MONASH University

Monash University, Low-cost, robust, high-activity water splitting electrodes R&D Project

Mid-term Activity Report, July 2020

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PROJECT SUMMARY AND SCOPE

This project brings together complementary expertise of ANU and Monash University in the engineering, design and characterisation of electrocatalysts to develop scalable methods for the fabrication of efficient, low-cost and robust electrodes for H_2 production from renewable energy sources via electrochemical water splitting. This process is central to the "Renewable hydrogen for export" goal, as the most feasible source of sustainable hydrogen. Despite recent progress, most research on electrochemical water splitting has focused on catalyst discovery with the use of often prohibitively sophisticated methods. In stark contrast, here we will build upon innovative fabrication techniques developed by the research partners, aiming to engineer efficient and cost-effective electrodes based on earth-abundant, low-cost elements such as iron. Key features of the project include: design of efficient large-area water splitting electrodes, demonstration of the scalability of the developed fabrication methods and exhaustive stability tests under technologically relevant conditions. High-performance water oxidation electrodes are also indispensable for other electrosynthesis processes including production of ammonia from dinitrogen. Thus, the project will eventuate in the development of innovative technologies, which are urgently needed for durable and cost-efficient H_2 and NH_3 production, resulting in immediate technological and commercial value.

Key anticipated outcomes of the project:

1 progression of the flame spray pyrolysis water splitting electrode fabrication technology to TRL4;
2 creation of a techno-economic model for the integration of the water splitting technology in a "Power to Gas" mode;
3 expanded connections to Australian and Japanese industrial partners in renewable hydrogen sector for commercialisation of the developed technologies, and establishing pathways for export of renewable Australian hydrogen; and
4 greater awareness in the public, government and industry sectors around the developments of renewable hydrogen technology in Australia.

Mid-term milestones for the period under report:

Milestone 2.1 Demonstration of water splitting electrodes operating at stabilised current densities of ≥20 mA cm^{-2} with efficiency ≥77% at 25-80°C.

Milestone 2.2 Demonstration of a water splitting system based on electrodes from Milestone 2.1 and showing degradation ≤10% over 2 weeks at 25°C.

Milestone 2.3 Design of the water electrolyser prototype that will operate at up to 100 °C, and at pH < 0.5 or pH > 13.5.

PROGRESS UPDATE

Over the reporting period, the work has focused on (i) the synthesis and characterisation of new catalysts, (ii) long-term tests of new catalysts, and (iii) design of an improved electrolyser device, consistent with the research plan. A broad range of new catalytic systems (oxides, sulphides and phosphides of non-noble metals like iron, nickel, cobalt, molybdenum, silver, lead and bismuth) has been fabricated using scalable methods. Most of these materials have enabled water splitting at an energy efficiency of at least 77%, as per Milestone 2.1. Selected catalysts have been demonstrated to suffer negligible losses in performance when tested over two weeks at ambient temperature, as required for Milestone 2.2. This is specifically demonstrated herein for two-electrode water splitting systems based on: (1) microwave-synthesised mixed nickel-molybdenum sulphides (cathode) and nickel-iron sulphides (anode), and (2) iron phosphides prepared by flame-spray pyrolysis and used both as an anode and cathode. To achieve Milestone 2.3, a new concept of an electrolyser device has been designed, and the preliminary prototype has been fabricated and tested.

The progress towards the project outcomes is also as expected. The flame-spray pyrolysis setup at ANU has been upgraded to enable the synthesis of a broader range of electrocatalytic materials, to support its progression towards TRL4 by the end of the project (Outcome 1). AGL and Monash have created and implemented a techno-economic model for the assessment of the feasibility of the use of hydrogen derived from electrolysis in various sectors (Outcome 2). Our connections to the industry partners are continuously expanding (Outcome 3); of a particular note are the expanding collaborations with Woodside Energy, ANT Energy Solutions and the Verdant Company. Finally, our outreach activities through various mechanisms are creating a greater awareness on the hydrogen economy (Outcome 4).

KEY HIGHLIGHTS AND DIFFICULTIES EXPERIENCED

While the restrictions due to the worldwide spread of the virus have affected the progress of our research through the temporary close down of the laboratories and significantly limited access to several key research facilities, timely establishment of the alternative work arrangements have minimised the impact of the global pandemic situation on the progress of the ARENA-funded project. Both Monash and ANU research teams are successfully achieving the goals identified in the research agreement.

The key highlights at this stage of the project include:

(1) Successful demonstration of the industry-ready flame-spray pyrolysis method for the fabrication of high-performance water splitting electrodes based on cheap and abundant nickel and iron that exhibit essentially no loss in their performance over two weeks of continuous electrolysis of alkaline water. The ANU flame-spray pyrolysis system is continuously upgraded to expand the synthetic capabilities to a broader range of electromaterials.

(2) Identification of three new families of unprecedently robust anode catalysts that operate with no detectable loss in activity at industrially-relevant temperatures of up to 80 °C in strongly acidic environment; some of these materials are directly applicable for the use in the technologically most promising proton-exchange membrane water electrolysers.

(3) Design and prototyping of a water electrolyser device that avoids the use of expensive ion-selective membrane and is capable of operation at both acidic and alkaline pH at temperatures up to 100 °C.

(4) Creation of a techno-economic model for the application of the 100% green hydrogen derived from renewables through the water electrolysis in various industry sectors. Implementation of this model has enabled identification of the key cost-determining parameters: (i) renewable electricity price, (ii) selling price for the generated hydrogen gas, (iii) cost of the electrolyser device.

COMMENTARY ON COMMERCIALISATION PROSPECTS

One of key features of the present ARENA-funded project is the collaboration between Monash researchers and the AGL Power Development team on the techno-economic analysis of the commercialisation prospects of the hydrogen derived through water electrolysis powered by renewable electricity. Through this, the three students and staff involved were exposed to a series of speakers from across AGL and associated companies for discussions on the following topics: Wholesale Electricity Markets, Physical Markets Trading in the NEM, AGL Futures Portfolio, Levelized Cost of Hydrogen, Hydrogen Energy Supply Chain Project (HESC), Valuations & Uncertainties in Hydrogen Projects, Technical Considerations of Hydrogen (Altona North Electrolyser) and the Western Sydney Gas Project (WSGP). Based on these discussions, extensive background readings and the mentorship of the AGL team, a basic financial model has been created and applied to three selected cases: (i) Feedstock synthesis for ammonia production: Queensland & Pilbara, (ii) Pulverised coal replacement for Green(er) Steel: Whyalla Steelworks, and (iii) Centralised production for transport and logistics: Melbourne Metropolitan Distribution (MMD).

The key outcome of this analysis was the identification of the cost of the water electrolysis devices, which is to a significant extent affected by the price of the electrodes, as a more significant parameter than the energy efficiency of electrolysers in terms of the cost-efficiency. In other words, development of electrodes that are not as efficient as the currently used noble-metal based ones, but orders of magnitude less expensive would substantially improve the cost-effectiveness of the technology. This outcome is in strong alignment with the aims of the present ARENA-funded project.

The above conclusion is already being confirmed through the rapidly expanding connections of the Monash-ANU teams with industry partners developing the sustainable water electrolysis technologies. Of a key importance here is the new project with Woodside Energy Inc. aiming to create efficient electrocatalysts for the hydrogen generation from sea water, as well as the emerging collaboration with the Verdant Company on the design of the electrolytic hygiene system based on the saline water electrolysis. Both of these developments are partially based on the outcomes of the present ARENA-funded project.

SUMMARY OF KNOWLEDGE SHARING ACTIVITIES COMPLETED

The outcomes of our research in the renewable energy technologies are continuously and broadly disseminated through various mechanisms and at different levels.

Of a particular note are our following activities in this domain:

(1) Hosting of delegations from academia, industry and government

Of a particular note are the following interactions:

- a significant number of visits of Monash researchers to Woodside headquarters in Perth and Woodside top-managers to Monash Clayton campus;

- a delegation from Germany led by the German Academy of Engineering and the German Industry Federation, the BDI focussed on Energy Futures based on hydrogen and ammonia;

- a delegation headed by Mr Hiroshi Kajiyama, Japanese Minister of Economy, Trade and Industry, along with the Australian Minister for Trade, Tourism and Investment, Senator Simon Birmingham;

- a delegation headed by the President of the National Academy of Engineering Korea Prof Oh-Kyong Kwon.

(2) Media highlights

Our work on the development of new low-cost, robust water splitting electrodes and devices has been broadly highlighted in various media:

- RSC Chemistry World [https://www.chemistryworld.com/news/uk-project-aims-to-cut-the-cost-of-producing-clean-green-hydrogen/4011788.article#/]

- Monash.Lens [https://lens.monash.edu/@science/2019/09/24/1376698/electrolysis-breakthrough-could-solve-the-hydrogen-conundrum]

- Nature Blog [https://chemistrycommunity.nature.com/users/253869-alexandr-simonov/posts/48277-intrinsically-stable-in-situ-generated-electrocatalyst-for-long-term-oxidation-of-acidic-water-at-up-to-80-c]

- Monash University News [https://www.monash.edu/science/news/current/monash-leads-the-way-in-a-green-chemistry-breakthrough-for-renewables/_nocache]

- PV-Magazine [https://www.pv-magazine-australia.com/2019/05/16/monash-researchers-achieve-green-hydrogen-breakthrough/]

- Renew Economy [https://reneweconomy.com.au/scientists-edge-closer-to-stable-cheap-green-hydrogen-production-78478/]

- Sustainability Matters [https://www.sustainabilitymatters.net.au/content/sustainability/case-study/researchers-closer-to-affordable-green-hydrogen-1543192365]

- National Resources Review
[https://www.nationalresourcesreview.com.au/news_article/australian-researchers-lead-the-way-in-a-green-chemistry-breakthrough-for-renewables/]

(3) Public presentations

- Dr Simonov has presented the experimental "Solar Fuels" rig to the public visitors during the Monash Open day.

- PhD candidate supervised by Dr Simonov, presented and advertised the renewable energy concepts and science in general for the International Women's Day (in Science) at Melbourne Girl's College.

- Youtube video highlighting the *operando* analysis of electrocatalysts
[https://www.youtube.com/watch?v=Z_UYpZC8xu0]

(4) Conference presentations

- **Self-healing electrocatalysts for stable oxidation of hot acidic water**. M. Chatti, J. L. Gardiner, M. Fournier, D. R. MacFarlane, R. K. Hocking, A. N. Simonov, *Cell Symposia - Next Generation Materials for Energy Applications*, Xiamen, China **Nov 2019**.

- **Three-dimensional Nanostructuring of Metal-Organic Frameworks for energy applications**. Keynote lecture by A. Tricoli. *ICONN - International Conference on Nanoscience and Nanotechnology*, Brisbane, **Feb 2020**.

- **Unlocking the Potential of Earth-Abundant Metal Oxides for Thermochemical Solar Fuel Production**. Invited presentation by A. Tricoli. *ACMM 26*, Canberra, **Feb 2020**.

- **Scalable Structuring of Efficient Earth-Abundant Electrocatalysts for Water Splitting and CO_2 Reduction**. Invited presentation by A. Tricoli. *ACES Symposium*, Canberra, **Feb 2020**.

The following presentation was cancelled due to the global travel ban:

- **Water Oxidation in Acidic Solutions: Beyond Noble Metals.** M. Chatti, J. L Gardiner, H. L. Du, D. Simondson-Tammer, D. R MacFarlane, A. N. Simonov. *237th Electrochemical Society (ECS) Meeting*, Montreal, Canada, **May 2020**.

Our interactions with a very broad audience with very different backgrounds through the activities above has clearly contributed to the increased awareness around the hydrogen economy and our developments in the sustainable hydrogen generation technologies among industry and general public. It was important to learn that the interest in H_2 production through electrolysis by industry has progress to a more substantial level with a clear intention to deeply investigate into the future opportunities. In particular, this resulted in several consulting projects on the hydrogen production opportunities we have been involved into by several Australian companies. Scientific presentations have broadened our research network; moreover, one of the new connections has resulted in the preliminary short collaboration with researchers from Europe.

(5) High profile publications

These publications highlight our vision on the development of the renewable fuels technologies:

- **A Roadmap to the Ammonia Economy** by D. R. MacFarlane, P. V. Cherepanov, J. Choi, B. H. R. Suryanto, R. Y. Hodgetts, J. M. Bakker, F. M. F. Vallana, A. N. Simonov. *Joule* 2020, https://doi.org/10.1016/j.joule.2020.04.004

- **Liquefied Sunshine: Transforming Renewables into Fertilizers and Energy Carriers with Electromaterials** by D. R. MacFarlane, Choi B. H. R. Suryanto, R. Jalili, M. Chatti, L. M. Azofra, A. N. Simonov. *Advanced Materials* 2020, https://doi.org/10.1002/adma.201904804

(6) Scientific publications

- **Enhancement of the photoelectrochemical water splitting by perovskite $BiFeO_3$ via interfacial engineering.** G. Liu, S. K. Karuturi, H. Chen, D. Wang, J. W. Ager, A. N. Simonov, A. Tricoli. *Solar Energy* **2020**, *202*, 198. https://doi.org/10.1016/j.solener.2020.03.117.

- **Hybrid Organic–Inorganic Materials and Composites for Photoelectrochemical Water Splitting**. Singh, S.; Chen, H.; Shahrokhi, S.; Wang, L. P.; Lin, C.-H.; Hu, L.; Guan, X.; Tricoli, A.; Xu, Z. J.; Wu, T. *ACS Energy Letters* **2020,** *5*, 1487. https://doi.org/10.1021/acsenergylett.0c00327.

- **Timescale and Electrode Effects Critical for the in situ X-ray Spectroscopic Analysis of Electrocatalysts: the Water Oxidation Case.** H. King, M. Fournier, S. A. Bonke, E. Seeman, M. Chatti, A. N. Jumabekov, B. Johannessen, P. Kappen, A. N. Simonov, R. K. Hocking. Photon-Induced, *Journal of Physical Chemistry C* **2019**, *123*, 28533. https://doi.org/10.1021/acs.jpcc.9b06944.

- **High Temperature One-Step Synthesis of Efficient Nanostructured $BiVO_4$ Photoanodes for Water Oxidation.** T. Tran-Phu, H. Chen, R. Bo, I. Di Bernardo, Z. Fusco, A. N. Simonov, A. Tricoli. *Energy Technology* **2019**, *7*, 1801052. https://doi.org/10.1002/ente.201801052.

- **Intrinsically stable *in situ* generated electrocatalyst for long-term oxidation of acidic water at up to 80 °C.** M. Chatti, J. L. Gardiner, M. Fournier, B. Johannessen, T. Williams, T. R. Gengenbach, N. Pai, C. Nguyen, D. R. MacFarlane, R. K. Hocking, A. N. Simonov. *Nature Catalysis* **2019**, *2*, 457. https://doi.org/10.1038/s41929-019-0277-8.

- **Earth-abundant transition metal oxides with extraordinary reversible oxygen exchange capacity for efficient thermochemical synthesis of solar fuels.** Gao, X.; Liu, G.; Zhu, Y.; Kreider, P.; Bayon, A.; Gengenbach, T.; Lu, T.; Liu, Y.; Hinkley, J.; Lipiński, W.; Tricoli, A.,. *Nano Energy* **2018,** *50*, 347. https://doi.org/10.1016/j.nanoen.2018.05.045.

LESSONS LEARNT AND NEXT STEPS

The key challenge of the project, as well as one of its key goals, is the eventual upgrade of the flame spray pyrolysis system beyond the existing capabilities, which are limited by the inherent specifications of the available equipment. This has been realised at the earliest stages of the project and we have now addressed the challenge by securing $600k funding for new equipment through the ARC Linkage Infrastructure, Equipment and Facilities scheme. A new advanced system with capabilities exceeding those initially planned will be installed in Prof Tricoli's laboratories by the end of 2021 and will be used to showcase the outcomes of the project.

Our knowledge sharing activities are attracting continued attention from potential Australian and overseas partners interested in hydrogen production through water electrolysis and in particular in our developments in the field. From the regular interactions with a range of companies we understand that the development of a whole device is critical, which has motivated us to intensify activity in this particular project work package recently. We have also gained an impression that large Australian industry (AGL, Woodside, WesCEF, etc.) are at an exploration, techno-economic analysis stage. At the same time, we are aware of and are partially involved in some more ambitious start-up activities aiming to create Australian water electrolysis plants.

We are enthusiastic about future follow-on projects building upon the results of the current ARENA-funded work. We have commenced negotiations with the international company ENI and Australian Government Department of Defence on possible collaborations for the creation of the hydrogen production systems for energy storage and for military needs, respectively. We are at the advanced stages of planning an R&D project with the Verdant Company – an Australian SME developing a new hygiene system operating through water electrolysis. Finally, we have already secured funding from Woodside Ltd for an R&D project aimed at the development of sea water electrolysis technology utilising the new technologies developed herein. The successful completion of the final stages of the present ARENA-funded project will ensure that these future collaborations will proceed efficiently and will significantly contribute to the development of the hydrogen technologies in Australia.