List of publications: Dr. James Birrell

2020

- Jagilinki, B.P., Ilic, S., Trncik, C., Tyryshkin, A.M., Pike, D.H., Lubitz, W., Bill, E., Einsle, O., **Birrell, J.A.**, Akabayov, B., Noy, D., Nanda, V. (2020). *In Vivo* Biogenesis of a *De Novo* Designed Iron−Sulfur Protein *ACS Synthetic Biology* 9(12), 3400-3407. https://doi.org/10.1021/acssynbio.0c00514
- Rodríguez-Maciá, P., Breuer, N., DeBeer, S., **Birrell, J.A.** (2020). Insight into the Redox Behavior of the [4Fe–4S] Subcluster in [FeFe] Hydrogenases *ACS Catalysis* 10(21), 13084-13095. https://doi.org/10.1021/acscatal.0c02771
- Sanchez, M.L.K., Konecny, S.E., Narehood, S.M., Reijerse, E.J., Lubitz, W., **Birrell, J.A.**, Dyer, R.B. (2020). The Laser-Induced Potential-Jump: a Method for Rapid Electron Injection into Oxidoreductase Enzymes *The Journal of Physical Chemistry B* 120(40), 8750-8760. https://doi.org/10.1021/acs.jpcb.0c05718
- Takeda, K., Kusuoka, R., **Birrell, J.A.**, Yoshida, M., Igarashi, K., Nakamura, N. (2020). Bioelectrocatalysis based on direct electron transfer of fungal pyrroloquinoline quinone-dependent dehydrogenase lacking the cytochrome domain *Electrochimica Acta* 359, 136982. https://doi.org/10.1016/j.electacta.2020.136982
- Oughli, A.A., Hardt, S., Rüdiger, O., **Birrell, J.A.**, Plumeré, N. (2020). Reactivation of sulfide-protected [FeFe] hydrogenase in a redox-active hydrogel *Chemical Communications* 56(69), 9958-9961. https://doi.org/10.1039/D0CC03155K
- Rodríguez-Maciá, P., Galle, L., Bjornsson, R., Lorent, C., Zebger, I., Yoda, Y., Cramer, S., DeBeer, S., Span, I., **Birrell, J.A.** (2020). Caught in the H_{inact}: Crystal Structure and Spectroscopy Reveal a Sulfur Bound to the Active Site of an O_2-stable State of [FeFe] Hydrogenase *Angewandte Chemie International Edition* 59(38), 16786-16794. https://doi.org/10.1002/anie.202005208
- Szczesny, J., **Birrell, J.A.**, Conzuelo, F., Lubitz, W., Ruff, A., Schuhmann, W. (2020). Redox polymer-based high current density gas diffusion H_2 oxidation bioanode using [FeFe] hydrogenase from *Desulfovibrio desulfuricans* in a membrane-free biofuel cell *Angewandte Chemie International Edition* 59(38), 16506-16510. https://doi.org/10.1002/anie.202006824
- Reijerse, E., **Birrell, J.A.**, Lubitz, W. (2020). Spin Polarization Reveals the Coordination Geometry of the [FeFe] Hydrogenase Active Site in Its CO Inhibited State *The Journal of Physical Chemistry Letters* 11(12), 4597-4602. https://doi.org/10.1021/acs.jpclett.0c01352
- Van Stappen, C., Decamps, L., Cutsail III, G.E., Bjornsson, R., Henthorn, J.T., **Birrell, J.A.**, DeBeer, S. (2020). The Spectroscopy of Nitrogenases *Chemical Reviews* 120(12), 5005-5081. https://doi.org/10.1021/acs.chemrev.9b00650
- **Birrell, J.A.**, Pelmenschikov, V., Mishra, N., Wang, H., Yoda, Y., Tamasaku, K., Rauchfuss, T.B., Cramer, S.P., Lubitz, W., DeBeer, S. (2020). Spectroscopic and Computational Evidence that [FeFe] Hydrogenases Operate Exclusively with CO-bridged Intermediates *Journal of the American Chemical Society* 142(1), 222-232. https://doi.org/10.1021/jacs.9b09745
- Chongdar, N., Pawlak, K., Rüdiger, O., Reijerse, E.J., Rodríguez-Maciá, P., Lubitz, W., **Birrell, J.A.**, Ogata, H. (2020). Spectroscopic and biochemical insight into an electron-bifurcating [FeFe] hydrogenase *Journal of Biological Inorganic Chemistry* 25(1), 135-148. https://doi.org/10.1007/s00775-019-01747-1

2019

- Reijerse, E.J., Pelmenschikov, V., **Birrell, J.A.**, Richers, C.P., Rauchfuss, T.B., Cramer, S.P., Lubitz, W. (2019). Asymmetry in the Ligand Coordination Sphere of the [FeFe] Hydrogenase Active Site is reflected in the Magnetic Spin Interactions of the Aza-Propanedithiolate Ligand *The Journal of Physical Chemistry Letters* 10(21), 6794-6799. https://doi.org/10.1021/acs.jpclett.9b02354
- Sanchez, M.L., Sommer, C., Reijerse, E., Birrell, J.A., Lubitz, W., Dyer, R.B. (2019). Investigating the Kinetic Competency of CrHydA1 [FeFe] Hydrogenase Intermediate States via Time-resolved Infrared Spectroscopy *Journal of the American Chemical Society* 141(40), 16064-16070. https://doi.org/10.1021/jacs.9b08348
- Schuller, J.M., **Birrell, J.A.**, Tanaka, H., Konuma, T., Wulfhorst, H., Cox, N., Schuller, S.K., Thiemann, J., Lubitz, W., Sétif, P., Ikegami, T., Engel, B.D., Kurisu, G., Nowaczyk, M.M. (2019). Structural adaptations of photosynthetic complex I enable ferredoxin-dependent electron transfer *Science* 363(6424), 257-260. https://doi.org/10.1126/science.aau3613
- Rodríguez-Maciá, P., Kertess, L., Burnik, J., **Birrell, J.A.,** Hofmann, E., Lubitz, W., Happe, T., Rüdiger, O. (2019). His-ligation to the [4Fe-4S] sub-cluster tunes the catalytic of [FeFe] hydrogenase *Journal of the American Chemical Society* 141(1), 472-481. https://doi.org/10.1021/jacs.8b11149

2018

- Rodriguez-Maciá, P., Reijerse, E.J., van Gastel, M., DeBeer, S., Lubitz, W., Rüdiger, O., **Birrell, J.A.** (2018). Sulfide Protects [FeFe] Hydrogenases from O_2 *Journal of the American Chemical Society* 140(30), 9346-9350. https://doi.org/10.1021/jacs.8b04339
- Oughli, A.A., Vélez, M., **Birrell, J.**, Schuhmann, W., Lubitz, W., Plumeré, N., Rüdiger, O. (2018). Viologen-modified Electrodes for Protection of Hydrogenases from High Potential Inactivation while Performing H_2 Oxidation at Low Overpotential *Dalton Transactions* 47(31), 10685-10691. https://doi.org/10.1039/C8DT00955D
- Chongdar, N., **Birrell, J.A.**, Pawlak, K., Sommer, C., Reijerse, E.J., Rudiger, O., Lubitz, W., Ogata, H. (2018). Unique Spectroscopic Properties of the H-Cluster in a Putative Sensory [FeFe] Hydrogenase *Journal of the American Chemical Society* 140(3), 1057-1068. https://doi.org/10.1021/jacs.7b11287

2017

- Pelmenschikov, V., **Birrell, J.A.**, Pham, C.C., Mishra, N., Wang, H., Sommer, C., Reijerse, E., Richers, C.P., Tamasaku, K., Yoda, Y., Rauchfuss, T.B., Lubitz, W., Cramer, S.P. (2017). Reaction Coordinate Leading to H_2 Production in [FeFe]-Hydrogenase Identified by Nuclear Resonance Vibrational Spectroscopy and Density Functional Theory *Journal of the American Chemical Society* 139(46), 16894-16902. https://doi.org/10.1021/jacs.7b09751
- Rodríguez-Maciá, P., Pawlak, K., Rüdiger, O., Reijerse, E.J., Lubitz, W., **Birrell, J.A.** (2017). Intercluster Redox Coupling Influences Protonation at the H-cluster in [FeFe] Hydrogenases *Journal of the American Chemical Society* 139(42), 15122-15134. https://doi.org/10.1021/jacs.7b08193
- **Birrell, J.A.**, Rüdiger, O., Reijerse, E.J., Lubitz, W. (2017). Semisynthetic Hydrogenases Propel Biological Energy Research into a New Era *Joule* 1(1), 61-76. https://doi.org/10.1016/j.joule.2017.07.009
- Rodríguez-Maciá, P., Reijerse, E., Lubitz, W., **Birrell, J.A.**, Rüdiger, O. (2017). Spectroscopic Evidence of Reversible Disassembly of the [FeFe] Hydrogenase Active Site *Journal of Physical Chemistry Letters* 8(16), 3834-3839. https://doi.org/10.1021/acs.jpclett.7b01608

- Rodríguez-Maciá, P., **Birrell, J.A.**, Lubitz, W., Rüdiger, O. (2017). Electrochemical Investigations on the Inactivation of the [FeFe] Hydrogenase from *Desulfovibrio desulfuricans* by O_2 or Light under Hydrogen-Producing Conditions *ChemPlusChem* 82(4), 540-545. https://doi.org/10.1002/cplu.201600508
- Sommer, C., Adamska-Venkatesh, A., Pawlak, K., **Birrell, J.A.**, Rüdiger, O., Reijerse, E.J., Lubitz, W. (2017). Proton Coupled Electronic Rearrangement within the H-Cluster as an Essential Step in the Catalytic Cycle of [FeFe] Hydrogenases *Journal of the American Chemical Society* 139(4), 1440-1443. https://doi.org/10.1021/jacs.6b12636

2016

- **Birrell, J.A.**, Wrede, K., Pawlak, K., Rodríguez-Maciá, P., Rüdiger, O., Reijerse, E.J., Lubitz, W. (2016). Artificial Maturation of the Highly Active Heterodimeric [FeFe] Hydrogenase from Desulfovibrio desulfuricans ATCC 7757 *Israel Journal of Chemistry* 56(9-10), 852-863. https://doi.org/10.1002/ijch.201600035
- **Birrell, J.A.**, Laurich, C., Reijerse, E.J., Ogata, H., Lubitz, W. (2016). Importance of Hydrogen Bonding in Fine Tuning the [2Fe-2S] Cluster Redox Potential of HydC from *Thermotoga maritima Biochemistry* 55(31), 4344-4355. https://doi.org/10.1021/acs.biochem.6b00341
- Kutin, Y., Srinivas, V., Fritz, M., Kositzki, R., Shafaat, H.S., **Birrell, J.**, Bill, E., Haumann, M., Lubitz, W., Högbom, M., Griese, J.J., Cox, N**.** (2016). Divergent assembly mechanisms of the manganese/iron cofactors in R2lox and R2c proteins *Journal of Inorganic Biochemistry* 162, 164-177. https://doi.org/10.1016/j.jinorgbio.2016.04.019

2015

- Fourmond, V., Stapf, S., Li, H.G., Buesen, D., **Birrell, J.**, Rüdiger, O., Lubitz, W., Schuhmann, W., Plumere, N., Léger, C. (2015). Mechanism of Protection of Catalysts Supported in Redox Hydrogel Films *Journal of the American Chemical Society* 137(16), 5494-5505. https://doi.org/10.1021/jacs.5b01194

2013

- **Birrell, J.A.**, Morina, K., Friedrich, T., Hirst, J. (2013). Investigating the function of [2Fe-2S] cluster N1a, the off-pathway cluster in complex I, by manipulating its reduction potential *Biochemical Journal* 456(1), 139-146. https://doi.org/10.1042/BJ20130606
- **Birrell, J.A.,** Hirst, J. (2013). Investigation of NADH binding, hydride transfer and NAD^+ dissociation during NADH oxidation by mitochondrial complex I using modified nicotinamide nucleotides *Biochemistry* 52(23), 4048-4055. https://doi.org/10.1021/bi3016873

2011

- **Birrell J.A.**, King M.S., Hirst J. (2011). A ternary mechanism for NADH oxidation by positively charged electron acceptors, catalyzed at the flavin site in respiratory complex I *FEBS Letters* 585(14), 2318-2322. https://doi.org/10.1016/j.febslet.2011.05.065
- Bridges H.R., **Birrell J.A.**, Hirst J. (2011). The mitochondrial-encoded subunits of respiratory complex I (NADH:ubiquinone oxidoreductase): identifying residues important in mechanism and disease *Biochemical Society Transactions* 39(3), 799-806. https://doi.org/10.1042/BST0390799

2010

- **Birrell J.A.**, Hirst J. (2010). Truncation of subunit ND2 disrupts the threefold symmetry of the antiporter-like subunits in complex I from higher metazoans *FEBS Letters* 584(19), 4247-4252. https://doi.org/10.1016/j.febslet.2010.09.017

2009

- **Birrell J.A.**, Yakovlev G., Hirst J. (2009). Reactions of the flavin mononucleotide in complex I: a combined mechanism describes NADH oxidation coupled to the reduction of $APAD^+$, ferricyanide, or molecular oxygen *Biochemistry* 48(50), 12005-12013. https://doi.org/10.1021/bi901706w