.org/10.1088/1361-651X/ad4d0d (with FHI and CCI).

9) Kumar, A.; Gil-Sepulcre, M.; Lee, J.; Bui, V.Q.; Wang, Y.; Rüdiger, O.; Kim, M. Y.; DeBeer, S.; Tüysüz, H., "Iridium single-atom-ensembles stabilized on Mn-substituted spinel oxide for durable acidic water electrolysis", *Adv. Mater.* **2024**, *36, 2414648* https://doi.org/10.1002/adma.202401648 (with CEC and KoFo).

10) Kumar, A.; Gil-Sepulcre, M.; Fandré, J. P.; Rüdiger, O.; Kim, M-G.; DeBeer, S.; Tüysüz, H. "Regulating Local Coordination Sphere of Ir Single-Atoms at the Atomic Interface for Efficient Oxygen Evolution Reaction", *J. Am. Chem. Soc.* **2024**, 146, 32953, https://doi.org/10.1021/jacs.4c08847 (Highlighted as the cover of the journal) (with CEC and KoFo).

11) Pfister, N.; Kraievska, I.; Rohner, C.; Dong, J.; Timpe, O.; Girgsdies, F.; Lunkenbein, T.; Khobragade, R.; De Bellis, J.; Schüth, F.; Trunschke, "A Facile Approach to Alumina-Supported Pt Catalysts for the Dehydrogenation of Propane", *Ind. Eng. Chem. Res.* **2024***, 63, 48, 20778–20786,* https://doi.org/10.1021/acs.iecr.4c02577 (with FHI and KoFo).

12) Li, R., Lewis R. J, Lopez-Martin, A., Morgan D. J., Davies T. E., Kordus, D., Cuenya, B., R., Hutchings, G. J., "Promoting H_2O_2 direct synthesis through Fe incorporation into AuPd Catalysts", Green Chem., **2025**, 27, 2065-2077 https://doi.org/10.1039/D5GC00134J (with CCI and FHI).

13) Williams, J. O., Ella Kitching, E., Rhea-Shree Patel, R-S., Mauß, J. M., Kley, K. S., Khobragade, R., de Bellis, J., Morgan, D., Slater, T., Schüth, F., Taylor, S. H., Dummer, N. F., Bender, M., Hutchings. G. J., "Selective acetylene hydrogenation over sol immobilisation prepared AgPd/Al_2O_3: influence of reaction conditions on catalyst activity", *ChemCatChem* **2025**, 17, 8, e202401794, https://doi.org/10.1002/cctc.202401794 (with CCI and KoFo).

14) Mauss, J.M., Kley, K.S., Khobragade, R., Tran, N.-K., de Bellis, J., Schüth, F., Scheffler, M., Foppa, L., "Modeling Time-On-Stream Catalyst Reactivity in the Selective Hydrogenation of Concentrated Acetylene Streams under Industrial Conditions via Experiments and AI", *ACS Catal.* **2025**, 15, 15, 12652-12665, https://doi.org/10.1021/acscatal.5c02226 (with FHI and KoFo).

15) Mauss, J.M., Leiting, S., Farès, C., Scott, A.G., Peredkov, S., DeBeer, S., Weidenthaler C., Schüth F., "A Heterogenized Molecular Catalyst for the Gas-Phase Cyclotrimerization of Acetylene to Benzene", *J. Am. Chem. Soc.* **2025**, 147, 45, 42088-42099 https://doi.org/10.1021/jacs.5c16274 (with CEC and KoFo).

16) Scott, A. G., Peredkov, S., Lopez-Martin, A., Lewis, R. J., Hutchings, G. J., DeBeer, S., "Evaluating Palladium 4d-to-2p X-ray Emission Spectroscopy for Characterizing Catalytically Relevant Species", *Inorg. Chem.* **2026**, 65, 3, 1801-1811, https://doi.org/10.1021/acs.inorgchem.5c04266 (with CEC and CCI).

17) Cartwright, J., Hosseini, H., Gunnarson, A., Lazaridou, A., Mauss, J.M., Davies, B., Pattisson, S., Lopez-Martin, A., Morgan, D.J., Dummer, N.F., Schüth, F., Hutchings, G.J., "Cationic Gold on Heteroatom Doped Carbon Supports for Vinyl Chloride Production", *Catal. Lett.* **2026**, 156, 104, https://doi.org/10.1007/s10562-026-05351-2 (with CCI and KoFo).

18) Lawes, N., Kowalec, I., Mediavilla-Madrigal, S., Aggett, K. J., Smith, L. R., Dearg, M., Slater, T. J. A., McCarthy, E., Rivera-Arrieta, H. I., Scheffler, M., Morgan, D. J., Willock, D. J., Beale, A. M., Logsdail, A. J., Dummer, N. F., Bowker, M., Catlow, R. C., Taylor, S. H., Hutchings, G. J., "The Important Role of Alloy-Oxide Interfaces in Controlling Methanol Formation in CO_2 Hydrogenation", *ACS Catal.* **2026**, 16, 3, 2209-2221, https://doi.org/10.1021/acscatal.5c06703 (with CCI and FHI).

19) Kowalec, I., Rivera-Arrieta, H., Lu, Z., Foppa, L., Scheffler, M., Catlow, C. R. A., Logsdail, A. J., "Role of monodentate formate in product selectivity for CO2 hyrogenation on Pd-based alloy catalysts", *Faraday Discuss.* **2026**, accepted, https://doi.org/10.1039/D5FD00125K (with CCI and FHI).

List of Research Papers Acknowledging FUNCAT

1) Dawson, S. R.; Pattisson, S.; Malta, G.; Dummer, N. F.; Smith, L. R.; Lazaridou, A.; Allen, C. S.; Davies, T. E.; Freakley, S. J.; Kondrat, S. A.; Kiely, C. J.; Johnston, P.; Hutchings, G. J. Sulfur Promotion in Au/C Catalyzed Acetylene Hydrochlorination. *Small* **2021**, *17* (16), 2007221. https://doi.org/10.1002/smll.202007221.

2) Richards, T.; Harrhy, J. H.; Lewis, R. J.; Howe, A. G. R.; Suldecki, G. M.; Folli, A.; Morgan, D. J.; Davies, T. E.; Loveridge, E. J.; Crole, D. A.; Edwards, J. K.; Gaskin, P.; Kiely, C. J.; He, Q.; Murphy, D. M.; Maillard, J.-Y.; Freakley, S. J.; Hutchings, G. J. A Residue-Free Approach to Water Disinfection Using Catalytic in Situ Generation of Reactive Oxygen Species. *Nat Catal* **2021**, *4* (7), 575–585. https://doi.org/10.1038/s41929-021-00642-w.

3) Lewis, R. J.; Ntainjua, E. N.; Morgan, D. J.; Davies, T. E.; Carley, A. F.; Freakley, S. J.; Hutchings, G. J. Improving the Performance of Pd Based Catalysts for the Direct Synthesis of Hydrogen Peroxide via Acid Incorporation during Catalyst Synthesis. *Catalysis Communications* **2021**, *161*, 106358. https://doi.org/10.1016/j.catcom.2021.106358.

4) Santos, A.; Lewis, R. J.; Morgan, D. J.; Davies, T. E.; Hampton, E.; Gaskin, P.; Hutchings, G. J. The Degradation of Phenol via in Situ H2O2 Production over Supported Pd-Based Catalysts. *Catal. Sci. Technol.* **2021**, *11* (24), 7866–7874. https://doi.org/10.1039/D1CY01897C.

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6) Qi, G.; Davies, T. E.; Nasrallah, A.; Sainna, M. A.; Howe, A. G. R.; Lewis, R. J.; Quesne, M.; Catlow, C. R. A.; Willock, D. J.; He, Q.; Bethell, D.; Howard, M. J.; Murrer, B. A.; Harrison, B.; Kiely, C. J.; Zhao, X.; Deng, F.; Xu, J.; Hutchings, G. J. Au-ZSM-5 Catalyses the Selective Oxidation of CH4 to CH3OH and CH3COOH Using O2. *Nat Catal* **2022**, *5* (1), 45–54. https://doi.org/10.1038/s41929-021-00725-8.

7) Huang, X.; Akdim, O.; Douthwaite, M.; Wang, K.; Zhao, L.; Lewis, R. J.; Pattisson, S.; Daniel, I. T.; Miedziak, P. J.; Shaw, G.; Morgan, D. J.; Althahban, S. M.; Davies, T. E.; He, Q.; Wang, F.; Fu, J.; Bethell, D.; McIntosh, S.; Kiely, C. J.; Hutchings, G. J. Au–Pd Separation Enhances Bimetallic Catalysis of Alcohol Oxidation. *Nature* **2022**, *603* (7900), 271–275. https://doi.org/10.1038/s41586-022-04397-7.

8) Dummer, N. F.; Sodiq-Ajala, Z.; Morgan, D. J.; Davies, T. E. Investigating the Preparation of Cu3Mo2O9 as a Photocatalyst. *Catalysis Communications* **2022**, *163*, 106414. https://doi.org/10.1016/j.catcom.2022.106414.

9) Barnes, A.; Lewis, R. J.; Morgan, D. J.; Davies, T. E.; Hutchings, G. J. Enhancing Catalytic Performance of AuPd Catalysts towards the Direct Synthesis of H2O2 through Incorporation of Base Metals. *Catal. Sci. Technol.* **2022**, *12* (6), 1986–1995. https://doi.org/10.1039/D1CY01962G.

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20) Richards, T.; Lewis, R. J.; Morgan, D. J.; Hutchings, G. J. The Direct Synthesis of Hydrogen Peroxide Over Supported Pd-Based Catalysts: An Investigation into the Role of the Support and Secondary Metal Modifiers. *Catal Lett* **2023**, *153* (1), 32–40. https://doi.org/10.1007/s10562-022-03967-8.

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NMR of Pd–Au Catalyzed Butadiene Hydrogenation. *ACS Catal.* **2024**, *14* (4), 2522–2531. https://doi.org/10.1021/acscatal.3c05968.

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