



# **15<sup>th</sup> INTERNATIONAL SYMPOSIUM HYDROGEN & ENERGY**

**Hydrogen Production, Hydrogen Storage, Hydrogen Applications, Theory and Modelling, Fuel Cells, Batteries, Synthetic Fuels, Functional Materials**

The 15<sup>th</sup> International Symposium “Hydrogen & Energy” follows the 14<sup>th</sup> Int. Symposium Hydrogen & Energy that took place 5<sup>th</sup> – 11<sup>th</sup> January 2020 in Sapporo, Japan together with the 1<sup>st</sup> International Symposium Hydrogenomics with more than 70 participants. It serves as an information platform of the fundamental science and technology and the frontiers of research on hydrogen and energy.

The symposium consists of top level invited keynote lectures reviewing the key elements of the hydrogen cycle, i.e. the hydrogen production, hydrogen storage and hydrogen combustion and fuel cells. Furthermore, contributions on the conversion of renewable energy in general and energy carriers besides and beyond hydrogen are very welcome. The world leading experts present the current research challenges and most important results in invited and contributing talks. Early stage and experienced researchers present their newest results and the open questions on posters as well as in a one slide presentation.

The symposium takes place in the **SEEBLICK HÖHENHOTEL**, in Emmetten, Switzerland.

The number of participants is limited to 70 without the accompanying persons.


## **22. - 26. January 2023**

**SEEBLICK HÖHENHOTEL**

Hugenstrasse 24, CH-6376 Emmetten, Switzerland

T: +41 41 624 41 41, e: [info@hotelseeblick.ch](mailto:info@hotelseeblick.ch)

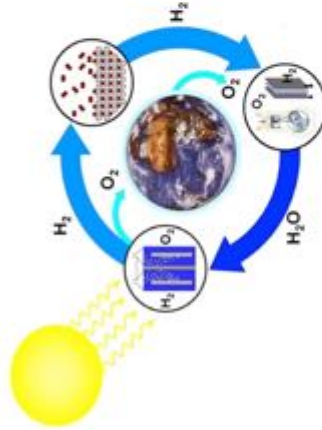
U: <http://www.hotelseeblick.ch>







**22. - 26. January 2023**  
**Seeblick Höhenhotel,**  
**Emmetten, Switzerland**



<http://hesymposium.ch/>

**SUBJECTS**

- Hydrogen production
- Hydrogen storage
- Fuel Cells
- Batteries
- Synthetic fuels
- Theory & modelling
- Applications

**ORGANIZER**

Prof. Dr. Andreas ZÜTTEL, Mrs. Ivana SUTER  
 Ecole Polytechnique Fédérale de Lausanne (EPFL)  
 Institut des sciences et ingénierie chimiques (ISIC),  
 CH-1015 Lausanne, Switzerland

**STEERING COMMITTEE**

Craig JENSEN, Hawaii, USA  
 Shin-ichi ORIMO, Japan  
 Min ZHU, China  
 Jinqu ZHANG, China  
 Andreas ZÜTTEL, Switzerland

**INVITED SPEAKERS**

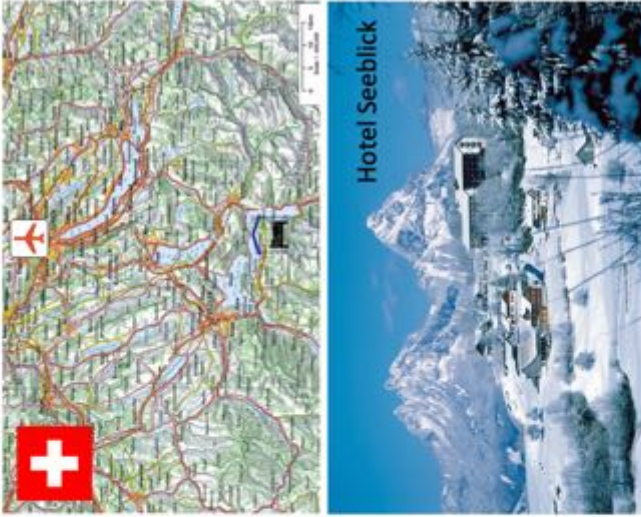
Berend SMIT, Switzerland  
 Robert SCHLÖGEL, Germany  
 Noris GALLANDAT, Switzerland  
 Shin-ichi ORIMO, Japan  
 Jihye PARK, S. Korea  
 Heena YANG, S. Korea  
 Björgvin Hjörvarsson, Sweden  
 Sabrina Sartori, Norway  
 Henning ZOZ, Germany

**PROGRAM**

	Su	Mo	Tu	We	Th	Fr
09:00						
12:00						
14:00	Recept.			Lunch		
17:00				social event		depart.
18:00	Din.	Dinner	Dinner	Dinner	Conf. dinner	
21:00		Poster	Poster			

*inv. lec. inv. talk, talk*

**LOCATION**



**SEEBLICK HÖHENHOTEL**

Hugenstrasse 24, CH-6376 Emmetten,  
 Switzerland

T: +41 41 624 41 41, e: info@hotelseeblick.ch  
 U: <http://www.hotelseeblick.ch>

**REGISTRATION**

Conference fee CHF 1200  
 incl. conference facilities, internet, proceedings  
 and social event, excursion, coffee breaks,  
 lunch, dinner, conference dinner, beverages at  
 poster sessions.  
 Conference fee (remote) CHF 250

Registration online:

<http://hesymposium.ch/>

Registration and abstract submission:  
 before 1<sup>st</sup> December 2022



# CONTENTS

## Timetable

9

## Abstracts 11

### PROGRAM

#### Sunday **22. 1. 2023 Chair: A. Züttel**

- 14:00 - 17:00 Registration  
Ivana SUTER
- 17:00 - 18:00 Opening of the 15<sup>th</sup> Int. Symposium Hydrogen & Energy  
Opening talk by Berend SMIT 'Big-data in chemical engineering: science beyond understanding'
- 18:30 - 20:00 Dinner

#### **23. 1. 2023 Monday morning Chair: Berend Smit**

- 09:00 - 09:50 Robert SCHLOEGL 'Catalysis as science and technology for the Hydrogen Age'
- 09:50 - 10:15 Thi Ha My PHAM 'In-situ synthesis of highly active Fe-doped Co-based catalyst for Oxygen Evolution Reaction'
- 10:15 - 10:45 Coffee break
- 10:45 - 11:10 Riku HORIE 'Kerosing production with various technologies in switzerland'
- 11:10 - 11:35 Jinqiu ZHANG 'High Catalytic Selectivity of Copper Nanowires for Ethylene Production from CO<sub>2</sub> Electrochemical Reduction'
- 11:35 - 12:00 Claudio PISTIDDA 'Recycling as the key for developing sustainable hydrogen storage materials'
- 12:00 - 12:15 Conference photo
- 12:15 - 14:00 Lunch

#### **Monday afternoon Chair: Robert Schlögl**

- 14:00 - 14:50 Jihye PARK 'Recent Trends in the Korean Hydrogen Industry'
- 14:50 - 15:20 Coffee break
- 15:20 - 15:45 Kun ZHAO 'Energetics and Growth Modes of Ni and Pd Nanoparticles onto Graphene'
- 15:45 - 16:10 Yuanyuan SHANG 'Recycling as the key for developing sustainable FeTi alloys for hydrogen storage'
- 16:10 - 16:35 Mark ALLENDORF 'From Nano to Macro and Back Again: Disruptive Science for Materials-Based Hydrogen Storage'
- 18:30 - 20:00 Dinner
- 20:00 - 21:30 **Poster session Chair: Andreas Borgschulte**

Manhui WEI 'An Advanced Al-Air Fuel Cell Using a Mesh-Encapsulated Anode via Al-Zn Energy Transfer'

Jessica RUFFINER 'Thermal Desorption of H<sub>2</sub> and CO<sub>2</sub> from High Surface Area Material'

Yasemen KUDDUSI 'Selective thermo-catalytic conversion of CO<sub>2</sub> and H<sub>2</sub> into ethylene'

Selim KAZAZ 'Ru-complex based polymeric photocathode for solar water splitting'

Kataoka YUTA 'Calculation of diffusion coefficients of H on metal surfaces'

Chia-Chieh SHEN 'Hydrogen Purification with LaNiAl<sub>5</sub>-Based Metal Hydrides'

Andreas ZÜTTEL 'ACHIEVEMENTS SCCER H&E Storage: Hydrogen Storage'

Andreas ZÜTTEL 'Analysis of the Energy Transition in Switzerland'

Andreas ZÜTTEL 'Renewable Energy Solutions for Switzerland'

Andreas ZÜTTEL 'The Economy of Renewable Energy'

Ulrike TRACHTE "EMERGENCY POWER SYSTEMS WITH FUEL CELLS AND HYDROGEN"

Emil Høj Jensen 'Effects of replacing La with Y on the crystal structure of La<sub>6-x</sub>Y<sub>x</sub>Ni<sub>6.5</sub>Mn<sub>0.33</sub>Al<sub>0.17</sub> materials'

**24. 1. 2023 Tuesday morning Chair: Sabrina Sartori**

09:00 - 09:50 Andreas BORGSCHULTE 'Proton Coupled Electron vs. Hydrogen Transport In Electrocatalysis'

09:50 - 10:15 Heena YANG 'K-water's Hydrogen business development'

10:15 - 10:45 Coffee break

10:45 - 11:10 Tai SUN 'Cycle and Regeneration Performance of Metal Hydride for Commercialized Storage and Compression System '

11:10 - 11:35 Rui LI 'Investigation on Hydrogen storage performance of AB<sub>2</sub> type alloy for 700bar Hydrogen compressor'

11:35 - 12:00 Cedric KOOLEN 'Electrochemical Wacker Process'

12:00 - 14:00 Lunch

**Tuesday afternoon Chair: Susana Garcia-Lopez**

14:00 -14:50 Sabrina SARTORI 'The Role of Secondary Phases and Element Substitutions in the Hydrogenation of Intermetallic Compounds'

14:50 - 15:20 Cedric KOOLEN 'Electrochemical Wacker Process'

15:20 - 15:45 Zohreh AKBARI 'Ruthenium-Supported Catalyst, a Potential New Catalyst for the Catalytic Hydrogen Combustion ''

15:45 - 16:10 Konstantinos BARDIS 'SIMULATION BASED DESIGN OF A METAL HYDRIDE COMPRESSOR USING REDUCED ORDER THERMAL MODELS AND COMPUTATIONAL FLUID DYNAMICS (CFD) '

- 15:45 - 16:10 Konstantinos BARDIS 'SIMULATION BASED DESIGN OF A METAL HYDRIDE COMPRESSOR USING REDUCED ORDER THERMAL MODELS AND COMPUTATIONAL FLUID DYNAMICS (CFD) '
- 16:10 - 16:35 Akhil PENMATHSA 'Simulation of Metal Hydride and Fuel Cell Based Hydrogen to Power Systems - 1D Model Based Thermal Management Optimisation'

**25. 1. 2023      Wednesday morning Chair: Chair: Björgvin Hjörvarsson**

- 09:00 - 09:50 Susana GARCIA-LOPEZ 'Materials discovery for energy-related applications: bridging process engineering and basic science'
- 09:50 - 10:15 Yunting WANG 'large-scale 3D nanostructured carbon for hydrogen storage'
- 10:15 - 10:45 Coffe break
- 10:45 - 11:10 'Steven SCHENK 'Membrane-less electrolysis'
- 11:10 - 12:00 Shin\_Ichi ORIMO 'Super-ionic conduction of mono-/di-valent cations and advanced battery application of complex hydrides: viewpoint from "HYDROEGNOMICS" project'
- 12:00 - 14:00 Lunch
- 14:00 -18:00 Social event
- 18:30 - 20:00 Dinner

**26. 1. 2023      Thursday morning Chair: Jihe Park**

- 09:00 - 09:50 Björgvin HJÖRVARSSON 'Using Model Systems to Obtain Understanding of Absorption And Diffusion of Hydrogen in Construction Materials'
- 09:50 - 10:15 Youngdon KO 'PLATINUM GROUP METAL-FREE DIRECT BOROHYDRIDE FUEL CELLS
- 10:15 - 10:45 Coffe break
- 10:45 - 11:10 Liping ZHONG 'Catalyst design and production for CO<sub>2</sub> methanation'
- 11:10 - 12:00 Henning ZOZ 'H<sub>2</sub>-Barbeque & H<sub>2</sub>-Cremation, bypassing fuel-cell conversion on route to stand-alone & subsidies free Hydrogen Energy Economy. '
- 12:00 - 12:15 Closing remarks

<b>SCIENCE OF HYDROGEN &amp; ENERGY AWARD</b>	51
<b>List of Participants</b>	59
<b>Information</b>	63



# SCHEDULE

Time	Sunday	Monday	Tuesday	Wednesday	Thursday	Friday
09:00 - 09:50		<b>Chair: B. Smit</b> Robert SCHLOEGL	<b>Chair: S. Sartori</b> Andreas BORGSCHULTE	<b>Chair: B. Hjörvarsson</b> Susana GARCIA-LOPEZ	<b>Chair: J. Park</b> Björgvin HIÖRVARSSON	
09:50 - 10:15		<i>Thi Ha My PHAM</i> Coffee break	<i>Heena YANG</i> Coffee break	Yunting WANG Coffee break	Youngdon KO Coffee break	
10:15 - 10:45		Riku HORIE	Tai SUN	Steven SCHENK	Liping ZHONG	
10:45 - 11:10		<i>Jinju ZHANG</i>	Rui LI	<i>Shin_Ichi ORIMO</i>	Henning ZOZ	
11:10 - 11:35		Claudio PISTIDDA	Cedric KOOLEN			
11:35 - 12:00		Conf. Photo			closing remarks	
12:00 - 14:00		Lunch	Lunch	Lunch		
	<b>Chair: A. Züttel</b>	<b>Chair: R. Schlögl</b>	<b>Chair: S. Garcia-Lopez</b>	<b>Chair: I. Suter</b>		
14:00-14:50		Jihye PARK	Sabrina SARTORI			
14:50 - 15:20		Coffee break	Coffee break			
15:20 - 15:45	Registration Ivana SUTER	Kun ZHAO	Zohreh AKBARI	Social event		
15:45 - 16:10		Yuanyuan SHANG	Konstantinos BARDIS			
16:10 - 16:35		<i>Mark ALLENDORF</i>	Akhil PENMATHSA			
16:35 - 17:00						
17:00 - 18:00	Berend SMIT					
18:30 - 20:00	Dinner	Dinner	Dinner	Conf. Dinner		
20:00 - 21:30		<b>Chair: A. Borgschulte</b> Poster				



# ABSTRACTS



## BIG-DATA IN SCIENCE AND ENGINEERING: SCIENCE BEYOND UNDERSTANDING

Berend SMIT<sup>a</sup>

<sup>a</sup>Laboratory of molecular simulation (LSMO), Institut des Sciences et Ingénierie Chimiques, Valais Ecole Polytechnique Fédérale de Lausanne (EPFL), Rue de l'Industrie 17, CH-1951 Sion, Switzerland

In many areas of science and engineering, we see big data being promoted as the tool that solves all our problems. Like all new developments, the promises are hyped. When the confetti's dust is settled, one can better assess how these novel methods can become useful tools for scientific research. In this lecture, we illustrate the use of data science in solving some scientific questions that were too complex to address using state-of-the-art theoretical approaches.

### State of the art

One of the aims of reticular chemistry is to design a metal-organic framework (MOF) that is optimal for a given application. This aim has inspired many chemists; to date, over 100,000 MOF crystal structures are reported in the Cambridge Structural Database<sup>1</sup> (CSD) for applications ranging from gas separations, gas storage, (photo) catalysis, and sensing to drug delivery.<sup>2,3</sup> The chemical design space of MOFs and related materials (e.g., covalent organic frameworks,<sup>4</sup> COFs; porous polymer networks, PPNs,<sup>5</sup> porous organic molecular crystals<sup>6</sup>) is enormous. Theoretically, one can combine an infinite number of possible linkers with many different metal nodes assembling in all kinds of structures.<sup>3,7</sup> In practice, however, one can only synthesize and test a small subset of all possible MOFs.

To complement the experimental efforts, computational screening studies<sup>8-16</sup> have been carried out using brute-force molecular simulation to predict the properties for a large set of experimental or *in silico*-generated MOF structures.<sup>17</sup> For example, Thornton et al.<sup>18</sup> screened 850,000 porous materials to explore the limits of hydrogen storage. Although we can screen many more materials than experiments, computational resources limit these studies to a fraction of all possible materials. For example, Kim et al.<sup>19</sup> showed that they could generate over 100 trillion MOFs. Even with the most efficient algorithm, near zero CPU time, it would be difficult to have faster I/O operations) than 1 ms per material (Python, current hardware, or 3,100 years to evaluate 100 trillion materials.

The fact that we have so many MOFs and so many applications creates many exciting challenges.<sup>20</sup> For example, screening studies have shown that materials synthesized for a particular application were top-performing for entirely different applications.<sup>21</sup> For instance, Al-PMOF was synthesized for its photo-catalytic activity,<sup>22</sup> but was later discovered to be promising for separating CO<sub>2</sub> from wet flue gases.<sup>23</sup> SBMOF-1 was synthesized<sup>24</sup> to capture CO<sub>2</sub> but turned out to be an excellent material for separating Xe from Kr.<sup>25</sup> UMCM-152 was first tested for H<sub>2</sub> adsorption<sup>26</sup> but was rediscovered as a record-breaking material for oxygen storage.<sup>27</sup> MOFs are synthesized with an application in mind, but then groups lack the capacity to test their novel MOFs for all possible applications. Similarly, for an applied group

interested in an application, it is nearly impossible to test the several novel MOFs that are being published every day.

### Data-science approaches

If one has to study so many materials, one needs novel methods for even the most simple tasks. For example, if one wants to do a machine learning study one typically needs a test and training set. Naively, one would select 1000 MOFs from the CSD and split them randomly in a test and training set. However, one would like to ensure that there are no similar structures in the test and training set, as nothing is easier for machine learning than reproducing the training set. As there are 100,000 MOF structures in the CSD, identifying identical structures by hand is impossible, so we need to develop algorithms to do this.<sup>28</sup> Interestingly, we found that one MOF was reported 1000 times in the CSD.

One also has to realize that even for MOFs, 100,000 structures are a small number of data points from a data-science perspective. For example, if we compare this with the number of data points collected in social sciences. Therefore, in chemistry, we always work within the low data limit. We show that we can compensate for our work in the low data regime by having machine learning build on chemical knowledge. We will discuss some machine-learning examples that started with no experimental data.

If we have designed our ideal MOF *in silico*, an unresolved question is whether we can synthesize this MOF and what are the optimal synthesis conditions. A machine-learning can leverage the fact that over 100,000 MOFs have been synthesized to make a model that can predict the most like structure to form for a given linker and metal node. However, the literature only reports successful experiments, and we will show the importance of learning from failed and partly successful experiments.<sup>29</sup>

### Outlook

This lecture will present several examples of how data science can be used to solve practical questions. This lecture aims to initiate a discussion on how data-science techniques can be used to solve scientific questions related to the H<sub>2</sub> energy landscape.



Berend SMIT

### Short CV

**Berend Smit** received an MSc in Chemical Engineering in 1987 and an MSc in Physics from the Technical University in Delft (the Netherlands). He received in 1990 his Ph.D. in Chemistry from Utrecht University (the Netherlands). He was a (senior) Research Physicist at Shell Research from 1988-1997, Professor of Computational Chemistry at the University of Amsterdam (the Netherlands) 1997-2007. In 2004 Berend Smit was elected Director of the European Center of Atomic and Molecular Computations (CECAM) in Lyon France. In 2007 he was appointed Professor of Chemical Engineering and Chemistry at U.C. Berkeley and Faculty Chemist at the Materials Sciences Division, Lawrence Berkeley National Laboratory. Since July 2014, he is a professor at EPFL.

## References

- 1 The Cambridge Crystallographic Data Centre (CCDC) (2021) <https://www.ccdc.cam.ac.uk/>
- 2 P. Z. Moghadam, A. Li, S. B. Wiggin, A. Tao, A. G. P. Maloney, P. A. Wood, S. C. Ward, and D. Fairen-Jimenez, *Development of a Cambridge Structural Database Subset: A Collection of Metal-Organic Frameworks for Past, Present, and Future* Chem Mater **29** (7), 2618 (2017) <http://dx.doi.org/10.1021/acs.chemmater.7b00441>
- 3 H. Furukawa, K. E. Cordova, M. O'Keeffe, and O. M. Yaghi, *The Chemistry and Applications of Metal-Organic Frameworks* Science **341** (6149), 974 (2013) <http://dx.doi.org/10.1126/Science.1230444>
- 4 H. M. El-Kaderi, J. R. Hunt, J. L. Mendoza-Cortes, A. P. Cote, R. E. Taylor, M. O'Keeffe, and O. M. Yaghi, *Designed synthesis of 3D covalent organic frameworks* Science **316** (5822), 268 (2007) <http://dx.doi.org/10.1126/science.1139915>
- 5 W. G. Lu, D. Q. Yuan, D. Zhao, C. I. Schilling, O. Plietzscht, T. Muller, S. Brase, J. Guenther, J. Blumel, R. Krishna, Z. Li, and H. C. Zhou, *Porous Polymer Networks: Synthesis, Porosity, and Applications in Gas Storage/Separation* Chem. Mat. **22** (21), 5964 (2010) <http://dx.doi.org/10.1021/cm1021068>
- 6 J. T. A. Jones, T. Hasell, X. F. Wu, J. Bacsá, K. E. Jelfs, M. Schmidtman, S. Y. Chong, D. J. Adams, A. Trewin, F. Schiffman, F. Cora, B. Slater, A. Steiner, G. M. Day, and A. I. Cooper, *Modular and predictable assembly of porous organic molecular crystals* Nature **474** (7351), 367 (2011) <http://dx.doi.org/10.1038/Nature10125>
- 7 H. Lyu, Z. Ji, S. Wuttke, and O. M. Yaghi, *Digital Reticular Chemistry* Chem-US **6** (9), 2219 (2020) <http://dx.doi.org/10.1016/j.chempr.2020.08.008>
- 8 H. Daglar and S. Keskin, *Computational Screening of Metal-Organic Frameworks for Membrane-Based CO<sub>2</sub>/N<sub>2</sub>/H<sub>2</sub>O Separations: Best Materials for Flue Gas Separation* J Phys Chem C **122** (30), 17347 (2018) <http://dx.doi.org/10.1021/acs.jpcc.8b05416>
- 9 C. E. Wilmer, M. Leaf, C. Y. Lee, O. K. Farha, B. G. Hauser, J. T. Hupp, and R. Q. Snurr, *Large-scale screening of hypothetical metal organic frameworks* Nat Chem **4** (2), 83 (2012) <http://dx.doi.org/10.1038/nchem.1192>
- 10 C. Wilmer and R. Snurr, in *Topics in Current Chemistry* (Springer Berlin Heidelberg, 2013), pp. 1 [http://dx.doi.org/10.1007/128\\_2013\\_490](http://dx.doi.org/10.1007/128_2013_490).
- 11 D. A. Gómez-Gualdrón, C. E. Wilmer, O. K. Farha, J. T. Hupp, and R. Q. Snurr, *Exploring the limits of methane storage and delivery in nanoporous materials* J. Phys. Chem. C. **118** (13), 6941 (2014) <http://dx.doi.org/10.1021/jp502359q>
- 12 S. Budhathoki, O. Ajayi, J. A. Steckel, and C. E. Wilmer, *High-throughput computational prediction of the cost of carbon capture using mixed matrix membranes* Energy Environ. Sci. (2019) <http://dx.doi.org/10.1039/C8EE02582G>
- 13 D. A. Gomez-Gualdrón, O. V. Gutov, V. Krungleviciute, B. Borah, J. E. Mondloch, J. T. Hupp, T. Yildirim, O. K. Farha, and R. Q. Snurr, *Computational Design of Metal-Organic Frameworks Based on Stable Zirconium Building Units for Storage and Delivery of Methane* Chem. Mater. **26** (19), 5632 (2014) <http://dx.doi.org/10.1021/cm502304e>
- 14 C. Simon, J. Kim, D. Gomez-Gualdrón, J. Camp, Y. G. Chung, R. L. Martin, R. Mercado, M. W. Deem, D. Gunter, M. Haranczyk, D. Sholl, R. Q. Snurr, and B. Smit, *The Materials Genome in Action: Identifying the Performance Limits for Methane Storage* Energy Environ. Sci. **8** (4), 1190 (2015) <http://dx.doi.org/10.1039/C4EE03515A>
- 15 C. M. Simon, J. Kim, D. A. Gomez-Gualdrón, Y. G. Chung, R. L. Martin, R. Mercado, M. W. Deem, D. Gunter, M. Haranczyk, R. Q. Snurr, and B. Smit, *Computer-aided search for materials to store natural gas for vehicles* Front. Young Minds **3** (11), 1 (2015) <http://dx.doi.org/10.3389/frym.2015.00011>
- 16 R. Anderson, J. Rodgers, E. Argueta, A. Biong, and D. A. Gomez-Gualdrón, *Role of Pore Chemistry and Topology in the CO<sub>2</sub> Capture Capabilities of MOFs: From Molecular Simulation to Machine Learning* Chem Mater **30** (18), 6325 (2018) <http://dx.doi.org/10.1021/acs.chemmater.8b02257>
- 17 P. G. Boyd, Y. J. Lee, and B. Smit, *Computational development of the nanoporous materials genome* Nat Rev Mater **2** (8), 17037 (2017) <http://dx.doi.org/10.1038/natrevmats.2017.37>
- 18 A. W. Thornton, C. M. Simon, J. Kim, O. Kwon, K. S. Deeg, K. Konstas, S. J. Pas, M. R. Hill, D. A. Winkler, M. Haranczyk, and B. Smit, *Materials Genome in Action: Identifying the Performance Limits of Physical Hydrogen Storage* Chem. Mat. **29** (7), 2844 (2017) <http://dx.doi.org/10.1021/acs.chemmater.6b04933>
- 19 S. Lee, B. Kim, H. Cho, H. Lee, S. Y. Lee, E. S. Cho, and J. Kim, *Computational Screening of Trillions of Metal-Organic Frameworks for High-Performance Methane Storage* Acs Appl Mater Inter **13** (20), 23647 (2021) <http://dx.doi.org/10.1021/acsami.1c02471>
- 20 D. Ongari, L. Talirz, and B. Smit, *Too Many Materials and Too Many Applications: An Experimental Problem Waiting for a Computational Solution* ACS Central Sci. **6** (11), 1890 (2020) <http://dx.doi.org/10.1021/acscentsci.0c00988>
- 21 A. Sturluson, M. T. Huynh, A. R. Kaija, C. Laird, S. Yoon, F. Hou, Z. X. Feng, C. E. Wilmer, Y. J. Colon, Y. G. Chung, D. W. Siderius, and C. M. Simon, *The role of molecular modelling and simulation in the discovery and deployment of metal-organic frameworks for gas storage and separation(dagger)* Mol Simulat **45** (14-15), 1082 (2019) <http://dx.doi.org/10.1080/08927022.2019.1648809>
- 22 A. Fateeva, P. A. Chater, C. P. Ireland, A. A. Tahir, Y. Z. Khimyak, P. V. Wiper, J. R. Darwent, and M. J. Rosseinsky, *A Water-Stable Porphyrin-Based Metal-Organic Framework Active for Visible-Light Photocatalysis* Angew Chem Int Edit **51** (30), 7440 (2012) <http://dx.doi.org/10.1002/anie.201202471>
- 23 P. G. Boyd, A. Chidambaram, E. Garcia-Diez, C. P. Ireland, T. D. Daff, R. Bounds, A. Gladysiak, P. Schouwink, S. M. Moosavi, M. M. Maroto-Valer, J. A. Reimer, J. A. R. Navarro, T. K. Woo, S. Garcia, K. C. Stylianou, and B. Smit, *Data-driven design of metal-organic frameworks for wet flue gas CO<sub>2</sub> capture* Nature **576** (7786), 253 (2019) <http://dx.doi.org/10.1038/s41586-019-1798-7>
- 24 D. Banerjee, Z. J. Zhang, A. M. Plonka, J. Li, and J. B. Parise, *A Calcium Coordination Framework Having Permanent Porosity and High CO<sub>2</sub>/N<sub>2</sub> Selectivity* Cryst Growth Des **12** (5), 2162 (2012) <http://dx.doi.org/10.1021/cg300274n>
- 25 D. Banerjee, C. M. Simon, A. M. Plonka, R. K. Motkuri, J. Liu, X. Chen, B. Smit, J. B. Parise, M. Haranczyk, and P. K. Thallapally, *Metal-organic framework with optimally selective xenon adsorption and separation* Nat. Comm. **7** (11831), 11831 (2016) <http://dx.doi.org/10.1038/ncomms11831>
- 26 J. K. Schnobrich, O. Lebel, K. A. Cychoz, A. Dailly, A. G. Wong-Foy, and A. J. Matzger, *Linker-Directed Vertex Desymmetrization for the Production of Coordination Polymers with High Porosity* J Am Chem Soc **132** (39), 13941 (2010) <http://dx.doi.org/10.1021/ja107423k>
- 27 P. Z. Moghadam, T. Islamoglu, S. Goswami, J. Exley, M. Fantham, C. F. Kaminski, R. Q. Snurr, O. K. Farha, and D. Fairen-Jimenez, *Computer-aided discovery of a metal-organic framework with superior oxygen uptake* Nat Commun **9** (2018) <http://dx.doi.org/10.1038/s41467-018-03892-8>
- 28 K. M. Jablonka, A. S. Rosen, A. S. Krishnapriyan, and B. Smit, *An Ecosystem for Digital Reticular Chemistry*. ChemRxiv (2022) <http://dx.doi.org/10.26434/chemrxiv-2022-4g7rx>
- 29 S. M. Moosavi, A. Chidambaram, L. Talirz, M. Haranczyk, K. C. Stylianou, and B. Smit, *Capturing chemical intuition in synthesis of metal-organic frameworks* Nat. Commun. **10** (1), 539 (2019) <http://dx.doi.org/10.1038/s41467-019-08483-9>

## CATALYSIS AS SCIENCE AND TECHNOLOGY FOR THE HYDROGEN AGE

Robert Schlögl

Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, D-14195 Berlin, Germany

### Hydrogen Age

It is now clear, that sustainable energy systems will consist of free electrons and molecular energy carriers likewise. Volatility of RES and the need to create global markets for RES require bulk long-term storage of solar energy that can only occur in molecular bonds. The first platform molecule in the transformation process of electrons to molecules (the reversal of combustion) is hydrogen. In the form of gas or as PCET product  $H^+ + e^-$  it will be further converted to allow easy handling (derivatives).

### Catalysis

Catalysis is the science and technology of controlling the kinetics of chemical transformations. Catalysts modify by specific interactions with reactants the energy profile of their interaction. The generation of hydrogen through electrolysis is a particular catalytic reaction in which the applied potential creates at the electrode metastable sites that react in a chemical reaction with water in the two half reactions.

### Material dynamics

Derivates of hydrogen can be formed with nitrogen (ammonia) or CO<sub>2</sub> (methanol, methane) to arrive at liquids referred to as "solar fuels" or "SAF". Here catalysts enable complex reaction networks leading to desired products and side reactions that need to be minimized. Chemical dynamics[1] between reagents and between catalyst and reagents enable these transformations. It is critical to design in future catalysts for such applications which is currently a dream. Our fundamental understanding about the mode of operation has improved enormously in the last decade. By using this understanding and application of operando spectro-microscopy and digital catalysis as modern toolboxes we begin to create a workflow for catalyst design based on knowledge rather than empirical know-how.

### References

- [1] Schlögl R., Chemische Batterien mit CO<sub>2</sub>. *Angew. Chem. Int. Ed.*, 2021. 60: p. 2-25.

---

#### Short CV



Robert Schlögl

Robert Schlögl is Director at the Fritz Haber Institute of the Max Planck Society in Berlin as well as was Founding Director at the Max Planck Institute for Chemical Energy Conversion in Mülheim a.d. Ruhr. Robert Schlögl's research focuses primarily on the investigation of heterogeneous catalysts, with the aim to combine scientific with technical applicability as well as on the development of nanochemically-optimized materials for energy storage. The application of knowledge-based heterogeneous catalysis for large-scale chemical energy conversion summarizes his current research focus.

He is President of the Alexander-von-Humboldt Foundation, Vice-President of the National Academy Leopoldina as well as an Honorary Professor at Technical University Berlin, at Humboldt University Berlin, at University Duisburg-Essen, at Ruhr University Bochum as well as a Distinguished Affiliated Professor at TU Munich and an Honorary Professor of Boreskov Institute of Catalysis. He is member at acatech and BBAW and other numerous international organizations, received numerous national and international awards as well as is partner in numerous European and international joint projects.

He is Author/co-author of more than 1200 publications, more than 550 presentations and invited talks as well as inventor of more than 20 patent families.

## IN-SITU SYNTHESIS OF HIGHLY ACTIVE FE-DOPED CO-BASED CATALYST FOR OXYGEN EVOLUTION REACTION

PHAM Thi Ha My

Laboratory of Materials for Renewable Energy (LMER), Institute of Chemical Sciences and Engineering (ISIC), Basic Science Faculty (SB), Ecole Polytechnique Fédérale de Lausanne (EPFL) Valis/Wallis, Energypolis, Rue de l'Industrie 17, CH-1951 Sion, Switzerland

EMPA Materials & Technology, CH-8600 Dübendorf, Switzerland

The Oxygen Evolution Reaction (OER) in water electrolysis requires high overpotential due to multiple steps involving four electrons. Herein, we reported a simple method for in-situ synthesis of Fe-doped Co-based catalyst that occurs in the same potential as OER and does not utilize polymer binder for electrode preparation [1]. The addition of  $\text{Co}^{2+}$  and  $\text{Fe}^{3+}$  in the alkaline solution and the application of an anodic potential induces a mixed OER-active state that exhibits an overpotential at  $10 \text{ mA cm}^{-2}$  of 329 mV, and a Tafel slope of  $28.2 \text{ mV dec}^{-1}$ .  $\text{Fe}^{3+}$  is incorporated into the Co-based phase by substitution at the  $\text{Co}^{3+}$  site. Our findings show that the presence of

Fe “doping” helps increase the surface area of the Co-based active phase by expanding the crystal lattice, while promoting the intrinsic OER activity of the Co-based catalyst by modulating the adsorption of  $\text{OH}^-$  onto the surface [2].

### References

- [1] T. H. Shen, L. Spillane, J. Vavra, T. H. M. Pham, J. Peng, Y. Shao-Horn, V. Tileli, *J. Am. Chem. Soc.* 2020, 142, 15876
- [2] C. G. Morales-Guio, L. Liardet, X. Hu, *J. Am. Chem. Soc.* 2016, 138, 8946



PHAM Thi Ha My

Thi Ha My PHAM is currently a PhD student at the Laboratory of Materials for Renewable Energy (LMER), in the Swiss Federal Institute of Technology, Lausanne. She obtained her Bachelor and Master degrees in 2017 and 2020 respectively, both from the department of Materials Science & Engineering, EPFL. After that, she moved to Sion to continue her PhD on developing electrocatalysts for energy applications. Thi Ha My is currently working in the National University of Singapore (NUS), as part of the EPFL Doc.Mobility program.



## KEROSING PRODUCTION WITH VARIOUS TECHNOLOGIES IN SWITZERLAND

Riku Horie

EPFL MSc Energy Science and Technology, Master Student

**Abstract:** The use of these Sustainable Aviation Fuels (SAF) allows the achievement of reducing the greenhouse gas emission during aviation, as it does not rely on coal and fossil fuels. Currently, to achieve this ambitious goal, in the aviation industry, there are technological innovations to back up the goal, and the SAF is one of the processes. This report reviews the economic cost of producing 100kL of kerosene per day in Switzerland using various production methodologies under the ASTM regulations. This includes the Power to Liquid (PtL) process producing hydrocarbon fuels via the synthesis of hydrogen and carbon monoxide, HEFA process, AtJ process, Biomass to Liquid (BtL) process etc. At the end, the report proposes the most suitable fuel for the aviation industry in Switzerland.

### Introduction

This study aims to analyse the currently best technology for kerosene production, by calculating capital expenditures, operating expenses, and revenue. The capital cost for each major component is estimated individually and scaled based on the facility size and construction cost of commercially existing plants.

### ASTM Specifications

ASTM specifications are set for checking if the fuel can fly from commercial flights. This ensures the safety and makes sure that the fuel is a reliable operation of aircraft. There are 4 steps, which are specifying the new fuel, establishing the fitness for purpose, testing the components and rig operability limits, and testing the aircraft, engine, and associated durability.

The initial fuels accepted by the ASTM specifications were SPK blends while the later ones include SPK in which aromatics and cycloalkanes were added. The carbon chain length and level of branching can vary dramatically.

### Type of Production Methodologies

The first methodology accepted was the Synthetic Paraffinic Kerosene with Aromatics (FT-SPK) approved in 2009. Its feedstock is Renewable biomass such as municipal solid waste (MSW), agricultural and forest wastes. It has a wide variety of waste and residue-based feedstocks. It is followed by the HEFA Hydrotreated Esters and Fatty Acids, approved in 2011. It uses lipid feedstocks such as animal and vegetable fats, waste cooking oil, and algae oil. It is followed by Synthesized isoparaffins (SIP), FT-SPK without Aromatics (FT-SPK/A), Alcohol to Jet (AtJ), Synthetic Paraffinic Kerosene (ATJ-SPK)

### Power to Liquid (PtL) Method

This type of SAF, which is produced in a process called PtL (Power-to-Liquid) process, collects hydrogen by using renewable energy sources such as solar PV and wind energy,

while it collects CO by the capture of CO<sub>2</sub>. Traditionally, SAFs of biofuel origin have been the mainstay of SAFs, but due to the limitations of their reserves, SAFs of CO<sub>2</sub> origin are now attracting more attention.

This study aims to analyse the currently best technology for kerosene production, by calculating capital expenditures, operating expenses, and revenue. The capital cost for each major component is estimated individually and scaled based on the facility size and construction cost of commercially existing plants.

There are 3 main chemical reactions involved in this process water electrolysis, RWGS, and FT synthesis, as shown below.

For these 3 chemical processes to be involved, 8 key components during the kerosene production are analysed. They are 1 Electricity generated by PV or wind energy, 2 Electricity storage, 3 Electrolysis for H<sub>2</sub> production, 4 CO<sub>2</sub> capture, 5 RWGS process for converting CO<sub>2</sub> into CO, 6 FT synthesis combining H<sub>2</sub> and CO for producing hydrocarbon, 7 Cleaning, and Upgrading, and 8 Converting into Kerosene.

### References

- [1] Iea. "Tracking Aviation 2020 – Analysis." IEA, <https://www.iea.org/reports/tracking-aviation-2020>.
- [2] European Commission. "Reducing Emissions from Aviation." Ec.europa.eu, 2021, [ec.europa.eu/clima/eu-action/transport-emissions/reducing-emissions-aviation\\_en](https://ec.europa.eu/clima/eu-action/transport-emissions/reducing-emissions-aviation_en).
- [3] How to Advance Cellulosic Biofuels Assessment of Costs, Investment Options and Policy Support -Final Version.
- [4] Diakakis, Stamatis. Sustainable Aviation Fuels Internship Project for DMT Environmental Technology.
- [5] Analysis of Natural Gas-to Liquid Transportation Fuels via Fischer-Tropsch OFFICE of FOSSIL ENERGY. 201



Riku HORIE

International Baccalaureate Diploma Programme (IBDP) (2016), Dubai International Academy. Bachelor of Engineering 2020, School of Creative Science and Engineering, International Program for Science and Engineering(IPSE), Department of Civil and Environmental Engineering, Waseda University, Tokyo, Japan, International Program for Science and Engineering(IPSE), Bachelor of Engineering, Department of Civil and Environmental Engineering, MSc Energy Science and Technology (2003), Master of Engineering, Orientation of Energy Management and Sustainability, École polytechnique fédérale de Lausanne (EPFL), Switzerland.

# HIGH CATALYTIC SELECTIVITY OF COPPER NANOWIRES FOR ETHYLENE PRODUCTION FROM CO<sub>2</sub> ELECTROCHEMICAL REDUCTION

Jinqiu Zhang, Shiji Zhang, Hua Bin, Yueping Xiong, Peixia Yang, Maozhong An

MIT Key Laboratory of Critical Materials Technology for New Energy Conversion and Storage, School of Chemistry and Chemical Engineering, Harbin Institute of Technology, Harbin, 150001, PR China

**Abstract** Electrochemical reduction reactions of CO<sub>2</sub> were carried out on copper nanowires catalysts that were loaded on carbon paper electrodes for production of ethylene. The copper nanowires were prepared by electrodeposition and oxidation-annealing-reduction processes. The effect of halogenation, oxidation, dealloying and alloying treatments on catalytic properties of copper catalysts were studied, respectively. The existence of cuprous ions and copper silver double active sites have a great influence on improving ethylene selectivity.

## Introduction

The electrochemical transformation of carbon dioxide into high valuable chemicals, such as ethylene, is a viable pathway using renewably sourced electricity. For CO<sub>2</sub> electrochemical reduction reaction, copper-based catalyst has a unique ability for production of multi-carbon products, which may be due to that copper has a negative adsorption energy for \*CO but a positive adsorption energy for \*H. A high concentration of intermediate \*CO on catalyst surface is favourable for C-C coupling. However, to achieve a high Faradaic Efficiency (FE) for the production of a specific C<sub>2</sub> product on copper catalyst is still a challenge. Herein, we explored copper nanowires on carbon paper as cathodic electrode for reduction of CO<sub>2</sub> to ethylene and discussed the influence of halogenation, oxidation, dealloying and alloying treatments.

## Experimental

Cu, Cu-Zn alloy or Cu-Ag alloy was electrodeposited on a piece of hydrophobic carbon paper as precursor. Cu nanowires were obtained by oxidation-annealing-reduction process. Potassium halide solutions were used in some experiments to convert copper into cuprous halide before the oxidation step. The removal of Zn from the Cu-Zn alloy is carried out synchronously in the oxidation step. For Cu-Ag alloy, Ag was remained after the reduction step. The catalytic performances of copper catalysts were tested in an electrolyte of 1 mol/L KOH at a constant potential by using a flow cell.

## Results and Discussion

After oxidation-annealing-reduction, Cu nanowires with diameter of about 50–200 nm grew on carbon fibers. The tops of about 10 nanowires were connected together to

form clusters. Oxidation is a necessary step for the growth of nanowires and it is helpful for providing oxygen vacancies. Halogenation and dealloying of Zn have influence on the concentration ratio of Cu<sup>+</sup> to Cu<sup>0</sup> in the catalysts. The Cu nanowires catalyst derived from KI modified copper (its TEM image was shown in Fig. 1a) and Cu-Zn alloy showed FEs for ethylene production over 50% and over 46% at -0.8V (vs. RHE), respectively. The presence of Ag in the Cu nanowires improved the local concentration of CO on the surface of the electrode and favoured C-C coupling. The Cu based nanowires derived from Cu-Ag alloy (its SEM image was shown in Fig. 1b) exhibited an improved FE for ethylene production, which was over 70% at -0.8V (vs. RHE).

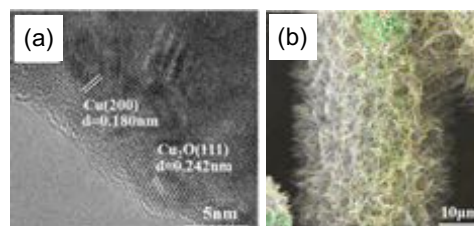


Fig. 1 (a) TEM image of copper nanowires derived from cuprous iodide. (b) SEM image of Cu-Ag alloy nanowires overlying EDS results where copper in yellow, silver in green, oxygen in purple and carbon in red.

## References

- [1] A. Bagger, W. Ju, A. S. Varela, P. Strasser, J. Rossmeisl. *ChemPhysChem*. 18, 3266 (2017)
- [2] M. Ma, K. Djanashvili, W.A. Smith. *Angew. Chem. Int. Ed.* 55, 6680 (2016)
- [3] T. Kim, G.T.R. Palmore. *Nat. Commun.* 11, 1(2020)



Jinqiu Zhang

Associate Prof. Dr. Jinqiu ZHANG was born in 1979 in Heilongjiang, China. Jinqiu Zhang graduated with a Ph.D in Chemical Engineering and Technology from Harbin Institute of Technology (HIT) in 2009. She works at Department of Electrochemical Engineering of HIT and her research filed is electrodeposition of functional materials.

Corresponding author: Jinqiu ZHANG, zhangjinqiu@hit.edu.cn, +86-451-86413721.

## Recycling as the key for developing sustainable hydrogen storage materials

Claudio Pistidda

Department of Materials Design, Institute of Hydrogen Technology, Helmholtz-Zentrum hereon GmbH, 21502, Geesthacht, Germany

Abstract Metals play a crucial role in supporting the global economy and the wellbeing of humankind. Supported by the constantly increasing demand for metal-based products, the extraction of mineral resources has increased, over the last decades, at a faster rate than economic growth. This trend is forecasted to steadily increase in the near future, thus leading to concerns over the exploitation of the Earth's natural resources and the environmental impact that the extraction of metals will have.[1,2] In this scenario, the recycling of metals from materials or products that have reached their end of life allows the saving of resources and energy while simultaneously preventing the depletion of natural sources and the release of harmful pollutants into the environment.

Hydrogen has attracted great interest in recent decades as an efficient energy carrier, capable of supporting the transition from fossil fuel-based to renewable-based energy sources.[3-6] However, due to its low volumetric density,[7] even if compressed or liquefied, the utilization of hydrogen for storing large quantities of energy is challenging.[8] The volumetric hydrogen density can be sensibly increased by chemically binding hydrogen to metals, metalloids, and metal alloys. To reduce the carbon footprint and environmental impact that the mining of metals for hydrogen storage purposes entails and to reduce their cost, at the Helmholtz-Zentrum Hereon we pursue the possibility of obtaining high-quality hydride-based materials from industrial metal waste. A complete overview of recent scientific breakthroughs in the synthesis and characterization of hydrogen storage materials made from recovered metal wastes will be presented.[9-17]

### References

- [1] Ayres, R. U. Metals recycling: economic and environmental implications. *Resources, Conservation and Recycling* 21, 145-173, doi:https://doi.org/10.1016/S0921-3449(97)00033-5 (1997).
- [2] Aznar-Sánchez, J. A., Velasco-Muñoz, J. F., García-Gómez, J. J. & López-Serrano, M. J. The Sustainable Management of Metals: An Analysis of Global Research. *Metals-Basel* 8, 805 (2018).

- [3] Dunn, S. On hydrogen futures: toward a sustainable energy system - Author's reply. *Int J Hydrogen Energ* 28, 135-135, doi:Pii S0360-3199(02)00060-5
- [4] Doi 10.1016/S0360-3199(02)00060-5 (2003).
- [5] Momirlan, M. & Veziroglu, T. N. Current status of hydrogen energy. *Renew Sust Energ Rev* 6, 141-179, doi:Pii S1364-0321(02)00004-7
- [6] Doi 10.1016/S1364-0321(02)00004-7 (2002).
- [7] Pistidda, C. Solid-State Hydrogen Storage for a Decarbonized Society. *Hydrogen* 2, doi:10.3390/hydrogen2040024 (2021).
- [8] Winter, C. J. Hydrogen energy - Abundant, efficient, clean: A debate over the energy-system-of-change. *Int J Hydrogen Energ* 34, S1-S52, doi:10.1016/j.ijhydene.2009.05.063 (2009).
- [9] Hoogers, G. Fuel cell technology handbook. (CRC press, 2002).
- [10] Jensen, J. O., Vestbo, A. P., Li, Q. & Bjerrum, N. J. The energy efficiency of onboard hydrogen storage. *J Alloy Compd* 446, 723-728, doi:10.1016/j.jallcom.2007.04.051 (2007).
- [11] Bergemann, N. et al. NaAlH<sub>4</sub> production from waste aluminum by reactive ball milling. *Int J Hydrogen Energ* 39, 9877-9882, doi:10.1016/j.ijhydene.2014.02.025 (2014).
- [12] Cao, H. et al. Conversion of magnesium waste into a complex magnesium hydride system: Mg(NH<sub>2</sub>)<sub>2</sub>-LiH. *Sustainable Energy and Fuels* 4, 1915-1923, doi:10.1039/c9se01284b (2020).
- [13] Hardian, R. et al. Waste Mg-Al based alloys for hydrogen storage. *Int J Hydrogen Energ* 43, 16738-16748, doi:10.1016/j.ijhydene.2017.12.014 (2018).
- [14] Le, T. T. et al. Efficient synthesis of alkali borohydrides from mechanochemical reduction of borates using magnesium-aluminum-based waste. *Metals-Basel* 9, doi:10.3390/met9101061 (2019).
- [15] Passing, M. et al. Development and experimental validation of kinetic models for the hydrogenation/dehydrogenation of Mg/Al based metal waste for energy storage. *Journal of Magnesium and Alloys*, doi:10.1016/j.jma.2021.12.005 (2022).
- [16] Pistidda, C. et al. Hydrogen storage systems from waste Mg alloys. *J Power Sources* 270, 554-563, doi:10.1016/j.jpowsour.2014.07.129 (2014).
- [17] Shang, Y. et al. Sustainable NaAlH<sub>4</sub> production from recycled automotive Al alloy. *Green Chemistry*, doi:10.1039/D1GC04709D (2022).

# AN ADVANCED AL-AIR FUEL CELL USING A MESH-ENCAPSULATED ANODE VIA AL-ZN ENERGY TRANSFER

Manhui Wei<sup>1,2,3</sup>, Keliang Wang<sup>1,4,\*</sup>, Pucheng Pei<sup>4</sup>, Yayu Zuo<sup>1</sup>, Liping Zhong<sup>2,3</sup>, Hengwei Wang<sup>1</sup>, Siyuan Zhao<sup>5</sup>

Affiliation 1. Beijing Institute of Technology 2. LMER, EPFL 3. EMPA 4. Tsinghua University 5. The Hong Kong Polytechnic University

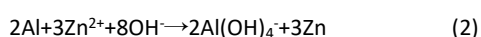
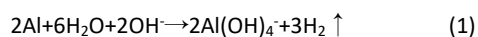
**Abstract** Al-air fuel cells (AAFCs) are regarded as the potential energy conversion systems due to the ultra-high theoretical capacity of 2980 mAh/g and specific energy of 8100 mWh/g for Al anodes. However, the anodic self-corrosion has severely limited the energy efficiency, which induces a great challenge to the commercial penetration of AAFCs. Herein, we propose an AAFC using a mesh-encapsulated anode via Al-Zn energy transfer, and further modify the alkaline electrolyte with a strong Lewis acid ZnCl<sub>2</sub>. Finally, a high capacity of 2322.91 mAh/g for AAFC are obtained at 20 mA/cm<sup>2</sup>, and the anode efficiency can reach 77.95%.

## Energy storage and conversion systems

Excessive consumption of fossil fuels has seriously deteriorated the atmospheric environment and forced the transformation of energy consumption in human beings. Therefore, the products in renewable energy market, including Li-ion batteries, proton-exchange membrane fuel cells and metal-air fuel cells are widely favoured and concerned. Metal-air fuel cells, in particular, have attracted more attention due to the advantages in consumption, emissions, cost, and efficiency. Nowadays, Al-air fuel cells (AAFCs) are expected to be the research focus due to the high capacity of 2980 mAh/g (close to Li), high specific energy of 21,870 Wh/L (2.32 times of Zn), abundant reserves and low density for Al anodes. Therefore, many research institutions and companies are racing to develop the high-performance AAFCs for electric vehicles, underwater power modules and military communication units.

## The mesh-encapsulated anode of AAFC

The energy loss of Al anode is attributed to the self-hydrophilic reaction [Eq. (1)]. By modifying the alkaline electrolyte with ZnO, the above problem can be effectively avoided [Eq. (2)].



However, the Zn film is relatively loose, unstable and gravitational. External vibration and turbulence can easily cause the protective layer to fall off and form dead-Zn, which brings challenges to the anti-corrosion of Al anode. Based on that, a structure of mesh-encapsulated anode is designed. The mesh size is 1.5 × 1.5 mm and the material is ASTM304. The mesh can not only be used as a fuel tank for Al anode, but also

can accept the fallen dead-Zn and utilize the energy of Zn to discharge. Hence, the share of all Al electrons involved in discharge is increased indirectly, and the energy conversion efficiency increased by more than 2 times.

## Modifying the alkaline electrolyte of AAFC with a strong Lewis acid ZnCl<sub>2</sub>

Although the dead-Zn is collected and utilized, the Zn film with a large number of holes and cracks still results in the non-maximization of the electrochemical energy conversion efficiency for Al metal. For improving the morphology of Zn film, a single inorganic strong Lewis acid ZnCl<sub>2</sub> replaces ZnO to modify the alkaline electrolyte. The protective effect for Al anode is further enhanced by the adsorption of the anion groups formed by Cl<sup>-</sup> in the alkaline electrolyte. The novel approach avoids the excessive increase of internal resistance caused by organic compounds, and does not adversely affect the energy output of cell. The modified electrolyte ensures that more energy can be used for discharge and higher output performance can be achieved, with a high capacity of 2322.91 mAh/g and a high anode efficiency of 77.95% at 20 mA/cm<sup>2</sup>.

## References

- [1] M. H. Wei, K. L. Wang, Y. Y. Zuo, et al. A high-performance Al-air fuel cell using a mesh-encapsulated anode via Al-Zn energy transfer. *iScience*, 2021, 24(11): 103259.
- [2] M. H. Wei, K. L. Wang, P. C. Pei, et al. An enhanced-performance Al-air battery optimizing the alkaline electrolyte with a strong Lewis acid ZnCl<sub>2</sub>. *Applied Energy*, 2022, 324: 119690.



Manhui Wei

Born in 1994 in Tianjin, China, Manhui Wei graduated with a B.E. in Marine Engineering from Dalian Maritime University (DMU) in 2017. He obtained an M.E. in Power Eng. & Eng. Thermophysics from Beijing Institute of Technology (BIT) in 2020, and continued to study for a Ph.D here under the supervision of Prof. Keliang Wang. Currently, he studies as a visiting PhD at Laboratory of Materials for Renewable Energy (LMER) of École Polytechnique Fédérale de Lausanne (EPFL), and is supervised by Prof. Andreas Züttel. His research interests include the anode/cathode/electrolyte design of metal-air batteries and proton-exchange membrane fuel cells.

## HYDROGEN STORAGE BY PHYSISORPTION

Jessica RUFFINER<sup>1,2</sup>, Noris GALLANDAT<sup>2</sup>, Heena YANG<sup>2</sup>, Andreas ZÜTTEL<sup>2</sup>

<sup>1</sup>) University of Fribourg, Physics Department, Pérolles, 1700 Fribourg, Switzerland

<sup>2</sup>) Laboratory of Materials for Renewable Energy (LMER), Institute of Chemical Sciences and Engineering (ISIC), Basic Science Faculty (SB), École polytechnique fédérale de Lausanne (EPFL) Valais/Wallis, Rue de l'Industrie 17, CH-1950 Sion, Switzerland

Materials with a large specific surface area or nano-porosity, e.g. carbon nanotubes, graphene, and metal organic frameworks, adsorb hydrogen (Van der Waals interaction) with an interaction energy of 5 – 8 kJ·mol<sup>-1</sup>H<sub>2</sub>. The entropy of hydrogen at 77K is 72 J·K<sup>-1</sup>·mol<sup>-1</sup>H<sub>2</sub>, therefore, the equilibrium pressure at 77K (-196°C) is 1.5 bar but steep increasing with increasing temperature (200 bar at -150°C). The amount of adsorbed hydrogen at 77K corresponds to 0.6 monolayer (1 ML<sub>H<sub>2</sub></sub> = 71'022 m<sup>2</sup>·mol<sup>-1</sup>).

### H<sub>2</sub> Adsorption

With the discovery of the carbon nanomaterials and the metal organic frameworks new materials are available [1] which exhibit a very large specific surface area up greater than 5000 m<sup>2</sup>·g<sup>-1</sup>. Such materials adsorb large amounts of hydrogen up to 0.05 mol H<sub>2</sub>·g<sup>-1</sup> (= 10 mass%) at liq. N<sub>2</sub> temperature (77 K). This capacity is larger than compressed hydrogen at 700 bar (5 mass%) or metal hydride storages (1 mass%). However, until now no such storage is on the market.

### BET model [2]

The equilibrium pressure of the hydrogen in the gas phase above the adsorbed hydrogen is given by the Van't Hoff equation.

$$\Delta G = \Delta H^0 - T \cdot \Delta S^0 + R \cdot T \cdot \ln\left(\frac{p}{p_0}\right)$$

In equilibrium  $\Delta G=0$ , the adsorption enthalpy  $\Delta H^0 = 5 - 8$  kJ·mol<sup>-1</sup>H<sub>2</sub>, and the entropy of hydrogen at T = 77K is 72 J·K<sup>-1</sup>·mol<sup>-1</sup>H<sub>2</sub>. R is the gas constant 8.314 J·K<sup>-1</sup>·mol<sup>-1</sup>. The amount of adsorbed hydrogen is determined by the BET-model.

$$\frac{n}{n_m} = \frac{c \cdot \beta}{(1-\beta) \cdot (1+(c-1) \cdot \beta)}, \quad c = e^{\frac{\Delta H_{ads} - \Delta H_v}{k \cdot T}}$$

n is the number of mol adsorbed hydrogen, n<sub>m</sub> is the number of mol H<sub>2</sub> in a monolayer, c is a temperature dependent parameter with the enthalpy of adsorption  $\Delta H_{ads}$  and the enthalpy of evaporation  $\Delta H_v$  and  $\beta = p/p_0$  the gas pressure divided by the saturation pressure.

### Experiment

A storage cylinder with a volume of 0.5 L is wrapped with a heating tape, isolated with silicon and immersed into liquid nitrogen. The amount of adsorbed hydrogen is measured as a function of pressure and temperature.

### Result (theoretical)

The hydrogen adsorption at 77K takes place at low pressure and only slightly increases with pressure (77K > critical temperature = 32K). At a pressure of 20 bar the gas phase already stores more hydrogen than the absorber and above 80bar the storage capacity of the empty cylinder is larger than that with the absorber.

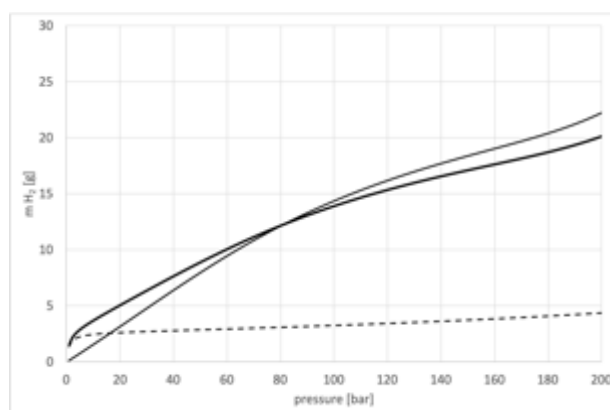


Fig. 1 Amount of hydrogen adsorbed (dotted line) on 187.5g HSAG 500 vs. the pressure at 78K in the cylinder (0.5 L). The corresponding amount of hydrogen in the gas phase of the empty cylinder (thin line) as well as the total amount of hydrogen (adsorbed and in the gas phase, thick line) are shown.

### References

- [1] Maurice Schlichtenmayer and Michael Hirscher, „Nanosponges for hydrogen storage“, J. Mater. Chem., 22 (2012), 10134.
- [2] Stephen Brunauer, P. H. Emmett, Edward Teller: Adsorption of Gases in Multimolecular Layers. In: Journal of the American Chemical Society. Band 60, Nr. 2 (1938), pp. 309–319, doi:10.1021/ja01269a023



#### Short CV

Born 23. 10. 1999 in Visp, Switzerland, Matura from Kollegium Spiritus Sanctus Brig 2020, BSc. in Physics, and Environmental Science from Science Faculty University of Fribourg 2023.

Jessica RUFFINER

## SELECTIVE THERMO-CATALYTIC CONVERSION OF CO<sub>2</sub> AND H<sub>2</sub> INTO ETHYLENE

Yasemen Kuddusi<sup>1,2</sup>, Andreas Züttel<sup>1,2</sup>

<sup>1</sup>Laboratory of Materials for Renewable Energy (LMER), Institute of Chemical Sciences and Engineering (ISIC), Basic Science Faculty (SB), École Polytechnique Fédérale de Lausanne (EPFL) Valais/Wallis, Energypolis, Rue de l'Industrie 17, 1951 Sion, Switzerland

<sup>2</sup>Empa Materials Science & Technology, 8600 Dübendorf, Switzerland

**Abstract:** Ethylene is a key chemical building block in the chemical industry with an annual production of around 200 million tons. It is a cornerstone in the production of polymers, adhesives, food supplements and pharmaceuticals. Its industrial production routes are fossil-based, energy-intensive and large CO<sub>2</sub> emitters. In this work, it is examined how CO<sub>2</sub> can be used as a source for ethylene production. We hereby focus maximizing the ethylene formation rate by means of Ga-based bifunctional catalysts. The incorporation of gallium oxide is found to have a positive effect on both activity and selectivity towards ethylene.

### Introduction

The rising levels of anthropogenic CO<sub>2</sub> concentrations in the atmosphere force scientists and engineers to rethink how high value-chemicals can be produced with a minimal carbon footprint. Carbon dioxide when used as a carbon feedstock along with green hydrogen retrieved from renewable resources offers a green pathway to produce hydrocarbons. Direct CO<sub>2</sub> hydrogenation to olefins follows either a methanol-mediated or a modified Fischer-Tropsch pathway. The selectivity in the latter is strongly limited by the Anderson-Schulz-Flory distribution<sup>1</sup>. An efficient catalyst for methanol-mediated CO<sub>2</sub> hydrogenation to olefins is bifunctional and should be active for both methanol synthesis and methanol dehydration/coupling under the same conditions<sup>1,2</sup>. In this work, we will investigate the effect of gallium oxide incorporation to the designed bifunctional catalyst on ethylene and light olefin formation rate from methanol mediated thermo-catalytic CO<sub>2</sub> hydrogenation.

### Experimental

Indium oxide (In<sub>2</sub>O<sub>3</sub>), gallium oxide (Ga<sub>2</sub>O<sub>3</sub>) and mixed oxide catalysts were prepared by coprecipitation of aqueous solutions of respective nitrate hydrate salts under vigorous mixing. The precipitates were aged, filtered, washed with deionized water, dried and then calcined. Both metal oxides and SSZ-13 zeolite were crushed and grinded separately. Then they were physically mixed.

Crystallinity and phases of the samples were checked by XRD. Electronic properties and surface oxygen vacancy concentrations were analyzed by XPS. Textural properties of the catalysts were retrieved from N<sub>2</sub> sorption experiments. For

acid side density of the samples, NH<sub>3</sub>-TPD and for surface basicity analysis, CO<sub>2</sub>-TPD was conducted. Surface metal hydrides and H<sub>2</sub> dissociation on the samples were analyzed by *in-situ* DRIFTS. Catalytic performance results were acquired from a microreactor coupled with a gas chromatography.

### Results and Discussion

By tuning of metal oxide content of the bifunctional catalyst, undesired CH<sub>4</sub> and CO formation were suppressed and light olefin formation was enhanced. With increasing atomic Ga ratio in the metal oxides of the bifunctional catalysts, C<sub>2</sub>H<sub>4</sub> selectivity increased. No C<sub>2</sub>H<sub>4</sub> was detected in the products for the same operating conditions for pure In<sub>2</sub>O<sub>3</sub>/SSZ-13 highlighting the role of gallium oxide.

The tuning of the product distribution of CO<sub>2</sub> hydrogenation to shorter chain hydrocarbons by gallium oxide incorporation is suggested to be linked to surface acid site density modulation and surface metal-hydride formation. It is postulated that the surface acid-base properties of mixed metal oxides play a decisive role in the C=C bond functionalization.

### References

- [1] Z. Ma and M. D. Porosoff, "Development of Tandem Catalysts for CO<sub>2</sub> Hydrogenation to Olefins," *ACS Catal.*, 9, 3, 2639–2656, 2019.
- [2] R.-P. Ye *et al.*, "CO<sub>2</sub> hydrogenation to high-value products via heterogeneous catalysis," *Nat. Commun.*, 10, 1, 5698, 2019.



Yasemen Kuddusi

Yasemen Kuddusi was born in 1995. She graduated as the 1<sup>st</sup> ranked student in her BSc of chemical engineering degree from ITU in 2019. Her BSc thesis was entitled as "Oxy-fuel pressurized fluidized bed combustion and CO<sub>2</sub> capture" under supervision of Prof. Hasancan Okutan. In 2021, she received her MSc of chemical engineering degree from UGent with a minor in Environment and Sustainable Development as one of the recipients of MasterMind Scholarship. Her MSc thesis work was entitled as "Experimental investigation into the effect of CO<sub>2</sub> on the oxidative coupling of methane" under supervision of Prof. Joris Thybaut and Prof. Pedro Mendes. Now, she is a 1<sup>st</sup> year PhD candidate in EPFL under supervision of Prof. Andreas Züttel working on enabling green synthesis of ethylene and acetylene from CO<sub>2</sub> hydrogenation.

## Ru-COMPLEX BASED POLYMERIC PHOTOCATHODES FOR WATER SPLITTING

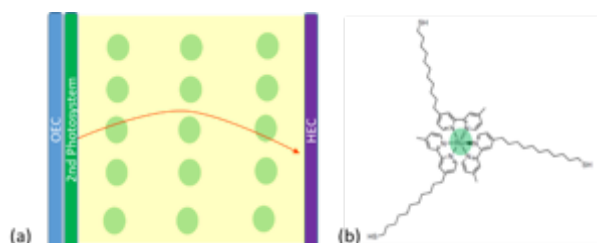
Selim Kazaz,<sup>a,b</sup> Andreas Borgschulte,<sup>a,b</sup> Daniel Denzler,<sup>c</sup> Stuart Robertson<sup>c</sup>

<sup>a</sup>Laboratory for Advanced Analytical Technologies, Empa – Swiss Federal Laboratories for Material Science and Technology, Überlandstrasse 129, CH-8600 Dübendorf, Switzerland; <sup>b</sup>Department of Chemistry, University of Zurich, Winterthurerstrasse 190, CH-8057 Zurich, Switzerland; <sup>c</sup>H2 Solar AG, Alter Postplatz 2, CH - 6370 Stans, Switzerland

Development of key components for Ru-based polymeric photocathode to combine the advantages of homogeneous and heterogeneous solar water splitting.

### Polymeric photocathodes

Photo-electrochemical water splitting has intrinsic advantages over established hydrogen production via photovoltaics coupled to electrolysis such as high electro-catalytic conversion due to low current densities and the lower demand of electrically conducting materials. However, current systems have not shown to be competitive due to a variety of challenges despite promising economic studies [1].



**Fig. 1:** (a) scheme of a photo-electrochemical cell based on a photocathode (hydrogen evolution catalyst, HEC, with polymeric photo-sensitizer) and photo-anode (oxygen evolution catalyst with 2<sup>nd</sup> photosystem). (b) shows the Ru(bpy)<sub>3</sub> monomer. The exact structure of the polymer and electronic conduction is not completely understood yet.

Recently, a novel system has been discovered showing significant photocatalytic activity [2]. The core of the device is a Ru(bpy)<sub>3</sub> based polymer opening a new opportunities for promising photo-electrochemical cells (Fig. 1 (a)). The monomer of the polymer consists of Ru complexed with thiol alkane functionalized bipyridine (Fig. 1 (b)). Advantages of the polymeric photocathode come from the fact that it combines both the advantages of homogeneous (molecular) systems and those of heterogeneous systems. However, as to be expected for a new system, various scientific and technological questions remain open.

### Scientific questions

- Upscaling of monomer synthesis for prototype development

- Structure of the polymer on the device
- Optical excitation and decay mechanism of Ru(bpy)<sub>3</sub> based polymer
- Energy and charge transfer mechanism
- Electronic conduction through metal polymer interfaces, charge separation
- Solar to hydrogen efficiency

### Results

Optimization of monomer synthesis

- Development of new synthesis route to overcome challenges of the complexation reaction: the long thiol alkane chains interact via van der Waals forces, which is a competitive interaction to the complexation
- New procedure allows gram scale production, which is sufficient to coat a square meter
- UV/Vis absorption and fluorescence lifetime measurements confirm good absorber properties
- Water splitting experiments under way

### Perspective

H2Solar intends to license or sell the technology, once proven, to industry and has this year agreed with Swiss energy suppliers the installation of such membranes affixed to motorway infrastructure, producing and storing hydrogen for transport. Costs are expected to be competitive against current market [1].

### References

- [1] B. Pinuad, et al., *Energy Environ. Sci.*, 2013, 6, 1983–2002
- [2] Patents WO 2009/056348 A1, and WO 2019/115012 A1



Selim Kazaz

Researcher at the Laboratory for Advanced Analytical Technologies at the Swiss Federal Laboratories for Materials Science and Technology (Empa). BSc and MSc degrees from the University of Zurich. Research interests revolve around solid-state chemistry and hydrogen spectroscopy for energy conversion and storage.

## CALCULATION OF DIFFUSION COEFFICIENTS OF H ON METAL SURFACES

Yuta Kataoka, Jun Haruyama, and Osamu Sugino

Institute for Solid State Physics, The University of Tokyo

Abstract : We calculated the diffusion coefficients of H on (111) surfaces of Cu, Ni, Pd, and Au. In the calculation, we combined the transition state theory with free energy surface obtained from 2 dimensional wave function of diffusing H. the quantum-classical crossover of diffusion coefficient is reproduced by this calculation.

### Introduction

Hydrogen (H) is known as a material with pronounced quantum effects and exhibits interesting behaviour in surface diffusion. At high temperatures, diffusion proceeds by thermal activity, whereas at low temperatures it proceeds by tunnelling. The temperature at which this diffusion mechanism transitions is called the crossover temperature. In the theoretical calculation, the diffusion coefficient was calculated using path integral molecular dynamics [1] and ring polymer molecular dynamics [2]. Since these methods are based on stochastic simulation, the computational cost becomes high at low temperatures. Therefore, this study proposes a calculation method that complements conventional stochastic simulations by calculating diffusion coefficients using a method that is not based on stochastic simulations.

### Calculation Methods

The diffusion coefficient between site A and site B was expressed as

$$D = \frac{a^2}{2} \frac{k_{A \rightarrow B} k_{B \rightarrow A}}{k_{A \rightarrow B} + k_{B \rightarrow A}}$$

where  $k_{A \rightarrow B}$  and  $k_{B \rightarrow A}$  is jump rate from A to B and jump rate from B to A, respectively. The jump rate was calculated based on transition state theory (TST). Since the free energy surface (FES) was available in our calculation, we used FES instead of potential energy surface (PES) in TST [3]. Jump rate from A to B was calculated using the distribution of H at transition state  $Q_{ts}$  and the distribution of H at site A,  $Q_A$ .

$$k_{A \rightarrow B} = \frac{1}{\sqrt{2\pi m \beta}} \frac{Q_{ts}}{Q_A},$$

where  $m$  and  $\beta$  is the mass of H and inverse temperature, respectively. The distribution was calculated from the wave

function obtained from 2-dimensional Schrödinger-like equation for H nuclei.

### Results

We calculate the diffusion coefficients of H on (111) surfaces of Cu, Ni, Pd, and Au (Fig.1). The crossover temperature is consistent with the one calculated from WKB based formula.

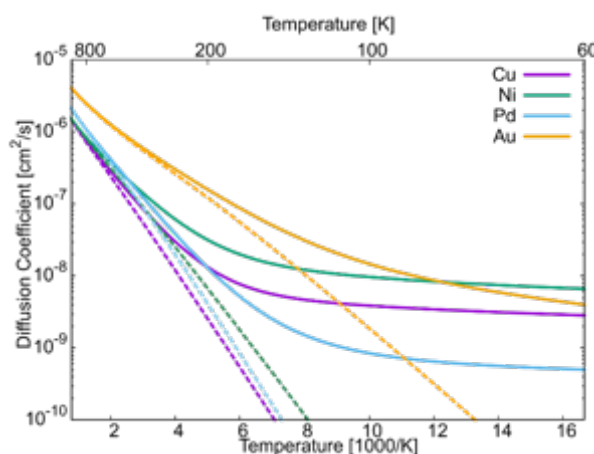


Fig. 1. Diffusion coefficients of H on (111) metal surfaces

### References

- [1] E. M. McIntosh, K. Thor Wikfeldt, J. Ellis, A. Michaelides, and W. Allison, *J. Phys. Chem. Lett.* **4**, 1565 (2013).
- [2] Y. V. Suleimanov, *J. Phys. Chem. C* **116**, 11141 (2012).
- [3] G. H. Vineyard, *J. Phys. Chem. Solids* **3**, 121 (1957).



Yuta Kataoka

CV Yuta Kataoka

2019 – 2021 : master's degree at Graduate School of Science, The University of Tokyo

2019 – Present : MERIT-WINGS, Tokyo University

2021 – Present : Ph.D, Graduate School of Science, The University of Tokyo



## HYDROGEN PURIFICATION WITH LaNiAl<sub>5</sub>-BASED METAL HYDRIDES

Chia-Chieh Shen<sup>1, 2\*</sup> and Jui-Yu Hsieh<sup>1</sup>

<sup>1</sup>Department of Mechanical Engineering, Yuan Ze University, Taiwan and <sup>2</sup>Fuel Cell Center, Yuan Ze University, Taiwan

Abstract;

Hydrogen purification with LaNiAl<sub>5</sub>-based metal hydrides was studied in a single reactor at operational temperature range of 20-70°C. Pressure-composition temperature (PCT) curves showed LaNiAl<sub>5</sub>-based have the absorption plateau pressure with approximately 1 atm at 30°C and desorption plateau pressure with 5 atm at 70°C, respectively. LaNiAl<sub>5</sub>-based alloys exhibited stable hydrogenation properties after 3000 cycles of hydrogen absorption and desorption, indicating that it is a suitable metal hydride candidate for application in hydrogen purifications. In this study, approximate 50 grams of commercial LaNiAl<sub>5</sub>-based alloy powders were filled into a single stainless steel reactor. Purification performance of hydrogen gas with starting purity of 99.99% was analyzed by a mass spectrometer. Operational parameters including reaction temperature, pressure and time were examined for designing an optimized hydrogen purifier.

### Introduction

High pure hydrogen is important for applications in fuel cells, semiconductors and food industries. Hydrogen purifications divided into two categories of physical and chemical methods. One of hydrogen purification method is to employ metal hydride materials to purify hydrogen gas to high pure of 99.9999%. However, poisoning, pulverization and disproportionation of metal hydride alloy are problems to restrict the development of metal hydride purification. Previously, one author of this study reported that substitution of Ni with Al in LaNi<sub>5</sub>-based alloy can remarkably hinder the disproportionation to keep its cyclic stability of hydrogenation and dehydrogenation [2]. The effect of impure hydrogen on the alloy poisoning of LaNiAl<sub>5</sub>-based has not been examined. Therefore, approximate 50 grams of commercial LaNiAl<sub>5</sub>-based alloy powders were filled into a single stainless steel reactor to study its purification performance.

### Experimental and results

Commercial 50 grams of LaNiAl<sub>5</sub>-based alloy powders were supplied from HyTec Co., Ltd., Taiwan [1]. They were filled into a single stainless steel reactor. Purification performance of hydrogen gas with starting purity of 99.99% was analyzed by a real time mass spectrometer (MS) measurement using a quadrupole MS (Agilent 5975B) with electron ionization.

Purification procedure was shown in Fig. 1. In beginning, when the starting hydrogen gas flowed into the reactor, cold water at T = 10-20 °C was supplied to remove the exothermic

heat released during the hydrogenation. After the hydrogenation complete, impurity gas valve was open to release the impurity gases while the water flow at medium temperature T = 20-30 °C was supplied to the purifier reactor. The outlet compositions of the desorbed gases were sampled by a MS detector. Then, closed the impurity gas valve and opened high purity hydrogen valve, the compositions of pure hydrogen gases were monitored by a MS detector during the dehydrogenation. The warm water at 50-70 °C was supplied to the reactor for maintain reactor temperature. Effect of reaction temperature, pressure and time were presented for the development of designing an optimized hydrogen purifier.

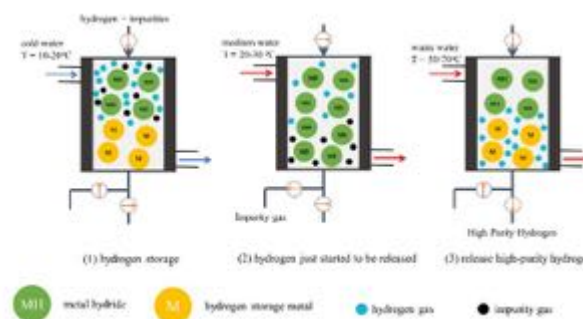


Fig. 1 Schematic of hydrogen purification using metal hydrides.

### Reference

- [1]. C.C. Shen, T.P. Perng, On the cyclic hydrogenation stability of an Lm(NiAl)<sub>5</sub>-based alloy with different hydrogen loadings, *J. Alloys Compd.*, 392 (2005) 187-191.



Chia-Chieh Shen

Dr. Chia-Chieh Shen is presently Associated Professor in Department of Mechanical Engineering and also Deputy Director of Fuel Cell Center at Yuan Ze University in Taiwan. He received his Ph.D. from Department of Materials Science and Engineering at National Tsing Hua University in Taiwan in 2006. After a postdoctoral researcher career, he joined the faculty of Yuan Ze University, as assistant professor in 2008. His research interests include metal hydrides (Ti-based, Mg-based and AB<sub>5</sub> type), fuel cell applications and thermohydrogenation. He has published over 20 international journal papers and 8 patents about metal hydrides.

## TRANSITION FROM FOSSIL TO RENEWABLE ENERGY WITH HYDROGEN

Andreas Züttel

Laboratory of Materials for Renewable Energy (LMER), Institute of Chemical Sciences and Engineering (ISIC), Basic Science Faculty (SB), École polytechnique fédérale de Lausanne (EPFL) Valais/Wallis, Rue de l'Industrie 17, CH-1950 Sion, Switzerland

**Abstract** The main challenge of the energy transition from abundant fossil to intermittent renewable energy is the conversion and storage of the renewable produced electricity in order to provide energy on demand. A entirely electric energy system is most efficient as compared to the conversion to hydrogen or synthetic fuels. However, seasonal storage of electricity is in batteries very expensive. Hydrogen can be transported over long distances and stored under ground and then used in combined cycle power plants for electricity production.

### CO<sub>2</sub> emissions and limited reserves

The global consumption of fossil fuels is increasing exponentially since forty years, doubling approximately every 27 years. Close to 50% of the emitted CO<sub>2</sub> remains in the atmosphere, i.e. nature is able to absorb 50% of the CO<sub>2</sub> emissions. However, until 2047 the world will emit the same amount of CO<sub>2</sub> as was emitted since 1850. The fossil resources are limited and will be consumed between 2047 and 2073. Therefore, a fast transition to renewable energy is required.

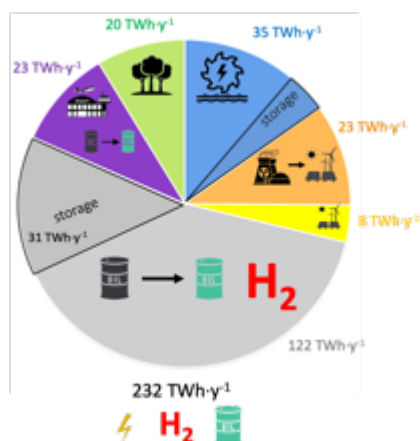


Fig. 1 Energy demand in Switzerland 2019

### Renewable energy

Beside the production of electricity from renewables the storage is essential for a future energy economy based on renewables in order to provide energy on demand from an intermittent source of energy and to shift energy from summer

to winter. The global renewable energy production is growing exponentially and if it continues like that will reach the world energy demand in 2035. The energy requirements are analysed on the example of Switzerland and the opportunities for the replacement of the fossil fuels with renewables are shown as well as the technical and economic consequences are described. In addition the opportunities for Australia to provide renewable energy for the world are discussed.

### Seasonal storage

The seasonal storage and the production of the fuel for aviation are the main challenges. Importing renewable energy during the winter time slightly reduces the storage requirement and the size of the photovoltaics needed, but large storage capacities in the hydroelectric storage lakes as well as for hydrogen remain a big technical challenge. Furthermore, the cost of the energy depends on the storage form and the overall conversion efficiency and has a significant economic impact.

### Hydrogen

Hydrogen plays a crucial role in the renewable energy economy since it is rather easy to produce, abundant and much more efficient than synthetic hydrocarbons. The future energy system will use electricity, hydrogen and synthetic fuels, depending on the requirements of the applications.

### References

- [1] Andreas ZÜTTEL, Noris GALLANDAT, Paul J. DYSON, Louis SCHLAPBACH, Paul W. GILGEN, Shin-Ichi ORIMO, "Future Swiss Energy Economy: the challenge of storing renewable energy", *Frontiers in Energy Research: Process and Energy Systems Engineering*, 9 (2022), <https://doi.org/10.3389/fenrg.2021.785908>

### Short CV



Andreas ZÜTTEL

Born 22. 8. 1963 in Bern, Switzerland. 1985 Engineering Degree in Chemistry, Burgdorf, Switzerland. 1990 Diploma in Physics from the University of Fribourg (UniFR), Switzerland. 1993 Dr. rer. nat. from the science faculty UniFR. 2004 Habilitation in experimental physics at the science faculty UniFR ([www.unifr.ch](http://www.unifr.ch)). President of the Swiss Hydrogen Association „HYDROPOLE“ ([www.hydropole.ch](http://www.hydropole.ch)). 2006 Head of the section “Hydrogen & Energy” at EMPA ([www.empa.ch](http://www.empa.ch)) and Prof. tit. in the Physics department UniFR. 2014 Full Professor for Physical Chemistry, Institut des Sciences et Ingénierie Chimiques, Ecole Polytechnique Fédérale de Lausanne EPFL ([www.lmer.epfl.ch](http://www.lmer.epfl.ch)), Switzerland. 2017 Co-Founder of GRZ Technologies Ltd. ([www.grz-technologies.com](http://www.grz-technologies.com)). 2020 Member of the Swiss Academy of Technical Science (SATW, <https://www.satw.ch>)

## Effects of replacing La with Y on the crystal structure of $\text{La}_{6-x}\text{Y}_x\text{Ni}_{6.5}\text{Mn}_{0.33}\text{Al}_{0.17}$ materials

Emil Høj Jensen <sup>1\*</sup>, Matylida Guzik <sup>1</sup>, Pamela Whitfield <sup>2</sup>, Sabrina Sartori <sup>1</sup>

1. Department of Technology Systems, University of Oslo, Gunnar Randers Vei 19, 2007 Kjeller, Norway
2. Excelsus Structural Solutions (Swiss) AG, Park InnovAARE 5234, Villigen, Switzerland

**Abstract:** In order to limit some of the major issues of using Mg in RE-Mg-Ni  $\text{A}_2\text{B}_7$ -type hydrogen storage alloys. Mg is being replaced with Y. The effects of single-substituted compounds are known, but for compounds with multiple element substitution. In here it is found that the addition of Y has an effect on where the other substituted elements are located in the structure, and that it induce the formation of a hexagonal-type phase at low amounts, but at higher amounts rhombohedral type structures are induced.

### Introduction

RE-Mg-Ni  $\text{A}_2\text{B}_7$ -type hydrogen storage alloys have gained increased interest in recent years due to the higher electrochemical storage capacity (~400 mAh/g) compared to commercial  $\text{AB}_5$ -type materials (theoretical capacity of 372 mAh/g) when used as the anode in Ni-Metal-Hydride batteries. An issue is that Mg has a high vapour pressure, making the exact composition challenging to control during production using conventional metallurgical production routes. At the same time, Mg is easily volatilized into ultra-fine powder particles, thus becoming a safety hazard [1]. A possible solution is to replace Mg with Y, since a similar crystal structure and electrochemical capacities are found [2]. Though the electrochemical stability of these materials needs to be improved [3].

### Findings

Here we report the location of the substituted Y element in the crystal structure of the primary hexagonal  $\text{Ce}_2\text{Ni}_7$ -prototype phase (space group  $\text{P6}_3/\text{mmc}$ ). It is known that for single substituted materials that Y prefer to enter specific sites initially [4,5]. Here a similar trend is found in that Y prefer to enter the  $\text{A}_2\text{B}_4$  subunit first, and subsequently the  $\text{AB}_5$  subunit secondly. This also affects which sites the Al and Mn elements are located. It is also found that Y induce

the formation of the hexagonal  $\text{Ce}_2\text{Ni}_7$ -prototype phase (space group  $\text{P6}_3/\text{mmc}$ ) initially, and with more Y added the rhombohedral  $\text{Gd}_2\text{Co}_7$  and  $\text{PuNi}_3$ -prototype phases (space group R-3m)

### References

1. Yan, H.; Xiong, W.; Wang, L.; Li, B.; Li, J.; Zhao, X. Investigations on  $\text{AB}_3$ -,  $\text{A}_2\text{B}_7$ - and  $\text{A}_5\text{B}_{19}$ -Type La Y Ni System Hydrogen Storage Alloys. *International Journal of Hydrogen Energy* 2017, 42, 2257–2264.
2. Baddour-Hadjean, R.; Meyer, L.; Pereira-Ramos, J.P.; Latroche, M.; Percheron-Guegan, A. An Electrochemical Study of New  $\text{La}_{1-x}\text{Ce}_x\text{Y}_2\text{Ni}_9$  ( $0 \leq x \leq 1$ ) Hydrogen Storage Alloys. *Electrochimica Acta* 2001, 46, 2385–2393.
3. Belgacem, Y.B.; Khaldi, C.; Boussami, S.; Lamoumi, J.; Mathlouthi, H. Electrochemical Properties of  $\text{LaY}_2\text{Ni}_9$  Hydrogen Storage Alloy, Used as an Anode in Nickel-Metal Hydride Batteries. *Journal of Solid State Electrochemistry* 2014, 18, 2019–2026.
4. Zhang, J.; Charbonnier, V.; Madern, N.; Monnier, J.; Latroche, M. Improvement of Reversible H Storage Capacity by Fine Tuning of the Composition in the Pseudo-Binary Systems  $\text{A}_2\text{-La Ni}_7$  (A = Gd, Sm, Y, Mg). *Journal of Alloys and Compounds* 2021, 852, 157008.
5. Paul-Boncour, V.; Crivello, J.C.; Madern, N.; Zhang, J.; Diop, L.V.B.; Charbonnier, V.; Monnier, J.; Latroche, M. Correlations between Stacked Structures and Weak Itinerant Magnetic Properties of  $\text{La}_2 - x \text{Y}_x \text{Ni}_7$  Compounds. *J Phys Condens Matter* 2020, 32, 415804.



Emil Høj Jensen

My name is Emil and I come from Denmark. I took my Bachelor in Nanoscience from the university of Aarhus where I graduated from in 2015. The project I worked on was a parameter study on the ratio of supercapacitor material, binder and activated carbon to find the optimal ratio. I took my masters through the Sino-Danish Center program in Nanoscience and Nanotechnology graduating in 2017 where I worked to fabricate free-standing bendable cathode electrodes for simpler and bendable Li-ion batteries. I am currently working on my PhD, focusing on the utilization of metal hydrides in hydrogen gas storage that can be coupled to the electric grid.

## EMERGENCY POWER SYSTEMS WITH FUEL CELLS AND HYDROGEN

Ulrike Trachte

Lucerne University of Applied Sciences and Arts - Engineering & Architecture

More than 15 years ago, a fuel cell system for uninterruptible power supply (UPS) with fuel cells (FC) was tested in the field on an antenna for telecommunications at the roof of Lucerne University of Applied Sciences and Arts - Engineering & Architecture. In Switzerland, this was the first application at an installation in operation. Hydrogen was used as fuel.

Further installations followed for applications in the telecommunications sector and for the POLYCOM security radio network. The systems were subjected to extensive stress tests with measurements in the field. Hydrogen handling and service aspects were included in the evaluation. The results demonstrated a high reliability of the systems and a high technical maturity of the systems.

However, the technology is (still) expensive and there is so far no widespread use in Switzerland.

### Introduction

According to a national risk analysis [1], the failure of mobile communications is one of the three biggest risks in Switzerland. Typically, batteries are used for emergency power for short downtimes and diesel generators for longer times. As an environmentally friendly alternative, fuel cells are suitable for emergency power applications thanks to their high electrical efficiency and clean and quiet operation for long operation times. In a nationally funded project [2], five fuel cell systems were long term tested in the field. The installed fuel cell systems had an electrical output of between two and six kilowatts. The systems were air-cooled. Hydrogen was supplied from 50 liter compressed gas cylinders.

### Approach

The FC systems were integrated into an existing UPS system or installed as a stand-alone system. At one site, the system was rebuilt as a stand-alone system using supercapacitors instead of batteries for start-up.

The systems were installed at different locations and are exemplary for different environmental conditions. Three systems were located indoor and one outdoor. One of the systems was located at an altitude of 2'400 m above sea level, another at a tunnel entrance, and two systems were installed in the open field. Thus, the air quality for the operation of the fuel cells was quite different depending on the location.

During the testing period reliability and operational suitability were tested. The tests were carried out remotely and on a regular basis. All sites were provided with measurement equipment. Performance data and ambient conditions were recorded continuously. Current data could be accessed in real time via remote monitoring.

### Results

After a total of seven years of operation the systems had a reliability of 99.6% to 100%. With the good reliability and stable operation, the systems fully met the expectations of the end-users. At the end of testing, there was no significant damage of the FC, and no signs of aging could be observed. All systems were still fully functional.

However, in Switzerland there is still potential for improvement in the service availability for FC products and in the handling of hydrogen, particularly in the service of cylinder supply and cylinder replacement.

### References

- [1] Bundesamt für Bevölkerungsschutz (BABS) (2020): Bericht zur nationalen Risikoanalyse. Katastrophen und Notlagen Schweiz 2020. BABS, Bern.
- [2] U. Trachte, P. Sollberger, T. Gisler: Langzeittest USV mit Brennstoffzellen, BFE, 2019.

---

#### Short CV



Ulrike Trachte

Study of Mechanical Engineering at University of Karlsruhe, Germany

1993 Degree Dipl.-Ing.

1993 – 1998 Project engineer in plant engineering in Germany

1999 – 2002 Project manager at SIG Transver AG, Switzerland

2003 – today Scientific engineer at Lucerne University of Applied Sciences and Arts



## RECENT TRENDS IN THE KOREAN HYDROGEN INDUSTRY

Jihye Park

Hyundai Motor Company, Korea

Hydrogen is an excellent energy carrier with potential for next-generation transportation and energy storage. However, several challenges remain before hydrogen's full potential can be realized. Because all sectors of the hydrogen industry – production, storage, transportation and utilization – are closely intertwined, consistent government policies or support are required for the sustainable growth of the industry. The Korean government is actively pursuing policies to revitalize the hydrogen economy, thereby expanding hydrogen market and achieving balanced development of hydrogen industry. Introducing the latest technology development trends of domestic companies including Hyundai Motor Group.

### Korean government's Hydrogen Roadmap

South Korea adopted the Hydrogen Economy Roadmap in 2019 [1-3]. In order to prepare the legal basis for the government's hydrogen promotion, the "Hydrogen Law" (Hydrogen Economy Promotion and Hydrogen Safety Management Act) was enacted in 2020 and implemented the following year. The Hydrogen Law stipulates several important industrial strategy elements, such as supporting hydrogen-centric companies through research and development (R&D) subsidies, loans, and tax exemptions. In 2022, the Korean government announced new policies and goals to foster the domestic hydrogen industry. The government's three major growth strategies ('3UP') are establishing global supply chain and creating large-scale hydrogen demand ('Scale-Up'), legal framework establishment ('Build-Up'), and technological innovation ('Level-Up').

### Hydrogen industry trends in Korea

Recently, trends in the Korean hydrogen industry are changing. Over the past few years, it has struggled to lead the industry in hydrogen utilization, particularly in fuel cell electric vehicles (FCEVs) and fuel cells for power generation and buildings. Now, from the perspective of an energy transition toward carbon neutrality, the Korean hydrogen industry is facing a new turning

point as more investments in infrastructure have been made and more companies and institutions have entered the fields of hydrogen production, storage and transportation.

### HMG's activities

In 2013, Hyundai Motor Group (HMG) succeeded in mass-producing fuel-cell electric vehicles (FCEVs) for the first time in the world. Since then, HMG's hydrogen project has shifted the paradigm, showing HMG's vision for a hydrogen society by introducing next-generation FCEVs, FC trucks & buses, and future mobility solutions [4].

### References

- [1] Hydrogen Economy Roadmap of Korea, January 2019, Government of Korea (<https://motie.go.kr>)
- [2] Jae-Eun Shin, Hydrogen technology development and policy status by value chain in South Korea, *Energies*, 15 (2022) 8983.
- [3] Troy Stangarone, South Korean efforts to transition to a hydrogen economy, *Clean Technologies and Environmental Policy*, 23 (2021) 509-516.
- [4] <https://tech.hyundaimotorgroup.com/>



Jihye Park

Jihye Park is a senior research engineer at Hyundai Motor Company. She received her BS and PhD in Metallurgical Engineering from Yonsei University in South Korea. As her postdoctoral fellow at Korea Institute of Science and Technology, she developed hydrogen storage materials and computational alloy design techniques. After joining Hyundai Motor Company, she was responsible for establishing technology strategy and driving business in the field of hydrogen storage and transportation. She is currently researching hydrogen storage and applications based on solid hydrogen storage materials.

# ENERGETICS AND GROWTH MODES OF NI AND PD NANOPARTICLES ON GRAPHENE/Ni(111)

Kun ZHAO<sup>1</sup>, John R. RUMPTZ<sup>2</sup>, Nida JANULAITIS<sup>2</sup> and Charles T. CAMPBELL<sup>1,2</sup>

<sup>1</sup>Department of Chemistry, and <sup>2</sup>Department of Chemical Engineering, University of Washington, Seattle, Washington 98195-1700, USA

The use of carbon supports for late transition metal nanoparticle catalysts has grown substantially in recent years due to efforts to develop electrocatalysts for clean energy applications and catalysts for new aqueous-phase biomass-related conversions, and due to the evolution of new carbon materials with unique properties (e.g., graphene, carbon nanotubes, etc.). However, much less is known about the bonding energetics of catalytic metal nanoparticles on carbon supports in comparison with oxide supports, which are more common for thermal catalysis.

Here we investigated the growth morphologies and heats of adsorption of Ni and Pd vapor deposited onto graphene/Ni(111) at 300 K and 100 K using He<sup>+</sup> low-energy ion scattering (LEIS) and single crystal adsorption calorimetry (SCAC). For Ni/graphene/Ni(111), the SCAC results showed at 300 K the heat of adsorption of Ni vapor increases rapidly from 336 kJ/mol initially to the heat of sublimation (430 kJ/mol) by 2 ML, and at 100 K from 230 kJ/mol to the heat of sublimation slower by 3.5 ML.

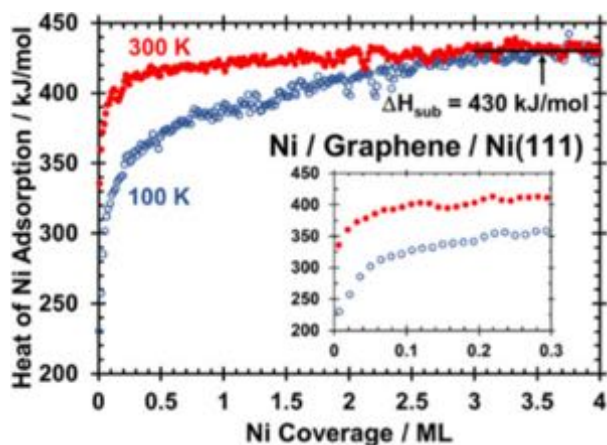


Figure 1. Differential heat of adsorption of Ni gas atoms onto graphene/Ni(111) as a function of Ni coverage at 300 K (red, filled points) and 100 K (blue, open points). The inset shows the low coverage regime (<0.3 ML) on an expanded scale.

The growth models derived from LEIS results suggested that Ni grows as flat-topped islands with a thickness of  $\sim 1.5$  nm when deposited at 300 K, and smaller hemispherical cap shape with a higher number density ( $2 \times 10^{16}$  particles/m<sup>2</sup>) when deposited

at 100 K. The particle size and morphology differences account for the differences in the heat of adsorption versus coverage at these two temperatures. The Ni chemical potential as a function of average particle diameter in the 0.5 to 4 nm range at 100 K was determined from the LEIS and SCAC measurements, and the Ni adhesion energy of 3.6 J/m<sup>2</sup> was determined from fitting the chemical potential vs diameter to a theoretical model.

For Pd/graphene/Ni(111), the heats of adsorption of Pd increase with coverage similarly to Ni at 300 K and 100 K and reach the heat of sublimation (377 kJ/mol) by 2 ML, with an initial heat of adsorption at 300 K (273 kJ/mol) that is 45 kJ/mol higher than at 100 K. The trends in the heat of adsorption are supported by the growth model from the LEIS results. Similar to Ni growth, but with smaller particle size and larger particle density than Ni, Pd grows as flat-topped islands at 300 K with a thickness of  $\sim 1$  nm, and hemispherical cap shape at 100 K with a larger number density ( $6 \times 10^{16}$  particles/m<sup>2</sup>) than at 300 K. The evolution of Pd chemical potential along with particle size was determined in the average particle diameter range of 0.6 – 2.5 nm at 100 K and the Pd adhesion energy was found to be 3.5 J/m<sup>2</sup>.

## Acknowledgement

The authors acknowledge the Department of Energy, Office of Basic Energy Sciences, under Grant Number DE-FG02-96ER14630, for support of this work.

## References

- [1] Rumptz, J. R.; Zhao, K.; Mayo, J.; Campbell, C. T. *ACS Catal.* **2022**, *12*,12632–12642.
- [2] Zhao, K.; Janulaitis, N.; Campbell, C. T. *submitted*, **2022**.



Kun ZHAO

Dr. Kun Zhao. 2012 B.S. in Applied Chemistry, and B.S. in Physics at Central China Normal University, Wuhan, China. 2015 M.S. in Physical Chemistry at Central China Normal University, Wuhan, China. 2020 PhD at EPFL in the group of Prof. Andreas Züttel with the thesis of Mechanisms of the Heterogeneously Catalyzed Reaction of CO<sub>2</sub> hydrogenation on Transition Metal Surfaces. 2021 to present, Postdoc Researcher at University of Washington, discovering the energetics and morphology of metal atoms and nanoparticles on graphene and metal oxide supports using advanced techniques of Single-Crystal Adsorption Calorimetry (SCAC) and Low-Energy Ion Scattering (LEIS) in ultrahigh vacuum (UHV) equipment.

## DEVELOPING SUSTAINABLE FETI ALLOYS FOR HYDROGEN STORAGE BY RECYCLING

Yuanyuan Shang<sup>1</sup>, Shaofei Liu<sup>2</sup>, Zhida Liang<sup>3, 4</sup>, Florian Pyczak<sup>3</sup>, Zhifeng Lei<sup>5</sup>, Tim Heidenreich<sup>1</sup>, Alexander Schökel<sup>6</sup>, Ji-jung Kai<sup>2, 7</sup>, Gökhan Gizer<sup>1</sup>, Martin Dornheim<sup>1</sup>, Thomas Klassen<sup>1, 8</sup>, Claudio Pistidda<sup>1</sup>

<sup>1</sup> Department of Materials Design, Institute of Hydrogen Technology, Helmholtz-Zentrum hereon GmbH, 21502, Geesthacht, Germany

<sup>2</sup> Department of Mechanical Engineering, City University of Hong Kong, 999077, Hong Kong, China

<sup>3</sup> Department of Metal Physics, Institute of Materials Physics, Helmholtz-Zentrum hereon GmbH, 21502, Geesthacht, Germany

<sup>4</sup> Department of Materials Science and Metallurgy, Cambridge, CB3 0FS, UK

<sup>5</sup> College of Materials Science and Engineering, Hunan University, 410082, Changsha, China

<sup>6</sup> Deutsches Elektronen-Synchrotron DESY, Notkestr. 85, 22607, Hamburg, Germany

<sup>7</sup> Center for Advanced Nuclear Safety and Sustainable Development, City University of Hong Kong, Hong Kong, China

<sup>8</sup> Helmut Schmidt University, Holstenhofweg 85, 22043, Hamburg, Germany

### Abstract

Intermetallic alloys such as FeTi have attracted ever-growing attention as a safe and efficient hydrogen storage medium. However, the utilization of high-purity metals for the synthesis of such materials poses considerable concerns over the environmental sustainability of their large-scale production. Here, attempting to drastically reduce the carbon footprint associated with the synthesis of FeTi alloys, without compromising their hydrogen storage properties, we report an approach for synthesising FeTi from industrial scraps of Fe (steels C45 and 316L) and Ti (Ti alloy Grade 2). Remarkably, at 50 °C in the range of hydrogen pressure between 0 bar and 100 bar, the alloys obtained by using C45-Ti Grade 2 and 316L-Ti Grade 2 can absorb a maximum amount of hydrogen of 1.61

wt.% and 1.50 wt.%, respectively (high-purity FeTi 1.70 wt.%). Moreover, depending on the type of steel utilized, the material's thermodynamic properties can be modified. Our findings pave a new pathway for developing high-performance, environmentally-sustainable FeTi alloys for hydrogen storage purposes using industrial metal wastes.

### References

[1] Shang, Y., Liu S., Liang Z., ... & Pistidda C. (2022). Developing sustainable FeTi alloys for hydrogen storage by recycling. (Accepted by *Communications Materials*)

### Short CV



Yuanyuan Shang

Yuanyuan Shang received her M.Eng. degree in materials science and engineering from the University of Science and Technology Beijing, under the supervision of Prof. Zhaoping Lu. She is now a Ph.D. student at Helmholtz-Zentrum Hereon. Her research interests mainly focus on developing hydrogen storage materials, i.e. Mg-based systems, NaAlH<sub>4</sub>, FeTi, NaBH<sub>4</sub>, and so on.



## From Nano to Macro and Back Again: Disruptive Science for Materials-Based Hydrogen Storage

Mark D. Allendorf

Sandia National Laboratories, USA

Hydrogen has the highest gravimetric energy density of any energy carrier and produces water as the only oxidation product, making it extremely attractive for both transportation and stationary power applications. However, its low volumetric energy density causes considerable difficulties, inspiring intense efforts to develop material-based storage using metal hydrides, liquid organic hydrogen carriers, and sorbents. The controlled uptake and release of hydrogen by these can be described as a series of challenges — optimal properties fall within a narrow range that can only be found in few materials and often involve significant tradeoffs. As a result, the slow pace of infrastructure development for hydrogen transport and storage is affecting both its economics and consumer appeal.

In this presentation I will discuss three current thrusts in our research that are transforming our approach to materials design and discovery:

1) Confinement of metal hydrides in non-innocent nanoporous hosts such as MOFs and COFs [1,2].

2) Co-design of materials, in which synthesis and characterization efforts partner with systems modeling to accomplish both forward and reverse engineering of new storage systems

3) Explainable machine learning, in which model prediction to validated material discovery was accomplished in only eighteen months [3].

Together, these strategies are enabling us to overcome challenges that have blocked discovery of successful storage materials for decades [4].

### References

- [1] V. Stavila, S. C. Li, C. Dun, M. A. T. Marple, H. E. Mason, J. L. Snider, J. E. Reynolds, F. El Gabaly, J. D. Sugar, C. D. Spataru, X. W. Zhou, B. Dizdar, E. H. Majzoub, R. Chatterjee, J. Yano, H. Schlomberg, B. V. Lotsch, J. J. Urban, B. C. Wood, M. D. Allendorf “Defying Thermodynamics: Stabilization of Alane Within Covalent Triazine Frameworks for Reversible Hydrogen Storage” *Angew. Chem. Int. Ed.* **2021**, *60*, 25815-25824.
- [2] Y. Cho, S. Li, J. L. Snider, M. A. T. Marple, N. A. Strange, J. D. Sugar, F. El Gabaly, A. Schneemann, S. Kang, M. Kang, H. Park, J. Park, L. F. Wan, H. E. Mason, M. D. Allendorf, B. C. Wood, E. S. Cho, V. Stavila “Reversing the Irreversible: Thermodynamic Stabilization of Lithium Aluminum Hydride Nanoconfined Within a Nitrogen-Doped Carbon Host” *ACS Nano* **2021**, *15*, 10163-10174.
- [3] M. Witman, G. Ek, S. Ling, J. M. Chames, S. Agarwal, J. Wong, M. D. Allendorf, M. Sahlberg, V. Stavila “Data-driven discovery and synthesis of high entropy alloy hydrides with targeted thermodynamic stability” *Chem. Mater.* **2021**, *33*, 4067.
- [4] M. D. Allendorf, V. Stavila, J. L. Snider, M. Witman, M. E. Bowden, K. Brooks, B. L. Tran, T. Autrey “Challenges to developing materials for the transport and storage of hydrogen” *Nat. Chem.* DOI 10.1038/s41557-022-01056-2.



Mark D. Allendorf

**Dr. Mark D. Allendorf** is Co-Director of the DOE Hydrogen Materials – Advanced Research Consortium (HyMARC) and a Senior Scientist at Sandia National Laboratories in Livermore, California. He holds an A.B. in chemistry (*Magna Cum Laude*) from Washington University in St. Louis and a Ph.D. in inorganic chemistry from Stanford University. At Sandia, his research focuses on the fundamental science and applications of metal-organic frameworks (MOFs) and on hydrogen storage. Current interests include metal hydrides and MOFs for hydrogen storage, chemical and radiation sensing, MOFs for electronic devices, and catalysts for biofuels production. His research has generated over 230 journal articles and proceedings papers, as well as thirteen patents. He is Past President and Fellow of The Electrochemical Society and has received Sandia awards for research, leadership, and teamwork, as well as a 2014 R&D100 Award for a novel approach to radiation detection.

## PROTON COUPLED ELECTRON VS. HYDROGEN TRANSPORT IN ELECTROCATALYSIS

Andreas Borgschulte,<sup>a,b</sup> Marin Nikolic,<sup>a,b</sup> Filippo Longo,<sup>a,b</sup> Emanuel Billeter,<sup>a,b</sup> Alessia Cesarini,<sup>a,c</sup> Selim Kazaz,<sup>a,b</sup> Mirushe Suloska,<sup>a,b</sup> Pavel Trtik<sup>d</sup>

<sup>a</sup>Laboratory for Advanced Analytical Technologies, Empa – Swiss Federal Laboratories for Material Science and Technology, Überlandstrasse 129, CH-8600 Dübendorf, Switzerland; <sup>b</sup>Department of Chemistry, University of Zurich, Winterthurerstrasse 190, CH-8057 Zürich, Switzerland; <sup>c</sup>Institute for Chemical and Bioengineering, Department of Chemistry and Applied Biosciences, ETH Zürich, Vladimir-Prelog-Weg 1-5/10, CH-8093 Zürich, Switzerland; <sup>d</sup>Laboratory for Neutron Scattering and Imaging, Paul Scherrer Institut, Forschungsstrasse 111, CH-5232 Villigen PSI, Switzerland

Abstract: Hydrogen is more than a reactant and/or adsorbate: it changes the physical and chemical properties of the (electro-) catalyst, specifically the electrical conductivity as a crucial property of redox catalysts.

### Hydrogen mobility as an enabler of hydrogen technology

The controllable hydrogen transport in matter is key parameter of the usability of hydrogen as an energy carrier. While it is obvious that hydrogen stored in a tank should not escape, but should move as efficient as possible in hydrogen selective membranes for hydrogen purification, the mobility of hydrogen varies over orders of magnitude on the atomic scale in conversion devices. I will highlight the various beneficial as well as detrimental effects of the ambivalent hydrogen allowing the greatly differing dynamics along the following practical examples: the Ni-MH battery, water splitting by Ni-electrodes, and hydrogen spillover in Ni-based catalysts. Despite their disparities, the unifying scientific question of the applications boils down to the question, why the transport of hydrogen consisting of a proton and an electron is different from electron coupled proton transport.

### Proton or electron mobility?

As a depictive entry, I present neutron tomography images of a Ni-MH battery. The principle of the Ni-MH battery relies on the electrochemical shuffling of hydrogen from one electrode to the other [1]:



M is a hydride forming metal alloy. Neutrons are sensitive to hydrogen, allowing following the change of the hydrogen distribution in the electrodes upon charging/discharging. In addition to the desired electro-chemical exchange of protons and electrons, neutron imaging also detects gaseous hydrogen, which leads to a battery discharge; i.e., reaction (1) can take place without transport of charges, i.e., by exchange of neutral

hydrogen. The peculiar electro-catalytic properties make Ni (oxy-) hydroxide surfaces also superior active electrodes for alkaline water electrolysis [2]. In particular, it is well known that highest performance for the oxygen evolution reaction is obtained only after prolonged cycling [3], i.e., exchange of H in Ni (oxy-) hydroxide. Using hard X-ray photoelectron spectroscopy (HAXPES), we were able to address the high electrical conductivity to the self-organisation of ion channels in the extended Ni (oxy-) hydroxide surface. Hydrogen spillover is a concept, in which hydrogen is transported via the surface of the oxide supporting the active metal catalyst [4]. Although obvious, that the high hydrogen mobility boosts catalytic conversion, we cannot confirm this idea using a novel high-throughput method based on neutron imaging. Instead, it appears that oxides containing practically immobile hydrogen are superior to oxides taking up hydrogen reversibly. The long established theoretical backbone of hydrogen spillover distinguishes between hydrogen transport and proton coupled electron transport. In the latter, no long-range hydrogen transport takes place. With this, we can close the line of thoughts from catalysis to electrolysis: also the oxygen evolution reaction on Ni is accelerated by hydrogen treatment, despite the fact that hydrogen is not supposed to take place in the reaction.

### References

- [1] Notten, van Beek, Chem. Ind. 54 (2000) 102
- [2] Klaus et al., J. Phys. Chem. C 119 (2015) 7243
- [3] Medway et al., J. Electroanalytical Chem. 587 (2006) 172
- [4] Prins, Chem. Rev. 112 (2012) 2714



Andreas  
Borgschulte

Physicist with focus on Applied Spectroscopy; PhD in physics from TU Braunschweig (D) in 2002, Postdoc VU Amsterdam (NL) and Helmholtzzentrum Geesthacht (D); since 2006 Group leader of the group Hydrogen Spectroscopy @ Empa, Lecturer at University Zürich and ETH Zürich.

## K-WATER'S HYDROGEN BUSINESS DEVELOPMENT

Heena YANG

Water Energy Research Institute, Korea Water Resources Corporation(K-water), 462-1 Jeonmin-dong, Yousung-Gu, Daejeon, Korea

Abstract

Green hydrogen is produced by renewable energy without greenhouse gas emissions. Korea Water Resources Corporation(K-water) has the largest renewable energy in Korea and plans to expand the green hydrogen production business through renewable energy. The hydrogen is produced using all of renewable energy from K-water by 2050, will be supplied nationwide to establish the hydrogen infrastructure. It will be a great success for Korea's energy independence.

### Introduction

K-water, established in 1967 as a water-specialized public company, has played a leading role in securing safe water in the country and ensuring water-oriented welfare for the people. K-water is also striving to cope with climate change, perform its social responsibility and resolve water-related issues around the world. Hydrogen is one of solution to respond to climate change, it can be produced through various routes, and used as a fuel. K-water has the largest amount of renewable energy (2,102 GWh/year from hydro, tidal, solar and wind power generation) in Korea and is also developing water-based renewable energy such as floating photovoltaic system and hydrothermal energy system.

Therefore, it is possible to play a key role in reducing greenhouse gas emissions by producing, and distributing green hydrogen using renewable energy. By 2026, it aims to install 3.3GW of floating solar power and supply 2.66 million tons of green hydrogen per year. Accordingly, various hydrogen demonstration projects are ongoing, and some of them are introduced.

### Hydropower based green hydrogen



Recently, K-water has begun construction of the 'Green Hydrogen Demonstration Facility', which produces green

hydrogen using the small hydro power generation of the water purification plant at the Water Purification Plant in Seongnam City. It signed a business agreement with Seongnam City, Hyundai Motor Company, and SK E&S on the establishment of a green hydrogen cycle (production-distribution-utilization).

This project is the first case in Korea to utilize renewable energy small hydro power generation. In the Water Purification Plant, water pressure is generated in the process of sending water from the Paldang Lake water intake to the water purification plant, and there is a 0.7MW small hydro power plant. It can be produced 69 tons of green hydrogen per year which is enough to charge 38 hydrogen cars for a day.

### Hydrogen business in the future

The hydrogen demonstration using small hydro power in Seongnam will be built without a hitch and will be expanded nationwide as a model case.

From 30% (by 2030) to 100% (by 2050) of small hydro power station will be used for hydrogen production. In addition, Sihwa Tidal Power Plant, the world's largest tidal power plant, will be a source to produce hydrogen by 2030. It will be a great achievement to build a hydrogen chain(production-supply) and contribution of hydrogen economy in Korea.



Heena YANG

Born in 1986 in Seoul, Republic of Korea, Heena YANG graduated with Ph.D. Degree in Materials Chemistry and Engineering from Konkuk University in 2016. During this time, she worked as an undergraduate research assistant in the field of nanostructured materials for proton exchange membrane fuel cells(PEMFCs). From 02/2017, she moved to Ecole Polytechnique Federale de Lausanne(EPFL) Valais as a Postdoc and started her work on the hydrogen storage materials such as complex hydrides and carbon based porous materials. Currently she works as a senior research at Korea water resources corporation(K-water), her work is focused on green hydrogen production system and its application.

## CYCLE AND REGENERATION PERFORMANCE OF METAL HYDRIDE FOR COMMERCIALIZED STORAGE AND COMPRESSION SYSTEM

Tai SUN

GRZ technologies SA, CH-1772 Grolley, Switzerland

**Abstract:** The cycle stability of the metal hydride is critical to the service life of commercialized hydrogen storage and compression system. A number of researches report the bad cycle performance of AB<sub>5</sub>-type metal hydrides, while some others report high cycle stability on AB<sub>5</sub> with high Ce-content. This work presents our experimental studies of the cycle performance of the AB<sub>5</sub> and AB<sub>2</sub> metal hydrides designed for industrial scale storage and compression. All AB<sub>5</sub> alloys show bad stability during cycling. Serious capacity degradation, plateau slope increase, plateau pressure deduction were observed even on alloys with optimized composition and preparation. This situation becomes worse when working at higher temperatures. Regeneration is proof to be effective in recovering capacity and plateau performance. However, the degradation rate of the AB<sub>5</sub> metal hydride becomes higher, with the increasement times of regeneration. In order to maintain the high-quality performance of our commercialized hydrogen storage and compression systems, we developed AB<sub>2</sub> alloys with high capacity and better performance. The degradation rate of the alloy is only 0.001wt%/1000cycles.

### References

- [1] G. Friedlmeier, A. Manthey, M. Wanner, and M. Groll, "Cyclic stability of various application-relevant metal hydrides," *Journal of Alloys and Compounds*, vol. 231, no. 1, pp. 880–887, Dec. 1995.
- [2] Tarasov, B.P., et al., Cycling stability of RNi<sub>5</sub> (R = La, La+Ce) hydrides during the operation of metal hydride hydrogen compressor. *International Journal of Hydrogen Energy*, 2018. 43(9): p. 4415-4427



Tai SUN

Dr. Tai Sun is now the material scientist of GRZ technologies SA. He has been working in the metal hydride for more than 13 years. Now he is the leader of the material science team of the company and in charge of the planning and management of hydrogen storage materials development and manufacture for the company's commercial hydrogen systems.

## INVESTIGATIONS ON HYDROGEN STORAGE PERFORMANCE OF AB<sub>2</sub>-TYPE METAL HYDRIDE FOR 865BAR HYDROGEN COMPRESSION

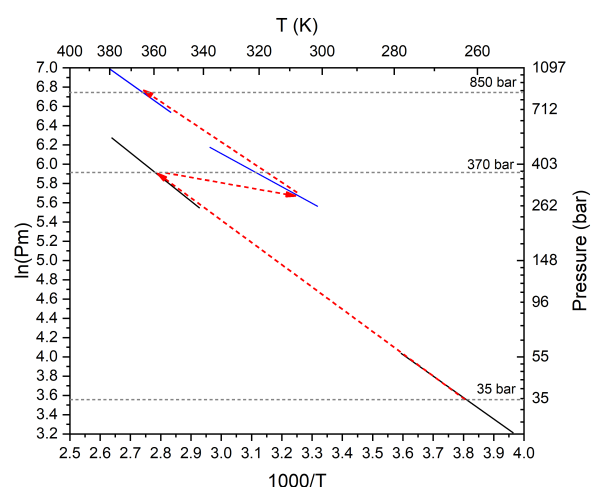
Rui Li<sup>1,2</sup>, Akhil Penmathsa<sup>1,2</sup>, Tai Sun<sup>2</sup>, Noris Gallandat<sup>2</sup>, Konstantinos Bardis<sup>2</sup>, Andreas Züttel<sup>1,\*</sup>

1. Laboratory of Materials for Renewable Energy (LMER), Institute of Chemical Sciences and Engineering (ISIC), Basic Science Faculty (SB), École Polytechnique Fédérale de Lausanne (EPFL) Valais/Wallis, Energypolis, Rue de l'Industrie 17, CH-1951 Sion, Switzerland

2. GRZ technologies SA, CH-1772 Grolley, Switzerland

Green hydrogen is considered as a prominent alternative to fossil fuels thanks to its emission-free use in hydrogen fuel cell vehicles in the transportation sector<sup>[1]</sup>. The refueling pressure of hydrogen fuel trucks is around 350bar, while the refueling pressure of hydrogen fuel passenger vehicles is done at approximately 865 bar<sup>[2]</sup>. Considering the safety and high pressure requirement during the refueling process, the development of compressors for hydrogen refueling stations has been investigated as an alternative<sup>[3]</sup>.

Compared to the traditional mechanical hydrogen compressors, metal hydride hydrogen compressors (MHHC) have certain advantages such as increased safety and lower maintenance requirements<sup>[4]</sup>. The purpose of this study is to develop a two-stage MHHC at 865bar. The MHHC compresses hydrogen from 35bar to 370bar in the first stage, and further to 865bar in the second stage. The effects of substitution of Ti by Zr, of Mn by Fe, and different Ni contents on the hydrogen storage performance of AB<sub>2</sub> alloys have been investigated. The most important results were the following: 1) With the increasing of Ni content, the B/A value increases, and the plateau slope of the alloy is the lowest when the Ni content is 0.18. 2)



With the increasing of Fe content, the plateau slope of the alloy first decreases and then increases; at an Mn content of 0.3, the alloy has the smallest slope. 3) In the study of A-side elements, the increase of Zr content will have a significant impact on the plateau pressure of the alloy. 4) Deviation between the experimentally measured PCT curve and the theoretical Van't Hoff equation, even after the inclusion of the fugacity effect<sup>[5]</sup>, has been demonstrated. Further investigation is required to properly judge the reason of this discrepancy.

### Reference

- [1] L. Schlapbach and A. Züttel, "Hydrogen-storage materials for mobile applications," vol. 414, 2001.
- [2] Q. Li et al., "Optimization of Ti-Zr-Cr-Fe alloys for 45 MPa metal hydride hydrogen compressors using orthogonal analysis," *J. Alloys Compd.*, vol. 889, p. 161629.
- [3] P. Liu, et al, "Hydrogen storage properties of (Ti<sub>0.85</sub>Zr<sub>0.15</sub>)<sub>1.05</sub>Mn<sub>1.2</sub>Cr<sub>0.6</sub>V<sub>0.1</sub>M<sub>0.1</sub>(M=Ni, Fe, Cu) alloys easily activated at room temperature," *Prog. Nat. Sci. Mater. Int.*, vol. 27, no. 6, pp. 652–657.
- [4] Z. Peng, et al. "Overview of hydrogen compression materials based on a three-stage metal hydride hydrogen compressor," *J. Alloys Compd.*, p. 23, 2022.
- [5] V. Charbonnier, et al. "Tuning the hydrogenation properties of Ti<sub>1+y</sub>Cr<sub>2-x</sub>Mn<sub>x</sub> laves phase compounds for high pressure metal-hydride compressors," *Int. J. Hydrog. Energy*, vol. 46, no. 73, pp. 36369–



Rui Li

### CV: Rui Li

Born in 1995 in Hubei, China, Rui Li graduated with a BA in Materials Science from the CTGU university in 2016. He then continued his postgraduate studies at South China University of Technology and obtained a master's degree in materials engineering in 2021. His master thesis and work is focused on the study of Ti-based hydrogen storage alloys. He is currently pursuing PhD in chemistry and chemical engineering at EPFL and GRZ technologies SA in the topic of the development and research of high-performance metal hydrides.

## Low-temperature non-equilibrium synthesis of anisotropic multimetallic nanosurface alloys for the electrochemical CO<sub>2</sub> reduction reaction

Cedric David KOOLEN<sup>a,b</sup>, Emad OVEISI<sup>c</sup>, Jie ZHANG<sup>d</sup>, Mo LI<sup>a,b</sup>, Jack K. PEDERSEN<sup>e</sup>, Jan ROSSMEISL<sup>e</sup>, Wen LUO<sup>f\*</sup>, Andreas ZUETTEL<sup>a,b</sup>

<sup>a</sup>Laboratory of Materials for Renewable Energy (LMER), Institute of Chemical Sciences and Engineering (ISIC), Basic Science Faculty (SB), École polytechnique fédérale de Lausanne (EPFL) Valais/Wallis, Energypolis, Sion, 1951, Switzerland.

<sup>b</sup>Empa Materials Science & Technology, Dübendorf, 8600, Switzerland.

<sup>c</sup>Interdisciplinary Centre for Electron Microscopy (CIME), École Polytechnique Fédérale de Lausanne (EPFL), CH-1015 Lausanne, Switzerland.

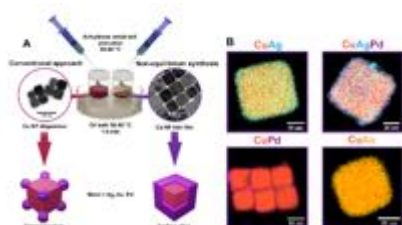
<sup>d</sup>Department of Chemistry, Faculty of Science, National University of Singapore (NUS), 119077 Singapore, Singapore

<sup>e</sup>Center for High Entropy Alloy Catalysis (CHEAC), Department of Chemistry, University of Copenhagen, 2100 København Ø, Denmark

<sup>f</sup>School of Environmental and Chemical Engineering, Shanghai University, Shanghai, 200444, China.

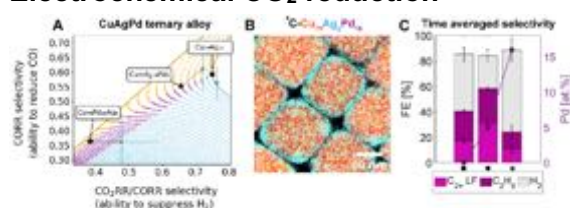
Multi-metallic nanoparticles (MMNPs) are of interest as functional materials for their highly tuneable properties. However, synthesizing homogeneously mixed MMNPs with immiscible components is limited to high temperature conditions. Here, we report a low-temperature ( $\leq 80$  °C) non-equilibrium synthesis of nano-surface alloys (NSAs) with tuneable size, shape and composition regardless of miscibility [1]. We further demonstrate our synthesis as a screening platform to investigate the effects of crystal facet and elemental composition by testing shaped NSAs as catalysts in the electroreduction of CO<sub>2</sub>. Finally, we resort to machine-learning (ML) to predict and synthesize both multi-carbon-product selective and phase stable Cu-Ag-Pd compositions [2].

### Synthesis



**Figure 1.** (A) Schematic illustration of the conventional and non-equilibrium galvanic replacement reaction, where multimetallic heterostructures and surface alloys were formed, respectively. (B) STEM-EDXS elemental maps of cubic Cu-Ag, Cu-Ag-Pd, Cu-Pd and Cu-Au NSAs prepared by the non-equilibrium method. Kinetic control allows to overcome miscibility gaps as evidenced by the Cu-Ag system.

### Electrochemical CO<sub>2</sub> reduction



**Figure 2.** Theory-guided optimization of the ternary alloy for extended phase-stability and C<sub>2</sub>+ selectivity in the

eCO<sub>2</sub>RR. (A) Activity-selectivity plot of CO<sub>2</sub>RR/CORR of the ternary alloy system. Orange colored dots indicate compositions with  $\geq 74$  at.% Cu, light blue and purple coloured with  $< 74$  at.% Cu and  $> 13$  at.% Ag and Pd, respectively. Black symbols (circle, star and square) denote the predicted values from the ML-based algorithm. Blue symbols and error bars indicate molar yields as calculated from experimental data in (C) (B) STEM-EDXS elemental map of as-synthesized C-Cu-Ag-Pd NSA with Ag:Pd equals 1:3. (C) Time averaged FEs of C<sub>2</sub>+ liquid fuels, C<sub>2</sub>H<sub>4</sub> and H<sub>2</sub> of the C-Cu<sub>79</sub>Ag<sub>16</sub>Pd<sub>5</sub>, C-Cu<sub>79</sub>Ag<sub>16</sub>Pd<sub>5</sub> and C-Cu<sub>79</sub>Pd<sub>16</sub>Ag<sub>5</sub> MMNPs, respectively.

### References

- [1] Koolen, C. D. *et al.* High-Throughput Sizing, Counting, and Elemental Analysis of Anisotropic Multimetallic Nanoparticles with Single-Particle Inductively Coupled Plasma Mass Spectrometry. *ACS Nano* (2022) doi:10.1021/acsnano.2c01840.
- [2] Pedersen, J. K., Batchelor, T. A. A., Bagger, A. & Rossmeisl, J. High-Entropy Alloys as Catalysts for the CO<sub>2</sub> and CO Reduction Reactions. *ACS Catal.* **10**, 2169–2176 (2020).



Cedric D. KOOLEN

Cedric D. KOOLEN is a doctoral assistant and safety engineer in the Laboratory of Materials for Renewable Energy (LMER), at the École Polytechnique Fédérale de Lausanne (EPFL) – Wallis-Valais headed by Prof. Dr. Andreas Züttel. His interests lie with CO<sub>2</sub> electrolysis and plasma-based techniques for the synthesis and characterization of nanoparticles.

# THE ROLE OF SECONDARY PHASES AND ELEMENT SUBSTITUTIONS IN THE HYDROGENATION OF INTERMETALLIC COMPOUNDS

Sabrina Sartori

Department of Technology Systems, University of Oslo, Norway

## Abstract

In this keynote talk we will discuss the role of secondary phases and element substitutions in intermetallic alloys, linking their hydrogenation performances with structural and microstructural properties. After setting the context with highlights on the factors that define capacity, thermodynamics, kinetics in the case of various classes of intermetallic alloys from literature, we will consider recent results from our investigations. For TiFe-compounds, we present the influence of specific microstructure and chemical composition of secondary phases on hydrogenation performances. In the case of La-Y-Ni-Mn-Al-type compounds we discuss the role of Y content in the phase formation and hydrogenation plateau pressures. The talk will offer some perspectives on the use of intermetallics for stationary applications.

## Content of the talk

Intermetallic compounds provide a viable solution to the challenge of energy storage from renewable sources, due to their ability to absorb and desorb hydrogen in a reversible way with a proper tuning of pressure and temperature conditions. Therefore, they are expected to play an important role in the clean energy transition and in the deployment of hydrogen as an efficient energy vector. An overview of properties and applications of various class of intermetallics will be given.

Recently it was shown that TiFe with 4 wt.% Zr greatly improved the first hydrogenation kinetics, after processing the sample via ball milling [1]. Here we report the use of scanning photoemission microscopy (ESCA Microscopy beamline at Elettra synchrotron facility, Trieste, Italy) to investigate the composition and chemical state of the various phases present in this alloy and how they change upon hydrogenation and dehydrogenation [2]. Our hypothesis is that the improvement in kinetics is caused by the specific microstructure and chemical composition of the secondary phase, and the variation of composition at the interface matrix/secondary phase. The as-cast alloy confirmed the higher abundance of zirconium at the edge of the zirconium-rich secondary phase. The edge is also the site of a Zr-Ti phase that was not detected using conventional SEM. For zirconium, the reduced/oxidized ratio is higher in the zirconium-rich region while for titanium it is higher in the region with low content of titanium. The hydrided sample showed the presence of a possible Zr-Fe hydride phase. In the dehydrided sample the TiFe phase was not oxidized, and in the Ti-Zr phase, oxidation is only on Zr. In the case of La-Y-Ni-Mn-

Al-system we performed a systematic study of a series of compounds with increased Y content, focusing on the analysis of material structural/microstructural properties and hydrogen sorption behaviour. Data collected at the synchrotron radiation powder X-ray diffraction (MCX beamline, Elettra, Italy) and neutron powder diffraction (BT-1, NIST, USA) were jointly analysed by Rietveld refinements using the Fullprof Suite program. Pressure-Composition-Temperature measurements were performed with a Hy-Energy PCTPro-2000 Sieverts apparatus to link the hydrogenation properties of the compounds with their phase composition.

## Conclusion

Intermetallics can be easily tailored with elemental substitution to favour activation, kinetics, cyclability, and to adjust the plateau pressure at system conditions of application. Our investigation showed that TiFe + 4 wt.% Zr alloy presents a wide range of different oxides. As the nature of the various oxide phases change upon hydrogenation/dehydrogenation, it may indicate that these oxides play a more important role in the hydrogenation than what was previously believed. For La-Y-Ni-Mn-Al-system it was found that higher Y content helps to maintain the material crystallinity during the hydrogenation cycles and increases its H-storage capacity.

## References

- [1] *et al.* S. Sartori, J. Huot. *J. Mater. Res. Technol.* **2019**, *8*, 1828–1834.
- [2] S. Sartori, *et al.*, J. Huot. *Inorganics* **2023**, *11*, pp 26



Sabrina Sartori

**Sabrina Sartori** is full professor of Physics at the University of Oslo (UiO), Norway, and leader of the section Energy Systems. She studied physical chemistry at the University of Padova and graduated with a PhD degree in materials science and engineering from the University of Bologna in 2003. Her current main research interests are focused on energy storage materials and hydrogen-based systems for the integration of renewable energy sources in stationary applications. She is leading the master program Renewable Energy Systems at UiO and is engaged in interdisciplinary collaborative projects with academic and industrial partners. Sartori is active in several science organizations, for instance she has been elected in the presidential line of the Materials Research Society for 2022-2024, serving as President in 2023.

# RUTHENIUM-SUPPORTED CATALYST, A POTENTIAL NEW CATALYST FOR CATALYTIC HYDROGEN COMBUSTION (CHC)

Zohreh Akbari<sup>1,2</sup>, Andreas Züttel<sup>1,2</sup>

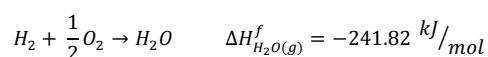
<sup>1</sup> Laboratory of Materials for Renewable Energy (LMER), Institute of Chemical Sciences and Engineering (ISIC), Basic Science Faculty (SB), École Polytechnique Fédérale de Lausanne (EPFL) Valais/Wallis, Energypolis, Rue de l'Industrie 17, 1951 Sion, Switzerland

<sup>2</sup> Empa Materials Science & Technology, 8600 Dübendorf, Switzerland

**Abstract** The high exothermicity of the hydrogen oxidation reaction makes it a great potential candidate to use in the heating sectors on industrial scales as well as in our daily life. Catalytic Hydrogen Combustion is a way to overcome the drawbacks of conventional combustion. In this study, the sub-nano-sized Ru-supported (< 1 nm) alumina catalyst is synthesized through the incipient wetness impregnation method, and its catalytic activity toward hydrogen and oxygen recombination reaction under lean hydrogen conditions is investigated. Stable catalytic activity after 45h, and complete hydrogen conversion with a conversion rate of 4 ml/min.gr<sub>cat</sub> under GHSV of 3000 h<sup>-1</sup> is achieved.

## Catalytic Hydrogen Combustion

Hydrogen is a carbon-free energy carrier with the largest energy density (33.3 kWh/kg) among all other energy sources. This chemical energy can be valorized by hydrogen and oxygen recombination through the following exothermic reaction:



Water, the only by-product of the reaction, makes hydrogen a potential future fuel. However, the application of conventional hydrogen combustion is hindered by drawbacks such as flame flashback risk and NO<sub>x</sub> emission. Catalytic Hydrogen Combustion (CHC) is a promising solution to overcome these drawbacks [1]. Pt and Pd are the state-of-the-art catalysts for the CHC, which can completely convert hydrogen into water under lean hydrogen conditions (< 4 vol% H<sub>2</sub> in the gas mixture) at room temperature (RT). However, by far, the utilization of Ru-based catalysts for the CHC has not been addressed.

## Ru-supported $\gamma$ -Alumina Synthesis and Characterization

As a result of a high surface area (BET surface area of 234 m<sup>2</sup>/gr), availability, and low cost,  $\gamma$ -alumina is chosen as the support material. In a typical synthesis, RuCl<sub>3</sub>.xH<sub>2</sub>O as the Ru precursor is dissolved in Et+DI water, and the sub-nano-sized Ru particles are synthesized through the incipient wet impregnation (IWI) method.

## Catalytic Hydrogen Conversion Performance

The catalytic performance of the synthesized Ru-based catalyst toward the CHC reaction is investigated using a plug-flow microreactor. The exhaust gas is then analysed using a Mass Spectrometer (MS). In this work, the effect of Cl ion contamination, Ru wt%, H<sub>2</sub> to O<sub>2</sub> ratio, GHSV, and H<sub>2</sub> vol% in the feed gas on the catalytic performance of the catalyst under the CHC reaction is studied. The obtained hydrogen conversion rate ( $X_{H_2}$ ) vs temperature curves are sigmoidal. Starting with the kinetically controlled regime, the activation energy is calculated using the Arrhenius equation.

$$X_{H_2} = \frac{H_{2,in} - \frac{N_{2,in}}{N_{2,out}} \times H_{2,out}}{H_{2,in}} \times 100$$

Results showed that although the catalyst is active at RT, a complete hydrogen conversion is granted at temperatures higher than 200°C under lean hydrogen conditions. Moreover, Cl ions removal significantly enhanced the catalytic activity. In addition, the Ru-based catalyst showed a stable catalytic performance at 240°C over 45h on stream. In the end, the mechanism and probable origins of the catalytic activity of the Ru-based catalyst toward the CHC reaction are proposed.

## References

- [1] Vogt U, Fumey B, Biemann M, Siong V, Gallandat N, Züttel A. *Catalytic Hydrogen Combustion on Porous SiC Ceramics*. Eur Fuel Cell Forum 2017:45–54.



Zohreh Akbari

Zohreh graduated with an M.Sc. degree in Materials Science and Engineering from the University of Tehran, Iran, as the 1<sup>st</sup> rank in 2018, where she was working on layered structured perovskite materials as an electrocatalyst for the ORR/OER reactions in solid oxide cells. For two years, she was a research assistant at the University of Tehran, working on state-of-the-art layered oxide materials for advanced Li-Ion batteries. Since April 2021, she has been a Ph.D. student at the Laboratory of Materials for Renewable Energy (LMER), where she is working on the design, synthesis and characterization of the supported catalysts for Catalytic Hydrogen Combustion (CHC) and studying their mechanistic and catalytic performance in the CHC.



## SIMULATION BASED DESIGN OF A METAL HYDRIDE COMPRESSOR USING REDUCED ORDER THERMAL MODELS AND COMPUTATIONAL FLUID DYNAMICS (CFD)

Konstantinos Bardis<sup>1</sup>, Akhil Penmathsa<sup>1,2</sup>, Noris Gallandat<sup>1</sup>, Tai Sun<sup>1</sup>

1. GRZ technologies SA, CH-1772 Grolley, Switzerland

2. Laboratory of Materials for Renewable Energy (LMER), Institute of Chemical Sciences and Engineering (ISIC), Basic Science Faculty (SB), École Polytechnique Fédérale de Lausanne (EPFL) Valais/Wallis, Energypolis, Rue de l'Industrie 17, CH-1951 Sion, Switzerland

**Abstract:** Green hydrogen is seen as a prerequisite to the clean energy transition for both the transportation and energy sector. The safe, compact and efficient compression and storage of hydrogen can accelerate the wider adoption of it. To this end, metal hydrides compressor offer an undeniable advantage in comparison to traditional mechanical compressors, since hydrogen is stored at low pressure and the possibility of leakages is significantly reduced. The process of hydrogen absorption and desorption is thermally controlled requiring the supply or removal of heat. Therefore, if such heating or cooling sources are freely available e.g. waste heat, river cooling etc., the overall efficiency of such compressors is higher.

In this study, such a compressor is thermally modelled and designed. It is a part of larger installation located in the pharmaceutical company Lonza Group AG (Visp, Switzerland) used for continuous compression and fueling of hydrogen tracks at 200 bar pressure and a maximum flow of 30 kg/h. Compression is carried out in two stages using two different materials and there two modules of low- and high-pressure stage guaranteeing the continuous supply of hydrogen. As a heating medium, steam is used, while, for cooling, water from the local river is utilized. The individual cells (cylindrical tubes) containing the metal hydride material are placed in a "shell-and-tube heat exchanger" type of arrangement within a bigger cylindrical container to form the overall compressor system (as show in the Figure). Around the cells is the flow of the thermal medium; baffles are used to further enhance the heat transfer and achieve the target compression ratio.

For the design of the compressor an hierarchical approach is adopted. Initially, the overall compressor characteristics are determined, such as the container diameter, the cells number

and diameter as well as its' length, using a simplified thermal model. After the main design parameters have been specified, detailed 3-D CFD simulations were carried out to obtain the baffles number and width. The results from the 3-D simulation were very illustrative about the optimum geometry, allowing for a significant increase of the compressor effective capacity (more than 20 %) with almost no increase in the design complexity and manufacturing/operation cost.

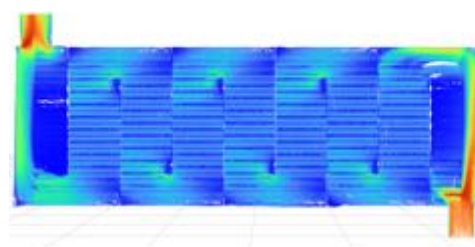


Fig. 1 Thermal picture of the compressor.



Dr. Konstantinos Bardis

### Short CV:

Born in 1992 in Athens, Greece, Konstantinos Bardis graduated with a Diploma degree in Naval Architecture and Marine Engineering from the National Technical University of Athens (NTUA). He completed his Doctoral studies in the Aerothermochemistry and Combustion Systems Laboratory of the Swiss Federal Institute of Technology of Zurich (ETH-Zurich) in September, 2020 under the supervision of Prof. Konstantinos Boulouchos. The topic of his dissertation was the Development of a Phenomenological Combustion Model for Prechamber Gas Engines. He worked in the ETH-Zurich until April, 2021 as a Post-Doctoral Researcher in the field of hydrogen combustion for heavy duty engines. He is currently employed in GRZ technologies SA as a thermal engineer.

## SYSTEM SIMULATION OF METAL HYDRIDE AND FUEL CELL-BASED HYDROGEN TO POWER SYSTEMS – 1D MODEL BASED THERMAL MANAGEMENT OPTIMIZATION

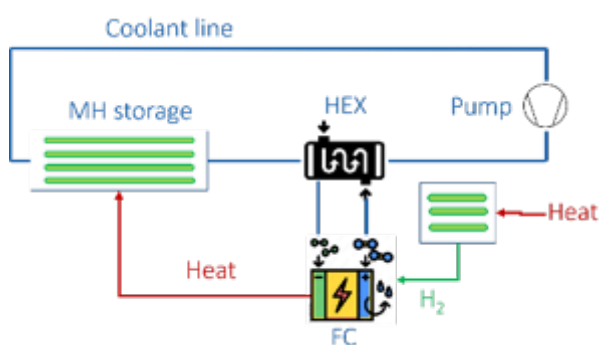
Akhil Penmathsa<sup>1,2,\*</sup>, Rui Li<sup>1,2</sup>, Konstantinos Bardis<sup>2</sup>, Noris Gallandat<sup>2</sup>, Tai Sun<sup>2</sup>, Andreas Züttel<sup>1</sup>

1. Laboratory of Materials for Renewable Energy (LMER), Institute of Chemical Sciences and Engineering (ISIC), Basic Science Faculty (SB), École Polytechnique Fédérale de Lausanne (EPFL) Valais/Wallis, Energypolis, Rue de l'Industrie 17, CH-1951 Sion, Switzerland  
2. GRZ Technologies SA, CH-1772 Grolley, Switzerland

Abstract: Metal hydrides are attractive for safe and reliable storage of hydrogen owing to their high storage density and low pressures. The thermodynamics of absorption/desorption of hydrogen allow thermal integration with fuel cell for efficient operation of hydrogen to power systems based on metal hydrides and fuel cell<sup>[1][2]</sup>.

### DASH

In this work, DASH (Dense And Safe Hydrogen) hydrogen to power system, based on metal hydrides and PEM fuel cell, developed by GRZ Technologies S.A is described<sup>[3]</sup>. Due to the thermal nature of the system, when the initial temperature of metal hydride and ambient air is low, the system cannot be started due to inadequate heat available for desorption and requires auxiliary means to provide heat of desorption. In this work different scenarios and candidate systems for startup are presented and studied by a system model. All the scenarios presented involve supplying heat to a fraction of metal hydrides initially by different techniques to desorb hydrogen and using waste heat from fuel cell to heat up remaining metal hydrides.



### 1D Model

A 1D model is used to describe the dynamics of metal hydride, incorporating heat and mass transfer along with chemical

kinetics<sup>[4]</sup>. A 0D model is used to describe the waste heat of fuel cell and integrated mathematically with the MH model to generate a 1D system model. Various functions of the required auxiliary startup system are described, solutions are formulated leading to different design candidates. 1D system model is used to simulate the startup system of DASH and operating limits are determined. Final design candidate is chosen among considered candidates and the operation and performance of the system is presented for real life conditions. Considering space limitations the design candidate with heated tank is ideal albeit requiring a complex control strategy for the startup process. The higher ambient temperature of surrounding air also improved the startup performance of the system.

### References

- [1] L. Schlapbach and A. Züttel, "Hydrogen-storage materials for mobile applications," vol. 414, 2001.
- [2] Nguyen, Huy Quoc, and Bahman Shabani. "Review of metal hydride hydrogen storage thermal management for use in the fuel cell systems." *International Journal of Hydrogen Energy* 46.62 (2021): 31699-31726.
- [3] <https://grz-technologies.com/dash-storage>
- [4] Mohammadshahi, S. S., E. MacA Gray, and C. J. Webb. "A review of mathematical modelling of metal-hydride systems for hydrogen storage applications." *international journal of hydrogen energy* 41.5 (2016): 3470-3484.



Akhil Penmathsa

### C.V. - Mr. Akhil Penmathsa

Born in 1996 in Hyderabad, India, Akhil Penmathsa graduated with a B.Tech. in Mechanical engineering from the SRM university in 2017. He then went on to pursue graduate studies at the Delft university of technology at Delft, The Netherlands where he obtained his MSc degree in Mechanical Engineering in 2021. His master thesis and work were focused on boundary layer flashback studies focusing on hydrogen combustion in gas turbines. He is currently pursuing PhD in chemistry and chemical engineering at EPFL and GRZ technologies SA in the topic of thermal management of metal hydrides storage and compression systems.

## MATERIALS DISCOVERY FOR ENERGY-RELATED APPLICATIONS: BRIDGING PROCESS ENGINEERING AND BASIC SCIENCE

Susana Garcia<sup>a</sup>

<sup>a</sup>Research Center for Carbon Solutions (RCCS), School of Engineering and Physical Sciences, Heriot-Watt University, EH14 4AS, Edinburgh, UK

Climate change is likely the greatest challenge that humanity will face this century. According to greenhouse gas emissions reduction scenarios, to avoid the most severe effects of climate change, achieving net-zero CO<sub>2</sub> emissions by 2050 is required. This is a very demanding landscape despite the striking development of renewable energy, since more than 80% of global primary energy is still fossil fuel-based. Most decarbonizing scenarios highlight the role of carbon capture, utilization and storage (CCUS) technologies, which are expected to play a relevant role in the next decades. For instance, natural gas reforming with CCUS is expected to be a cost-effective option for an industrial-scale low-carbon hydrogen production, so-called blue hydrogen. In line with the EU hydrogen strategy, it can therefore help lay the foundation for much higher use of hydrogen across the whole economy. To accelerate the discovery, development, and deployment of novel advanced materials for carbon capture applications, it is critically important that efforts between experimentalists, theoreticians, and process engineers are coordinated. The PrISMa project (<https://prisma.hw.ac.uk>) addresses this challenge by integrating materials design with process design and environmental considerations to allow for tailor-making carbon capture solutions optimally tuned for local sources and sinks.

### State of the art

CCUS is a key technology for achieving the global emissions reduction targets because of its role in power and industrial decarbonization [1, 2]. Decarbonisation from a variety of industrial emission sectors highlights a marked need for capture technologies that can be optimized for different sources of CO<sub>2</sub> and integrated in an equally diverse range of applications of captured CO<sub>2</sub> as a feedstock. At high Technology Readiness Levels (TRLs), there are substantial efforts focusing on optimizing a single particular carbon capture technology (e.g. amine-based capture) for a single typical stationary source (e.g., coal-fired power plants). However, significant gains in energy efficiency and other economic benefits as well as environmental impacts can be obtained if we tailor make a capture technology for a particular CO<sub>2</sub> source and a particular CO<sub>2</sub> destination, such as utilization or transport via pipeline, or ship to permanent storage. Such tailoring requires a systematic view of separation methodologies, microscopic processes, and engineering design.

### Our innovative approach

The innovative aspect of this work is the integration of recent developments in material science to generate a large number of novel materials with process design and techno-economic and environmental analyses. The lack of such integration has been identified as one of the key bottlenecks that limit the prospect of novel materials for CCUS technologies to reach the market. Here, we present a methodology for systematic knowledge exchange between material science and process engineering.

### Materials Discovery by bridging process engineering and basic science

In the PrISMa platform, advanced techno-economic material screening models are used to identify and quantify the relevant process key

performance indicators (KPIs), e.g., CO<sub>2</sub> purity, recovery, productivity, and energy consumption, that should lead to improved carbon capture processes. These performance indicators are further translated into targets for the design of novel materials. This allows us to deeply understand the material properties and requirements underpinning sorbent-based carbon capture processes. This platform integrates, material screening, process design, techno-economics, and life-cycle analysis, and provides us with a holistic assessment of the potential for cost reduction. A series of case studies have been investigated where CO<sub>2</sub> is captured from different point sources (e.g. natural gas and coal-fired power plants, cement plants) and sent for geological storage. By interrogating the vast materials and process design space with the PrISMa platform, we were able to identify materials that outperform current benchmark ones. We also make use of big-data science and developed multiscale workflows that enable us to find correlations between the properties of materials and their performance in a process [3]. Our results so far confirm the importance of bridging materials discovery with process design for accelerating the deployment of advanced sorbent-based carbon capture technologies.

We plan to extend our approach to support low-carbon hydrogen production through CCUS, and we expect this approach will have a long-term impact on the way we integrate fundamental science with process engineering.

### References

- [1] B. Smit, S. Garcia, *Europhysics News* **2020**, *51* (2), 20-22. DOI: 10.1051/eprn/2020203.
- [2] J. R. Fernández, S. Garcia, E. S. Sanz-Pérez, *Industrial & Engineering Chemistry Research* **2020**, *59* (15), 6767-6772. DOI: 10.1021/acs.iecr.0c01643.
- [3] S. M. Moosavi et al., *Nat. Mater.* **2022**. DOI: 10.1038/s41563-022-01374-3.



Susana Garcia

**Susana García** is Professor of Chemical and Process Engineering and Deputy Head of the Institute of Mechanical, Process and Energy Engineering at Heriot-Watt University. She is also the Associate Director in Carbon Capture and Storage at the Research Centre for Carbon Solutions (RCCS), an interdisciplinary world leading engineering centre, inspiring and delivering innovation for the wider deployment of technologies needed to meet necessary carbon targets. Her current research focuses on advancing materials and separation processes for energy, industrial and environmental applications. She ambitions to change the paradigm on how novel processes based on advanced materials are developed through the integration of process engineering and basic science.

# LARGE-SCALE SYNTHESIS OF GO/MWCNTS COMPOSITE FOR HYDROGEN STORAGE

Yunting Wang, Andreas Züttel

<sup>a</sup>École polytechnique fédérale de Lausanne (EPFL) Valais/Wallis, Laboratory of Materials for Renewable Energy (LMER), Institute of Chemical Sciences and Engineering (ISIC), CH-1950 Sion, Switzerland

<sup>b</sup>Empa Materials Science and Technology, 8600 Dübendorf, Switzerland

## Abstract

Here we proposed a large-scale synthesis method for GO/MWCNTs composite as hydrogen storage material. This method comprises a feeding/mixing step wherein  $\text{KMnO}_4$  and graphite are fed into  $\text{H}_2\text{SO}_4$  separately and then mixed to prepare a graphite/oxidant mixture, an oxidation step comprising oxidizing the graphite/oxidant mixture through two-step oxidations to obtain a graphene oxide dispersion, and a composite synthesis step, comprising mixing, sonicating and stirring the graphene oxide dispersion with a sonicated dispersion of multi-walled carbon nanotubes to obtain the final product. As a result, the morphology and structure of GO/MWCNTs composite synthesized by large-scale method exhibit high similarity to that synthesized by traditional method. GO/MWCNTs exhibited a 3D nanostructure composed of MWCNTs linked to the graphene oxide layers. The hydrogen capacity of GO/MWCNTs can be more than 5 wt.% at ambient temperature and 50 bar. Therefore, this large-scale synthesis method is promising for industrial applications to enable the process of industrialization and to build small storage units for the investigation of the properties of the new storage system.

## Introduction

Hydrogen ( $\text{H}_2$ ) is a clean form of energy that has the potential to fuel vehicles. However, efficient hydrogen storage for developing a sustainable hydrogen economy remains a significant challenge. [1] Graphene oxide and multi-walled carbon nanotubes (GO/MWCNTs) composite with a 3D nanostructure shows an excellent hydrogen storage capacity, which can be up to 5 wt.% at 50 bar and room temperature. [2] This material can replace high-pressure vessels in the future, enables small-scale applications e.g. lightweight cars, as well as allows easy and safe distribution of hydrogen at low pressure or in small cartridges. However, the synthesis of this carbon nanostructure material currently only allows producing small amounts of less than 1 gram in the lab. Among the composite synthesis procedures, the development of a large-scale continuous process to synthesize GO materials and the GO/MWCNTs composite are big challenges.

## Large-scale synthesis method

GO/MWCNTs composite was synthesized by the following steps, including the pre-treatment of graphite, mixing of graphite with oxidants, and the oxidation process for the synthesis of GO, and the following composite synthesis step. Particularly, for the dissolution of  $\text{KMnO}_4$  in  $\text{H}_2\text{SO}_4$ , two glass jacketed bottles build a continuously stirred reactor, which

allows longer residence times and the necessary heat removal. In the oxidation process, a continuous flow reactor increased the contact area and improved the heat exchange.

## GO/MWCNTs composite for hydrogen storage

The results of SEM, TEM, XRD, and Raman indicated the GO/MWCNTs composite was successfully synthesized by the large-scale synthesis process. The MWCNTs were aggregated on the graphene layer to form a 3D nanostructure. The GO/MWCNTs composite shows a hydrogen storage capacity of ~5.0 wt.% under room temperature and 50 bar, which is the same as the small-scale composites. It is worth noting that the adsorption capacity will increase to around 8.0 wt.% as the pressure increases to 90 bar.

## References

- [1] Allendorf, M.D., Stavila, V., Snider, J.L., Witman, M., Bowden, M.E., Brooks, K., Tran, B.L. and Autrey, T., 2022. Challenges to developing materials for the transport and storage of hydrogen. *Nat. Chem.*, 14(11), 1214-1223.
- [2] Yang, H., Lombardo, L., Luo, W., Kim, W. and Züttel, A., 2018. Hydrogen storage properties of various carbon supported  $\text{NaBH}_4$  prepared via metathesis. *Int. J. Hydrog. Energy*, 43(14), 7108-7116.



Yunting Wang

## Short CV

Dr. Yunting Wang is a postdoc scientist from École polytechnique fédérale de Lausanne (EPFL) Valais/Wallis. She received her PhD degree in Environmental Material at China University of Mining and Technology of Beijing and carried out Joint PhD research at Korea University in South Korea, and focused on developing novel nanomaterials/electrocatalysts for electrochemical energy conversion and wastewater treatment. She is now working on the hydrogen storage materials, for example, 3D carbon materials.

## REMA – MEMBRANE-LESS ELECTROLYSER

Steven A. Schenk (1), Ioakeim Sioutis (1), Pooria Hadikhani (2), Demetri Psaltis (1)

(1) Optics laboratory, École Polytechnique Fédérale de Lausanne (EPFL), Lausanne, Switzerland

(2) Computational Science & Engineering Laboratory, ETH Zurich, Zurich, Switzerland

### Abstract

Clean hydrogen can be produced by water electrolysis. Commercial electrolyzers rely on a physical barrier called membrane or separator to separate hydrogen and oxygen products. Membrane-less electrolyzers use fluid mechanics to maintain the gas product separated. Therefore, these electrolyzers do not need membranes or separators. By avoiding the use of a membrane, these systems could work with reduced losses induced by membranes, provide flexibility in the catalysts used and the reaction operated, simplify its construction and its design, decrease the price of the system and increase its attractiveness, and increase the efficiency of the system. However, products separation is a challenging task in membrane-less electrolyzers. In this study, a millimeter scale membrane-less electrolyser is introduced based on a proven micro-scale technology from the laboratory of optics at EPFL. The scaled-up stack of this technology is necessary to make the production of hydrogen economically interesting. 99.99% purity hydrogen production at larger scale has been maintained by an appropriate fluid channel design and allow to operate a current density above 500mA/cm<sup>2</sup>. And a membrane-less electrolyzer stack has been designed, fabricated and tested for higher hydrogen production validating the technology for larger scale and industrialized hydrogen production applications.

### Introduction

Green hydrogen is seen as the Swiss knife of decarbonization because if we make it cheap enough it can be used in many different applications. The challenges to get cheap green hydrogen are various along its value chain. Here we focus on its production from water and electricity by the means of an electrolyser. Nowadays, commercial electrolyser efficiency reaches up to 70% efficiency for a consequent investment cost. To reduce the price of hydrogen and make a viable solution for the energy transition, cheaper, more efficient, more robust and easy industrialized production of electrolyser are needed. We see here an opportunity for membrane-less electrolyser to fill a gap in this field.

### Scaling-up

In the last decade, membrane-less electrolyser has been investigated at a micro-scale, demonstrating the possibility to produce high quality hydrogen at high efficiency without the need of a membrane [1-2]. The scaled-up of this technology to a millimeter scale fluidic channel has shown the possibility to maintain a separation of the gases produced using fluid mechanics, see fig. 1. With a 99.99% hydrogen production and a simplified and more robust system, millimeter scale membrane-less electrolyzer can be then produced by conventional fabrication method permitting them to target industrial application.

### Stack

Industrial application of electrolysis for hydrogen production relies on the possibility to stack electrolysis cells to be able to produce larger amount of hydrogen and reduce its price by sharing one balance of stack. Membrane-less electrolyser stacking challenges are combining the stacking of the fluidic behavior and the electrochemical behavior in a compact construction. A 4 cells, 28 channels, membrane-less stack has been designed, built and tested to show the stacking capacity of this technology, see fig. 2. By an appropriate fluid channel design and mechanical design, the separation of product has been maintained at high quality and the hydrogen production is increased.

### References

- [1] Hadikhani, Pooria, et al. "A membrane-less electrolyzer with porous walls for high throughput and pure hydrogen production." *Sustainable energy & fuels* 5.9 (2021): 2419-2432.
- [2] Hashemi, S. Mohammad H., et al. "A versatile and membrane-less electrochemical reactor for the electrolysis of water and brine." *Energy & Environmental Science* 12.5 (2019): 1592-1604



### CV of Steven Alexandre Schenk

Bachelor in Mechanical Engineering (2012 – 2016), EPFL, Lausanne, Switzerland. Master in Mechanical Engineering (2016-2019) EPFL, Lausanne, Switzerland, Master Thesis (2019), MIT, Boston, United States. *Scientific Assistant* (2020 -Now) Laboratory of Optics, EPFL, Lausanne, Switzerland

# Super-ionic conduction of mono-/di-valent cations and advanced battery application of complex hydrides: viewpoint from “HYDROEGNOMICS” project

Shin-ichi ORIMO<sup>1</sup>

<sup>1</sup> WPI-AIMR / Institute for Materials Research, Tohoku University, Sendai 980-8577, Japan

Hydrogen in materials exhibits a wide range of concentration, high mobility, quantum nature, and superior chemical reactivity. All these features of hydrogen originate from its bonding and size flexibilities. The goal of the MEXT (Ministry of Education, Culture, Sports, Science and Technology, Japan) project is to develop a new materials science on hydrogen and hydrides as a guideline to “fully utilize” the diverse functionalities of hydrogen in materials [1].



One of the research targets of this project is a series of complex hydrides exhibiting various energy-related properties [2]. So far, we have reported the systematic studies on lithium super-ionic conduction and all-solid-state lithium-ion battery using an optimized solid-solution phase of complex hydrides  $\text{LiCB}_9\text{H}_{10}/\text{LiCB}_{11}\text{H}_9$  [3]. A detailed molecular dynamics simulation on the order-disorder phase-transition behavior, re-orientational anion motion, and cation conductivity was recently reported on the related system [4].

In addition to the mono-valent cations, lithium and sodium [5], we have been also focusing on the di-valent cations, magnesium [6] and calcium. We have been developing a highly stable and efficient Ca electrolyte composed of a new complex hydride  $\text{Ca}(\text{CB}_{11}\text{H}_{12})_2$  for RT-operating calcium-ion battery [7]. This  $\text{Ca}(\text{CB}_{11}\text{H}_{12})_2$  electrolyte exhibits excellent electrochemical performances; that is, the high conductivity, wide potential window, and reversible Ca plating/stripping with high Coulombic efficiency. Furthermore, we are studying complex hydrides with pseudo-rotational anion motion, such as  $\text{Li}_5\text{MoH}_{11}$  with  $[\text{MoH}_9]^{3-}$ , as new candidates of super-ionic conductors of various cations [8].

## References

- [1] Referred to as “HYDROGENOMICS (hydrogenomics) project”, and see please; <https://hydrogenomics.jp/>
- [2] R. Mohtadi and S. Orimo, *Nat. Rev. Mater.* 2 (2017) 16091.
- [3] S. Kim, H. Oguchi, N. Toyama, T. Sato, S. Takagi, T. Otomo, A. Dorai, N. Kuwata, J. Kawamura, S. Orimo, *Nat. Comm.* 10 (2019) 1081.
- [4] K. Sau, T. Ikeshoji, S. Kim, S. Takagi, S. Orimo, *Chem. Mater.* 33 (2021) 2357.
- [5] K. Yoshida, T. Sato, A. Unemoto, M. Matsuo, T. Ikeshoji, T.J. Udovic, S. Orimo, *Appl. Phys. Lett.* 110 (2017) 103901.
- [6] K. Kisu, S. Kim, M. Inukai, H. Oguchi, S. Takagi, S. Orimo, *ACS Appl. Ener. Mater.* 3 (2020) 3174.
- [7] K. Kisu, S. Kim, T. Shinohara, K. Zhao, A. Züttel, S. Orimo, *Sci. Rep.* 11 (2021) 7563.
- [8] S. Takagi, T. Ikeshoji, T. Sato, S. Orimo, *Appl. Phys. Lett.* 116 (2020) 173901.



Shin-ichi ORIMO

Shin-ichi ORIMO received his Ph.D. in 1995. He was a JSPS research fellow, a research associate in Hiroshima University, and a guest researcher in Max-Planck Institute for Metal Research awarded by Alexander von Humboldt Fellowship and MEXT Fellowship. He worked as the Special Advisor to the University President, and is currently Director of WPI-AIMR, and Head of Research Section of Institute of Materials Research (IMR), Tohoku University. He received “Metals Meritorious Award (Japanese Institute of Metals, 2011)”, “The Commendation for Science and Technology (The Minister of MEXT, 2012)”, “Hydrogen & Energy Award (2015)”, “Honda Frontier Award (2021)”, and so on. He is also a Guest Professor, High Energy Accelerator Research Organization (KEK).

<http://www.hydrogen.imr.tohoku.ac.jp/>

Corresponding author: Shin-ichi ORIMO, Email: shin-ichi.orimo.a6@tohoku.ac.jp, Tel. (+81)22-215-2093.

# USING MODEL SYSTEMS TO OBTAIN UNDERSTANDING OF ABSORPTION AND DIFFUSION OF HYDROGEN IN CONSTRUCTION MATERIALS

Björgvin Hjörvarsson

Uppsala University, Materials Physics, Uppsala Sweden

Hydrogen is widely used as a chemical agent and its importance for energy storage is steadily increasing. Consequently, understanding the interaction of hydrogen with materials is essential in many perspectives. In this contribution I will discuss ideas which can be used as a base for understanding absorption and diffusion of hydrogen in materials. The discussion starts by analysing the influence of the local atomic concentration in transition metal alloys on the hydrogen absorption, followed by discussion on the effect of imperfections such as grain boundaries. The role of large angle grain boundaries on absorption and hydrogen embrittlement will be dwelled upon, illustrating the fascinating interplay of symmetry and boundaries. Finally, the relation between crystalline order and absorption will be mentioned.

## Background

The development of material related technology has enabled new avenues, and sometimes unexpected understanding. For example, we can now observe and identify atoms on a surface, as well as mapping the internal chemical composition in alloys, as illustrated in Figure 1. This type of detailed information on the local concentration of elements enables *e.g.* prediction of changes in the spatial dependence of the local hydrogen concentration, as well as elastic and magnetic interaction of the atoms in alloys [1]. Not only has the analysis of materials developed, deposition techniques now allow controlled growth of fractions of monolayers, forming single crystals or

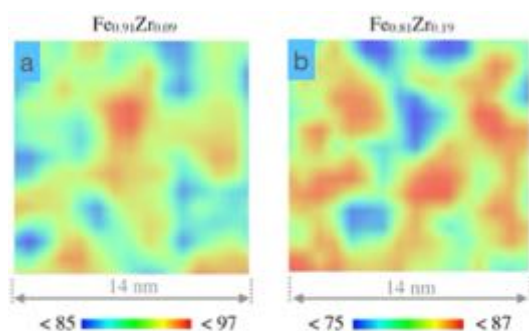


Figure 1. Illustration of the atomic distribution in random alloys of  $Fe_{1-x}Zr_x$ . The resolution in the analysis is  $1 \text{ nm}^3$ , which is a compromise between resolution and statistical certainty using Atom Probe. The figure is adapted from reference [1].

amorphous layers with desired elemental distribution, which

can even be patterned to form three dimensional heterostructures [2].

This progress, in combination with the detailed information available on the effects of interfaces [3], strain [4], clamping [5], and finite size [1] on the hydrogen uptake, allows us to predict how randomness and defects influence the hydrogen uptake in construction materials. The theoretical framework which is used for the discussion is based upon the work of Nørskov and Alefeldt [6].

These ideas will be used to discuss the underlying effects of actual challenges such as hydrogen embrittlement and hydrogen storage, highlighting the use of fundamental sciences addressing societal challenges such as the storage and transport of energy.

## References

- [1] Ryota, Gemma, et al. Scientific Reports (Nature Publisher Group); London Vol. 10, Iss. 1, (2020)
- [3] Erik Östman, et al. Nature Physics (2018), doi:10.1038/s41567-017-0027-2 (2018)
- [3] B. Hjörvarsson, et al. Phys. Rev. B **43**, 6440 (1990)
- [4] S. Olsson, et al. J. of Physics: Cond. Matter **13**, 1685-98 (2001).
- [5] B. Hjörvarsson, et al. J. of Appl. Physics **9**, 73-85, (1997)
- [6] Alefeld, G. Ber. Bunsenges. Phys. Chem. **76**, 746 (1972)  
J.K. Nørskov Phys. Rev. B **26**, 2785 (1982)



Professor Björgvin Hjörvarsson is heading the Materials Physics program (<https://physics.uu.se/research/materials-physics/>) at the Department of Physics, at Uppsala University. His research concerns the underlying principles of absorption and transport of hydrogen in materials, especially the impact of confinement and composition on the obtained properties. This knowledge is of relevance for storage of hydrogen as well as design of any device where hydrogen has a function or a presence. Changes in physical properties of materials can also be profound upon absorption of hydrogen, *e.g.* mechanical, magnetic and optical properties. Understanding and utilization of these changes is therefore expected to be of vital importance in the utilization of hydrogen for both energy storage as well as processing of materials. Hjörvarsson is an elected member of the Royal Swedish Academy of Sciences and the Royal Society of Sciences in Uppsala.

## PLATINUM GROUP METAL-FREE DIRECT BOROHYDRIDE FUEL CELLS

Youngdon Ko<sup>1,2</sup>, Junkil Park<sup>3</sup>, Xiong Zhang<sup>4,5</sup>, Liqun Kang<sup>6</sup>, Thi Ha My Pham<sup>1,2</sup>, Victor Boureau<sup>7</sup>, Cuong Pham-Huu<sup>4</sup>, Jihan Kim<sup>3</sup>, Liping Zhong<sup>1,2</sup>, Andreas Züttel<sup>1,2</sup>

Affiliation 1. LMER, EPFL 2. EMPA 3. KAIST, 4. University of Strasbourg 5. DICP 6. MPI 7. CIME, EPFL

**Abstract** Catalyst replacement in direct borohydride fuel cells (DBFCs) is studied for reducing the price of catalysts. The platinum group metals (PGMs) are replaced with a nickel catalyst and transition metal with nitrogen-doped carbon materials (M-N-C). The oxygen reduction reaction (ORR) and hydrogen peroxide reduction reaction (PRR) activity of Fe-N-C and Co-N-C are compared. It shows that the Co-N-C is the more suitable catalyst in DBFC cathode due to its durability.

### Hydrogen storage and utilization

Hydrogen storage and utilization are the technologies to achieve carbon-neutral energy systems with renewable energy sources. The demand for safe and high-density hydrogen storage methods increasing attention such as material-based hydrogen storage. Among the various materials that have been investigated, complex hydrides can be a candidate material for high gravimetric hydrogen storage and using hydrogen reasonable temperature ranges (Room temperature to 200 °C). The utilization of hydrogen technology needs to investigate efficiently producing electricity and heat with compatible cost. Direct borohydride fuel cells (DBFCs) are investigated by converting the chemical energy of sodium borohydride and hydrogen peroxide to electricity and heat.

### Palladium replaced with nickel catalyst in DBFC anode

The nickel catalyst can substitute expensive palladium catalysts even with high performance and efficient fuel utilization. The complex anode reaction with anion-exchange ionomer (AEI) and cation-exchange ionomer (CEI) is evaluated in half-cell and single-cell configurations. The ionomer type produces high (AEI) or low local pH (CEI) at the active site of the catalyst in the single-cell configuration, generating different catalytic reactions. The selective catalytic activities for the borohydride oxidation reaction (BOR) and hydrogen oxidation reaction (HOR) are the key parameters for achieving good performance. Furthermore, fuel utilization and H<sub>2</sub> evolution measurement in a single-cell configuration provide more information on the complex anode reaction in DBFC.

### Platinum replaced with M-N-C catalyst in the DBFC cathode

The M-N-C materials are used in the DBFC cathode for hydrogen peroxide reduction reaction (PRR). The PRR activity and durability of M-N-C are evaluated with half-cell and membrane electrode assembly (MEA) configurations. The Fe-N-C has higher activity on PRR than Co-N-C. However, the Co-N-C is more stable than Fe-N-C under the DBFC operation condition. The post-mortem XPS and Raman spectroscopy are measured to observe M-N-C degradation. In addition, the density functional theory (DFT) calculation supports the Co-N-C stability on the catholyte. In the DBFC durability test, Fe-N-C shows 18.6% performance loss after the accelerated durability test, whereas Co-N-C shows a more stable performance only 6.7% performance loss.

### References

- [1] Y.D. Ko, J. Park, X. Zhong, L. Kang, THM. Pham, V. Boureau, C. Huu, J. Kim, L. Zhong<sup>†</sup>, A. Züttel, Activity and Durability of M-N-C catalysts for Oxygen Reduction Reaction and Hydrogen Peroxide Reduction Reaction in Platinum Group Metal-Free Direct Borohydride Fuel Cells, *In preparation*.
- [2] Y.D. Ko, L. Lombardo, M. Li, THM. Pham, H.N. Yang, A. Züttel<sup>†</sup>, Selective Borohydride Oxidation Reaction on Nickel Catalyst with Anion and Cation Exchange Ionomer for High-Performance Direct Borohydride Fuel Cells, *Advanced Energy Materials*, (2022) 2103539.



Youngdon Ko

Born in 1992, Republic of Korea. Youngdon Ko graduated B.Sc. and M.Sc. degree from Konkuk University in 2019, Republic of Korea. Currently, he is a Ph.D. student at Prof. Andreas Züttel's group in EPFL. His research topics are investigating hydrogen storage and utilization using complex hydride materials and direct borohydride fuel cells (DBFCs). The various catalysts are studied to replace platinum group metal catalysts in fuel cells such as nickel and transition metal with nitrogen-doped carbon materials (M-N-C).



## DESIGN AND SYNTHESIS OF CATALYST FOR CO<sub>2</sub> METHANATION PILOT

Liping Zhong<sup>1,2\*</sup>, Thi Ha My Pham<sup>1,2</sup>, Zohreh Akbari<sup>1,2</sup>, Youngdon Ko<sup>1,2</sup>, Solaimon Mohamad<sup>1,2</sup>, Yasemen Kuddusi<sup>1,2</sup>, Noris Gallandat,<sup>1,2,3</sup> Andreas Züttel<sup>1,2</sup>

1. Laboratory of Materials for Renewable Energy (LMER), Institute of Chemical Sciences and Engineering (ISIC), Basic Science Faculty (SB), École Polytechnique Fédérale de Lausanne (EPFL) Valais/Wallis, Energypolis, Rue de l'Industrie 17, CH-1951 Sion, Switzerland

2. Empa Materials Science & Technology, CH-8600 Dübendorf, Switzerland

3. GRZ technologies SA, CH-1772 Grolley, Switzerland

\*Corresponding author: liping.zhong@epfl.ch

### Abstract

The conversion of CO<sub>2</sub> and green hydrogen to methane with high selectivity via Sabatier reaction has attracted much attention for replacing the natural gas fuel of clean fuel. This process validates not only the application of H<sub>2</sub> green fuel but also re-utilization of CO<sub>2</sub>. [1] However, the high efficiency of CO<sub>2</sub> methanation requests well-designed reactor and idealistic catalyst material. An idealistic CO<sub>2</sub> methanation catalyst needs to be active and selective at low temperature and meanwhile has a long life-time for the utilization. [2] In this work, we demonstrate the strategy and process for designing and producing an idealistic catalyst for a CO<sub>2</sub> methanation pilot of 200KW. The process includes the selection of active metal phase and support, the development of economic synthesis process and the scale-up production. As shown in Figure 1, our lab designed and synthesized catalyst has shown a superior reactivity compared to the commercial catalyst.

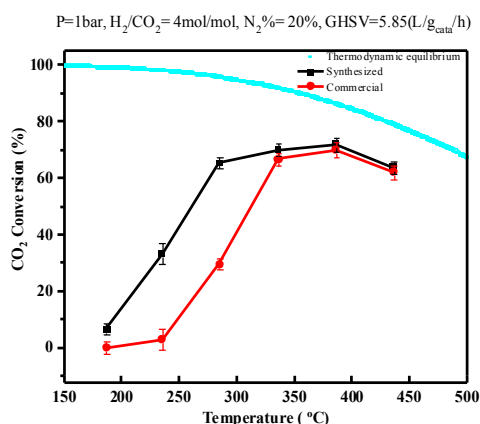


Figure 1. The CO<sub>2</sub> light-off conversion of synthesized and commercial catalysts evaluated at different temperatures.

In a scientific view, we have also demonstrated that the CO<sub>2</sub> conversion and CH<sub>4</sub> selectivity is significantly affected by the metal-support interaction of catalyst and the metal particle size. [3] [4] Herein, we have developed a synthesis method for tuning the particle size and the interaction between metal and support. A series of characterization methods were used to understand the mechanism.

### References

- [1] Ashok, J. et al. A review of recent catalyst advances in CO<sub>2</sub> methanation processes. *Catalysis Today* 356, 471–489 (2020).
- [2] Mutschler, R., Moiola, E., Luo, W., Gallandat, N. & Züttel, A. CO<sub>2</sub> hydrogenation reaction over pristine Fe, Co, Ni, Cu and Al<sub>2</sub>O<sub>3</sub> supported Ru: Comparison and determination of the activation energies. *Journal of Catalysis* 366, 139–149 (2018).
- [3] Chen, S. et al. Raising the CO<sub>x</sub> Methanation Activity of a Ru/γ-Al<sub>2</sub>O<sub>3</sub> Catalyst by Activated Modification of Metal-Support Interactions. *Angewandte Chemie - International Edition* 59, 22763–22770 (2020).
- [4] Kwak, J. H., Kovarik, L. & Szanyi, J. CO<sub>2</sub> reduction on supported Ru/Al<sub>2</sub>O<sub>3</sub> catalysts: Cluster size dependence of product selectivity. *ACS Catalysis* 3, 2449–2455 (2013).



Liping ZHONG

Liping Zhong is a postdoc researcher in Laboratory of Materials for Renewable Energy (LMER) at EPFL working with Professor Andreas Züttel. She was born in 1992 in Yunnan, China. She received her B.S. in Environmental Engineering from the University of Jinan in 2014 and her Master's training in Environmental Engineering in Kunming University of Science and Technology from 2014 to 2017. She has obtained her PhD degree in University of Strasbourg in 2020 under the supervision of Dr. Zafeiratos. Since her Master's study, she has been working in the field of transition-metal-based catalysts for CO and CO<sub>2</sub> conversion in H<sub>2</sub> atmospheres. In particular, she has mastered advanced technologies for designing and monitoring active phase of catalyst under real reaction conditions. Currently, she is contributing to design and synthesis of catalysts for CO<sub>2</sub> methanation in a pilot scale.

## H<sub>2</sub>-BARBEQUE & H<sub>2</sub>-CREMATION, BYPASSING FUEL-CELL CONVERSION ON ROUTE TO STAND-ALONE & SUBSIDIES FREE HYDROGEN ENERGY ECONOMY.

Henning Zoz<sup>1</sup>, Shengyu Lai<sup>2</sup>, Albert Hesse<sup>3</sup>

<sup>1</sup>Zoz Group, Wenden, Germany,

<sup>2</sup>Zhongshan Guanjian Metal Products Co., Ltd, Zhongshan City, China,

<sup>3</sup>Albert Hesse Familienstiftung, Wenden, Germany

Almost 10 years ago, Zoz was nominated for the German Environmental Award (2013) with Power-to-Gas-Fuel (P2G2F®). Since gasoline and diesel represent the cost-peak in fossils, P2G2F® was and is expected to becoming one of the first economic applications in hydrogen energy technology. Still today, this is not achieved, the diesel- engine remains the most economic and ecologic drive system of mankind. P2G2F® particularly fails at the still too high reconversion cost utilizing fuel-cells. Hydrogen for fueling combustion engines fails on the cost of the required pre-compression, the hydrogen turbine additionally on the high-temperature materials that are either not or only available at very high cost. ODS/NFA materials from nuclear fusion (19YAT, 20YAI and 14YWT, namely Zoz-PM2000, PM2017 and PM2018) may help in near future. Hydrogen transportation sector, even after decades, does not see any significant products that can stand without permanent subsidies and/or political market interventions, which is not acceptable. No matter if the CO<sub>2</sub>-szenario is true or fairytale, fossils are too costly and too valuable to just burn away.

### Power Plant + Hydrogen = H2F2Go = human, efficient and environmentally friendly cremation

If reconversion is still too costly, for the time being, technologies where this is not required, are most attractive. In result, the inventions Power Plant and H2F2Go (DE 10 2022 122 862 + 863 # 08.09.2022) describing CO<sub>2</sub>-free Hydrogen cremation, were claimed where Hydrogen is replacing fossil gas in a burner to producing heat. Since late 2022, modern industrial countries such as Germany are worried about "getting through winter", which also describes an unprecedented high demand for energy self-sufficient systems for all areas of life.

### HydrogenGasgrill + Electrolyser + H2Tank2Go® = Power to Gas to Heat + Power

Addressing this additional eco-market demand, the invention Hydrogen Gasgrill with Electrolyser (H2Grill2Go # 07.12.2022) was claimed where again Hydrogen is replacing fossil fuel to producing heat but also provides energy for mobility and home-heating from multiple small solid-state tanks H2Tank2Go®. Power is provided by photovoltaic and wind energy via a buffer battery, rainwater quality is sufficient, only sun, wind and rain are needed. Once applying ideal H<sub>2</sub> combustion, even rainfall is converted into purest water. All three inventions require neither electricity for an electric drive motor nor a fuel gas at correspondingly high volumetric energy density in order to feed a combustion engine. Pressurized storage of hydrogen in these cases is not an option due to high compression cost. Stand-

alone clean replacement is not expected to require any economic subsidies, given market-drivers should be sufficient.



Fig. 1 Powder manufacturing installations at Zoz

Virtually bypassing so far insuperable barriers, the combination of a thermoprocessing plant with regenerative energy generation, electrolysis, H<sub>2</sub>-solid-state storage (virtually pressureless) and H<sub>2</sub>-burner (P2G2H, H=heat), H<sub>2</sub>-Cremation and H<sub>2</sub>-Grill can therefore serve as an economically operated bridging technology at enormous importance.

### References

- [1] joint patent-applications 08.09.2022: <https://gmbh.zoz.de/patents/>
- [2] joint patent-application 07.12.2022: <https://gmbh.zoz.de/patents/>



Henning ZOZ

Dr. (IPN) Henning Zoz was born 1.4.1964, is the CEO of Zoz Group, headquartered at Wenden. Zoz manufactures process engineering equipment as well as nanostructured materials for nanotechnology from nuclear to hydrogen and so in electromobility. Zoz was Professor in Mexico & Japan till 2014, in 2011 elected in South Westfalia as the Manager of the Year and holds multiple patents & awards. Zoz is married, 58 years old and father of five children.

# **SCIENCE OF HYDROGEN & ENERGY AWARD**

The “Science of Hydrogen & Energy” award is a prize, just similar to the Nobel prize, for an extraordinary contribution to the sciences of hydrogen. The aim is to award a prize to a distinct scientist for his scientific work of a life time.

2007



**Prof. Dr. Ronald Griessen**

2008



**Prof. Dr. Louis Schlapbach**

2009



**Dr. Gary Sandrock**

2009



**Prof. Dr. Jens Norskov**

2010



**Prof. Dr. Rüdiger Bormann †**

2011

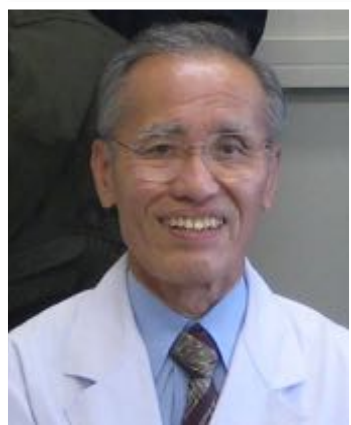


**Prof. Dr. Ivor Rex Harris †**

2012



**Prof. Dr. Rainer Kirchheim**



**Prof. Dr. Koji Hashimoto**



**Prof. Dr. Mogens MOGENSEN**

2013



**Mr. Katsuhiko HIROSE**

2014



**Prof. Dr. Hans GEERLINGS**

2014



**Prof. Dr. Qidong WANG †**

2014



**Prof. Dr. Andreas ZÜTTEL**

2015



**Prof. Dr. Bernard DAM**

2015



**Prof. Dr. Shin-Ichi ORIMO**

2015



**Dr. Michael HIRSCH**

2015



**Prof. Dr. Bjørn HAUBACK**

2016



**Dr. Young Whan CHO**

2016



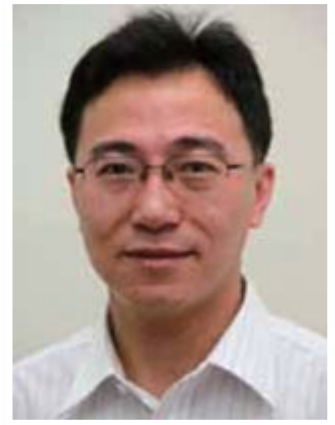
**Prof. Dr. Craig JENSEN**

2016



**Prof. Dr. Torben R. JENSEN**

2016



**Prof. Dr. Min ZHU**

2017



**Prof. Dr. Ping CHEN**

2017



**Dr. Robert BOWMAN**

2018



**Prof. Dr. Michael GRÄTZEL**

2019



**Prof. Dr. Henning ZOZ**

2020



**Dr. Martin DORNHEIM**

2020



**Dr. Michael LATROCHE †**

## SCIENCE OF HYDROGEN & ENERGY AWARD 2023



**Prof. Dr. Robert SCHLÖGL**

Prof. Dr. Robert Schlögl (born February 23, 1954) has been Director at the Fritz Haber Institute of the Max Planck Society, Berlin since 1994 and since 2011 Founding Director and Managing Director at the Max Planck Institute for Chemical Energy Conversion (MPI CEC), Mülheim an der Ruhr, Germany.

Robert Schlögl is a chemist and catalysis researcher. His research focuses on heterogeneous catalysis and materials for energy storage concepts. With his work he has contributed to a new understanding of catalytically active materials. Most recently, he has been working on future energy systems and the complex challenges of the energy transition.

Robert Schlögl and his team research energy conversion processes in nature and the importance of catalysts in these processes. It is about questions of generation, storage and transport of energy. In nature, energy is stored through photosynthesis. In the process, carbon dioxide and water are converted into organic molecules such as sugar and oxygen. However, photosynthesis cannot be replicated using synthetic chemistry, the molecules involved are too sensitive.

The scientists around Robert Schlögl therefore want to understand the basic chemical reactions of these processes in order to be able to use them for new energy systems. In individual research projects, for example, they deal with the conversion of

Light into electrical energy, storage materials for hydrogen, the catalytic splitting of water and the further development of fuel cells.

Catalysts play a major role in all of these processes. For example, solar energy cannot be stored without catalytic converters. The aim of Robert Schlögl's research is the development of new, more efficient catalysts. He attaches great importance to the sustainability of the processes. Substances used as catalysts must be available and accessible in sufficient quantities on earth. He has also developed a process that could be used to significantly reduce energy consumption in the chemical industry using carbon nanomaterials. The chemical raw material styrene can thus be produced more energy-efficiently than before.

In his research, Schlögl works in an interdisciplinary manner and combines scientific model studies with the high-performance systems of technical catalysis. He developed new methods with which dynamic phenomena at interfaces can be observed. As a result, catalysts for industry can be developed more effectively.

# SCIENCE OF HYDROGEN & ENERGY AWARD 2023



**Prof. Dr. Berend Smit**

Prof. Dr. Berend Smit (born November 8, 1962) received an MSc in Chemical Engineering in 1987 and an MSc in Physics from the Technical University in Delft (the Netherlands). He received in 1990 cum laude Ph.D. in Chemistry from Utrecht University (the Netherlands). He was a (senior) Research Physicist at Shell Research from 1988-1997, Professor of Computational Chemistry at the University of Amsterdam (the Netherlands) 1997-2007. In 2004 Berend Smit was elected Director of the European Center of Atomic and Molecular Computations (CECAM) in Lyon France. In 2007 he was appointed Professor of Chemical Engineering and Chemistry at U.C. Berkeley and Faculty Chemist at the Materials Sciences Division, Lawrence Berkeley National Laboratory.

Since July 2014, he is a full professor at EPFL.

Berend Smit's research focuses on the application and development of novel molecular simulation techniques, with an emphasis on energy-related applications.

Together with Daan Frenkel he wrote the textbook [Understanding Molecular Simulations](#) and together with Jeff Reimer, Curt Oldenburg, and Ian Bourg, the textbook [Introduction to Carbon Capture and Sequestration](#).

Carbon Capture is the topic I started working on after I moved to Berkeley. Separating CO<sub>2</sub> from flue gasses is an important topic, much more important than most people realize. Our addiction to fossil fuels has caused alarmingly high CO<sub>2</sub> levels in the atmosphere. As it is very unlikely we will stop using fossil fuels in the coming years, Carbon Capture and storage is the only way to mitigate an even further increase in CO<sub>2</sub> levels.

Our research focuses on using molecular simulations to find the optimal material for carbon capture. At present we focus on metal organic frameworks. These materials are ideal for molecular simulations. We know the crystal structure and one can envision many more materials than one can realistically synthesize. In addition, the chemistry in these materials is very different from what our intuition tells us. In short, much work exiting work to do.

A few highlights were our molecular simulations were able to give us a better understanding of the properties of materials that are of interest for carbon capture

Which MOF is the best for Carbon Capture? With our molecular simulations we wanted to screen millions of materials to find the best for carbon capture, but before we could do this we needed a metric to compare two materials. Finding such a metric was not easy, but with some help from EPRI we found a good metric that allowed us to screen millions of zeolites. In our [Nature Materials](#) article you see how the best zeolite looks like

MTV-MOFs are MOFs synthesized with different linkers, but the conventional experimental methods do not allow us to tell the exact location of these linkers. In a [Report in Science](#) we describe how we could solve this issue of apportionment using a combined NMR and computational study.

An example of how different the chemistry in some of the MOFs can be, we found out by looking at the adsorption of CO<sub>2</sub> in MOF-74. This material has a so-called open metal site. In MOFs without such open metal sites the force fields in the literature predict the adsorption isotherms very well, but the same force fields are off by two orders of magnitude if there is an open metal site. With [Laura Gagliardi's group](#) in Minnesota we developed a method to derive force fields from quantum chemistry calculations. Our [Nature Chemistry](#) publication shows that this approach gives a good prediction of these isotherms.



## BEST POSTER AWARD

2007



**Ms. Alondra TORRES TRUEBA**

2012



**Mr. Andreas BLIERSBACH**

2013



**Mr. Moreno DE RESPINIS**

2014



**Mr. Yixiao FU**

2015



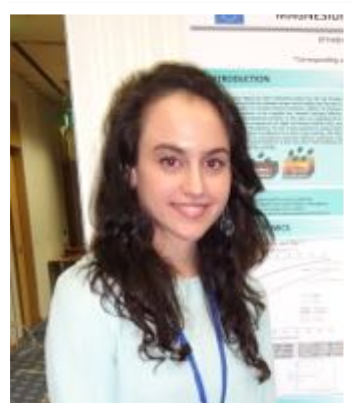
**Dr. Shunsuke KATO**

2015



**Mr. Nikolai BILISKOV**

2016



**Ms. Efi HADJIXENOPHONTOS**

2016



**Ms. Guanqiao LI**

2017



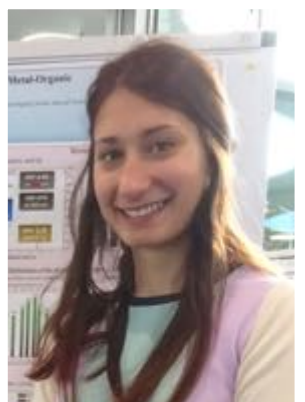
**Ms. Marina CHONG**

2017



**Ms. Katherine HURST**

2018



**Ms. Stavroula (Alina)  
KAMPOURI**

2019



**Dr. Young-Su LEE**

2019



**Mr. Marco CALIZZI**

2020



**Mr. Masaaki KITANO**

# PARTICIPANTS

Name	Address	Work phone, mobile, email
Ms. Zohreh AKBARI	EPFL Rue de l'Industrie 17 1950 Sion, Switzerland	T: +41 21 693 3857 m: +41 77 905 0632 e: zohreh.akbari@epfl.ch
Dr. Mark ALLENDORF	Sandia National Laboratories 7011 East Avenue 94550 Livermore, United States	T: +1 (925) 294 2895 m: e: mdallen@sandia.gov
Dr. Konstantinos BARDIS	GRZ Technologies SA Route de la Gruyere, 23 1700 Fribourg, Switzerland	T: m: +41 76 529 2772 e: konstantinos.bardis@grz-technologies.com
Dr. Andreas BORGSCHULTE	Empa Überlandstrasse 129 8600 Dübendorf, Switzerland	T: m: e: andreas.borgschulte@empa.ch
Prof. Dr. Susana GARCIA-LOPEZ	Heriot-Watt University, Institute of Mechanical Process and Energy Engineering Room 2.12, James Nasmyth Building EH14 4AS Edinburgh, UK	T: +44 131 451 8083 m: +44 7476 93 0920 e: s.garcia@hw.ac.uk
Prof. Dr. Björgvin HJÖRVARSSON	Uppsala University Box 516 751 20 Uppsala , Sweden	T: m: +46 70 425 0715 e: bjorgvin.hjorvarsson@physics.uu.se
Mr. Riku HORIE	EPFL FMEL Vortex, Route de Praz-Veguey 29 - BP 927, 1022 Chavannes-pres-Renens 1015 Lausanne, Switzerland	T: m: e: dortohoriesv20@gmail.com
Mr. Emil Høj JENSEN	University of Oslo Gunnar Randers Vei 19 2007 Kjeller, Norway	T: m: +47 935 83 271 e: emilhoj@its.uio.no
Mr. Selim KAZAZ	Empa Überlandstrasse 129 8600 Dübendorf, Switzerland	T: m: e: selim.kazaz@empa.ch

Name	Address	Work phone, mobile, email
Mr. Youngdon KO	EPFL Rue de l'Industrie 17, LMER 1950 Sion, Switzerland	T: +41 21 695 8215 m: e: youngdon.ko@epfl.ch
Mr. Cedric KOOLEN	EPFL Rue de l'industrie 17 1950 Sion, Switzerland	T: m: +41 76 202 5649 e: cedric.koolen@epfl.ch
Ms. Yasemen KUDDUSI	EPFL Rue de l'Industrie 17 1951 Sion, Switzerland	T: m: +41 78 215 5734 e: yasemen.kuddusi@epfl.ch
Mr. Rui LI	GRZ technologies SA Route du P.A.A 27 1772 Grolley, Switzerland	T: m: +41 78 249 1100 e: li.rui@grz-technologies.com
Mr. Dima MUKHIN	accompanying Kun ZHAO  , USA	T: m: e:
Prof. Dr. Shin_Ichi ORIMO	Tohoku University 2-1-1 Katahira, Aoba-ku 980-8577 Sendai, Japan	T: m: e: orimo@imr.tohoku.ac.jp
Dr. Jihye PARK	Hyundai Motor Company Uiwang-si, Gyeonggi-do 16082, Korea, Republic of	T: m: e: jihyepark@hyundai.com
Mr. Akhil PENMATHSA	GRZ Technologies SA Route Joseph Chaley 41 1700 Fribourg, Switzerland	T: m: +41 78 241 7324 e: akhil96ajith97@gmail.com
Ms. Thi Ha My PHAM	EPFL Rue de l'Industrie, 17 1950 Sion, Switzerland	T: m: +41 78 799 5530 e: thi.pham@epfl.ch
Dr. Claudio PISTIDDA	Helmholtz-Zentrum hereon GmbH, Dept. Materials Design, Inst. of Hydrogen Technology Max-Planck-Str. 1 21502 Geesthacht, Germany	T: m: e: claudio.pistidda@hereon.de

<b>Name</b>	<b>Address</b>	<b>Work phone, mobile, email</b>
Ms. Jessica RUFFINER	EPFL Chemin Saint Marc 7 1700 Fribourg, Switzerland	T: m: +41 77 445 6434 e: jessica.ruffiner@unifr.ch
Prof. Sabrina SARTORI	University of Oslo Welhavens gate 21A 0316 Oslo, Norway	T: m: +47 98 676 975 e: sabrina.sartori@its.uio.no
Mr. Steven SCHENK	LO - EPFL Rue de carouge 21 1205 Genève, Switzerland	T: +41 21 693 7605 m: e: steven.schenk@epfl.ch
Prof. Dr. Robert SCHLOEGL	Fritz-Haber-Institut der Max-Planck- Gesellschaft Faradayweg 4-6 14195 Berlin, Germany	T: +49 30 8413 4409 m: +49 151 2922 6328 e: acsek@fhi-berlin.mpg.de
Ms. Yuanyuan SHANG	Helmholtz-Zentrum Hereon Max-Planck-Straße 1 21502 Geesthacht, Germany	T: +49 (4152) 87 2687 m: e: yuanyuan.shang@hereon.de
Prof. Dr. Chia-Chieh SHEN	Yuan Ze University No. 135, Yuandong Rd., Taoyuan City, Taiwan, China	T: m: e: ccshen@saturn.yzu.edu.tw
Prof. Dr. Berend SMIT	EPFL Rue de l'industrie 17 1950 Sion, Switzerland	T: m: e: berend.smit@epfl.ch
Mr. Tai SUN	GRZ Technologies SA P.A.A 27 1772 Grolley, Switzerland	T: m: +41 78 213 1537 e: tai.sun@grz-technologies.com
Ms. Ivana SUTER	EPFL Rue dell'industrie 17 1950 Sion, Switzerland	T: +41 21 695 8304 m: +41 78 916 6904 e: ivana.suter@epfl.ch
Ms. Ulrike TRACHTE	Hochschule Luzern – Technik & Architektur, Maschinentechnik Technikumstrasse 21 CH-6048 Horw Schweiz	T: +41 41 3493 249 e: ulrike.trachte@hslu.ch

<b>Name</b>	<b>Address</b>	<b>Work phone, mobile, email</b>
Dr. Yunting WANG	EPFL LMER Rue de l' industrie 17 LMER 1950 Sion, Switzerland	T: m: e: yunting.wang@epfl.ch
Mr. Manhui WEI	EPFL Rue de l'Industrie 17, LMER 1950 Sion, Switzerland	T: m: +41 76 239 7360 e: manhui.wei@epfl.ch
Dr. Heena YANG	K-water Resource Corporation, Carbon Neutrality Planning 200, Sintanjin-ro, Daedeok-gu 34114 Daejeon, South Korea	T: +82 10 8985 0729 e: heena.yang@kwater.or.kr
Mr. Kataoka YUTA	The University of Tokyo 5-1-5 Kashiwanoha Kashiwa, Japan	T: m: e: y.kataoka@issp.u-tokyo.ac.jp
Dr. Jinqiu ZHANG	Harbin Institute of Technology No.92 Xidazhi St. Harbin, China	T: m: +86 1394 518 9262 e: zhangjinqiu@hit.edu.cn
Dr. Kun ZHAO	University of Washington 747 16th Ave E 98125 Seattle, United States	T: +1 206 643 9579 m: e: quen.zhao@gmail.com
Dr. Liping ZHONG	EPFL Rue dell'industrie 17 1950 Sion, Switzerland	T: m: +41 78 220 0832 e: liping.zhong@epfl.ch
Dr. Henning ZOZ	ZOZ GmbH Maltoz Strasse Wenden, Germany	T: +49 276 297 560 m: e: office@zoz.de
Prof. Dr. Andreas ZÜTTEL	EPFL Valais/Wallis I17 1 G1, Rue de l'Industrie 17 1950 Sion, Switzerland	T: +41 21 695 8210 m: +41 79 484 2553 e: andreas.zuettel@epfl.ch

# Information

## HISTORY OF THE INTERNATIONAL SYMPOSIUM HYDROGEN & ENERGY

15<sup>th</sup> International Symposium Hydrogen & Energy, January 24<sup>th</sup> - 29<sup>th</sup> 2021 was postponed to 22. - 27. January 2023 due to the global Corona virus situation.



14<sup>th</sup> International Symposium Hydrogen & Energy, January 5<sup>th</sup> - 10<sup>th</sup> 2020 combined with 1<sup>st</sup> Int. Symposium Hydrogenomics  
Hotel Monterey Edelhof, Sapporo, Japan  
Hydrogen & Energy Award for Martin DORNHEIM, Michele LATROCHE  
Best poster award for Masaaki KITANO



13<sup>th</sup> International Symposium Hydrogen & Energy, January 20<sup>th</sup> - 25<sup>th</sup> 2019  
GYEONG WON JAE AMBASSADOR, 200, Techno park-ro, Yeonsu-gu, Incheon, Korea  
Hydrogen & Energy Award for Henning ZOZ, Germany  
Best Poster Award sponsored by HYDROPOLE for Young-Su LEE, KIST, Korea and Marco CALIZZI, EPFL, Switzerland



12<sup>th</sup> International Symposium Hydrogen & Energy February 11<sup>th</sup> - 16<sup>th</sup> 2018  
SwissTech Convention Center, EPFL, Lausanne, Switzerland  
Hydrogen & Energy Award for Michael GRÄTZEL  
Best Poster Award for Stavroula (Alina) KAMPOURI



11<sup>th</sup> International Symposium Hydrogen & Energy February 26<sup>th</sup> - March 3<sup>rd</sup> 2017  
HILTON WAIKOLOA VILLAGE, 9-425 Waikoloa Beach Dr, Waikoloa Village, HI 96738, USA  
Hydrogen & Energy Award for Robert BOWMAN and Ping CHEN  
Best Poster Award for Marina CHONG and Katherine HURST



10<sup>th</sup> International Symposium Hydrogen & Energy 21. - 25. February 2016  
Laforet Zao Resort & Spa, 2-1 Nanokahara Togatta Onsen, Zao Town, Katta-gun, Miyagi Prefecture  
Opening talk by Andreas ZÜTTEL, "Do we need hydrogen?"  
Hydrogen & Energy Award for Young Whan CHO, Min ZHU, Craig JENSEN and Torben R. JENSEN  
Best Poster Award for Efi HADJIXENOPHONTOS and Guanqiao LI



9<sup>th</sup> International Symposium Hydrogen & Energy 25. - 30 January 2015  
Hotel Seeblick, Emmetten, Switzerland  
Opening talk by Klaus LACKNER, 'Closing the Carbon Cycle with Synthetic Fuels and Capture of Carbon Dioxide from Ambient Air'  
Hydrogen & Energy Award for Bernard DAM, Shin-Ichi ORIMO, Michael HIRSCHER, Bjørn HAUBACK  
Best Poster Award for Shunsuke KATO and Best H2FC Poster award for Nikola BILISKOV



8<sup>th</sup> International Symposium Hydrogen & Energy, 16. - 21. February 2014  
Xinghu Dadao, Zhaoqing, 526060 Guangdong, P. R. China  
Opening talk by Andreas ZÜTTEL, 'Closing the Cycle with Hydrogen'  
Hydrogen & Energy Award for QiDong WANG and Andreas ZÜTTEL  
Best Poster Award for Yixiao FU "Study on the hydrogen exchange behavior in the metal hydride-LiBH4 composite"



7<sup>th</sup> International Symposium Hydrogen & Energy, January 21 - 25, 2013  
Seminar- und Wellnesshotel Stoos, Switzerland  
Opening talk by Katsuhiko HIROSE, 'Hydrogen as energy vector for fuel for future transport and energy optimization'  
Hydrogen & Energy Award for Katsuhiko HIROSE and Hans GEERLINGS  
Best Poster Award Moreno DE RESPINIS



6<sup>th</sup> International Symposium Hydrogen & Energy, January 22 - 27, 2012  
Seminar- und Wellnesshotel Stoos, Switzerland  
Opening talk by Mogens Bjerg MOGENSEN, 'Electrolysis and Recycling of Co2 into Co2-neutral Fuels'  
Hydrogen & Energy Award Mogens Mogenson  
Best Poster Award Andreas BLIERSBACH





5<sup>th</sup> International Symposium Hydrogen & Energy, January 23 - 28, 2011  
Seminar- und Wellnesshotel Stoos, Switzerland  
Opening talk by Paul EKINS, "Hydrogen Energy: Policy Responses to Economic and Social Challenges"  
Hydrogen & Energy Award Koji HASHIMOTO  
Best Poster Award Alondra TORRES TRUEBA



4<sup>th</sup> Symposium Hydrogen & Energy, January 24 - 29, 2010  
Hotel Hirschen, Wildhaus, Switzerland  
Opening talk by Boulouchos Konstantinos, "PROPERTIES, RISKS AND POTENTIAL OF HYDROGEN AS FUEL FOR COMBUSTION ENGINES"  
Hydrogen & Energy Award Rüdiger BORMANN, Rex HARRIS and Rainer KIRCHHEIM



3<sup>rd</sup> Symposium Hydrogen & Energy, January 25 - 30, 2009,  
Hotel Alpenblick in Braunwald, Switzerland  
Opening talk by Heinz Berke, "Metal-Induced and Metal-Free Reactions of Dihydrogen as a Base for Chemical Hydrogen Storage"  
Hydrogen & Energy Award Gary SANDROCK and Jens NORSKOV

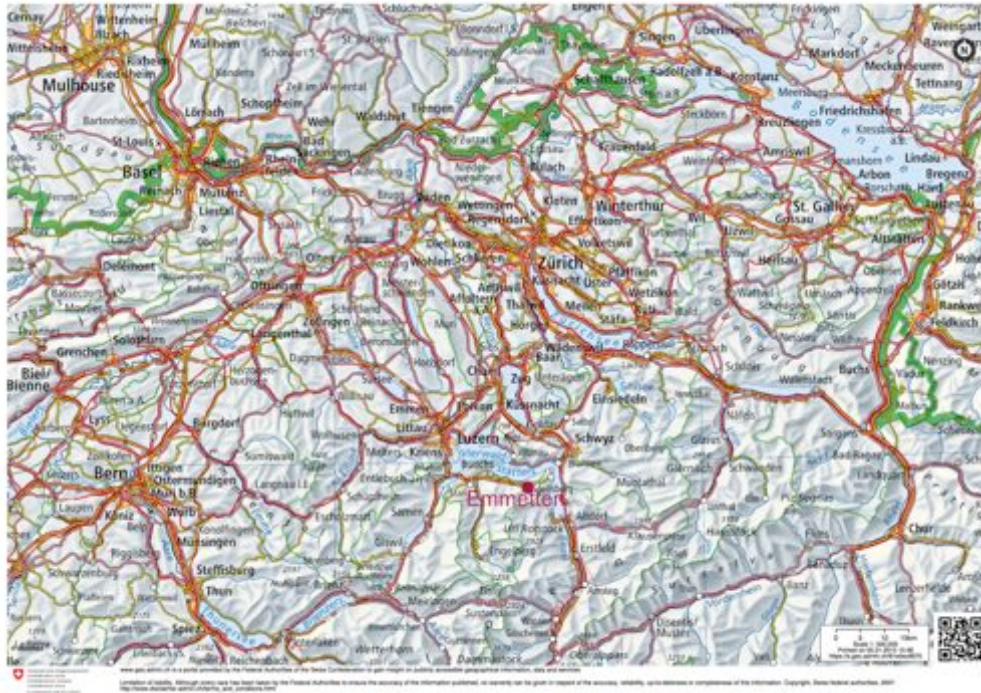


2<sup>nd</sup> Symposium Hydrogen & Energy, January 21 - 25, 2008  
Hotel Alpenblick in Braunwald, Switzerland  
Opening talk by Louis SCHLAPBACH "History of Hydrogen"  
Hydrogen & Energy Award Louis SCHLAPBACH

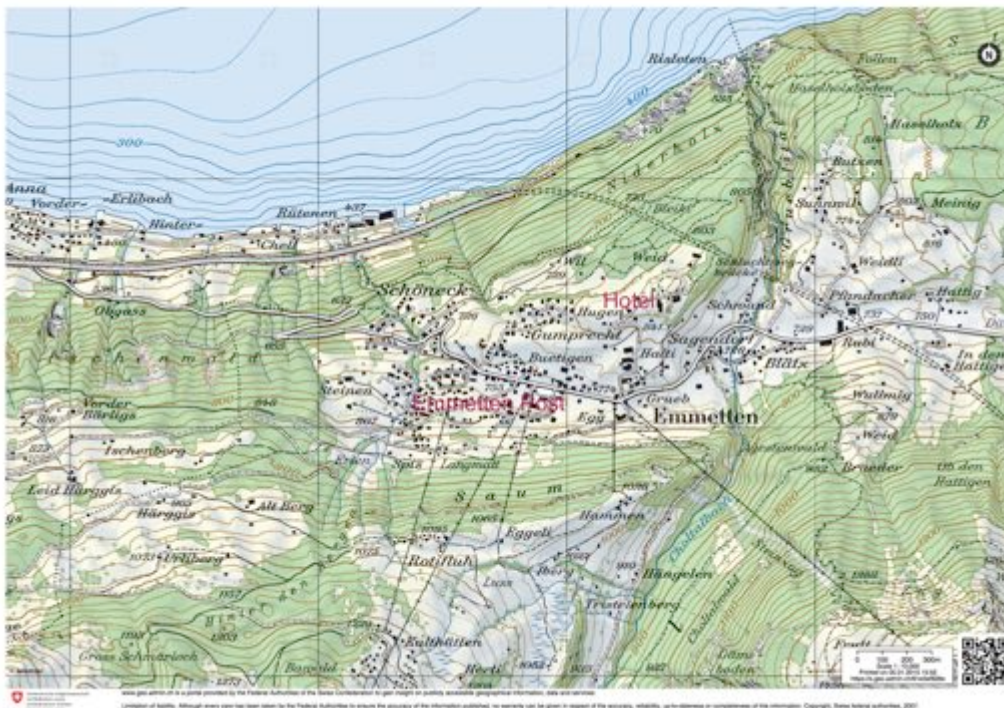


1<sup>st</sup> Symposium Hydrogen & Energy, January 21 - 25, 2007  
EMPA, Dübendorf, Switzerland  
Opening talk by Andreas ZÜTTEL "Hydrogen and Energy"

# MAPS






Map from Zürich (upper left corner) to Emmetten (center bottom)



Map of the region Emmetten

# Travel to Emmetten from Zürich airport:

Please go to the ticket counter in the airport and ask for a ticket to Emmetten (roundtrip). Please also ask the person at the counter to print you the timetable for your connection e.g.:








Station/Stop	Date	Time	Platform	Travel with	Comments
Zürich Flughafen	So 25. 1. 15	dep 13:38	3	IR 3268	Direction: Luzern 
Luzern		arr 14:51	6		☺
Luzern		dep 15:10	12	IR 2976	Direction: Engelberg 
Stans		arr 15:23	1		
Stans		dep 15:26		Bus 311	Direction: Seelisberg 
Emmetten Post		arr. 15:57			

Duration: 2:19; runs daily

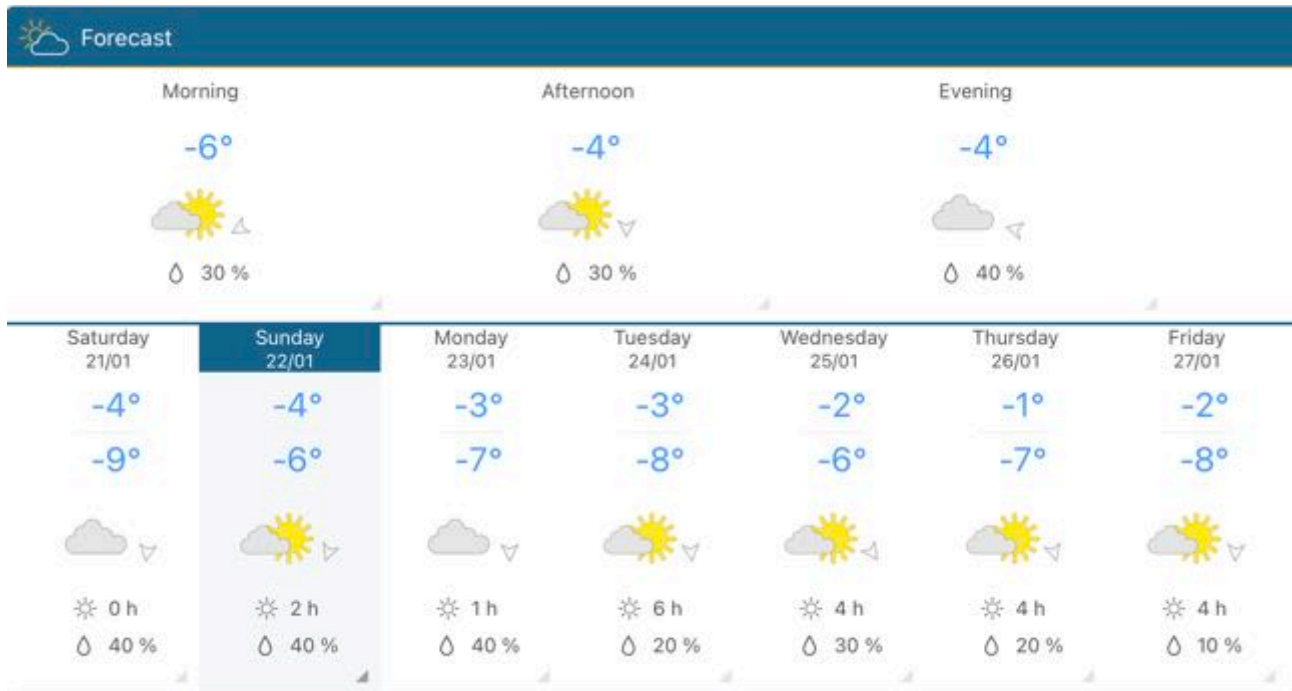
<http://www.sbb.ch/en/home.html>



## EMERGENCY TELEPHONE NUMBERS

		country code for Switzerland +41...
	POLICE	117
	FIRE FIGHTERS	118
	AMBULANCE	144
	RESCUE HELICOPTER (REGA)	1414
	Ivana SUTER Administration / Organizer	+41 78 916 69 04
	Andreas ZÜTTEL Organizer	+41 79 484 2553
	SEEBLICK HÖHENHOTEL Hugenstrasse 24 CH-6376 Emmetten email: <a href="mailto:info@hotelseeblick.ch">info@hotelseeblick.ch</a> URL: <a href="http://www.hotelseeblick.ch">http://www.hotelseeblick.ch</a>	+41 41 624 41 41

# WEATHER in Emmetten



Temperature [°C]



# SOCIAL EVENTS



## Rütli

Bus to Beckenried, Ship to the "Tellplatte" and short walk to "Rütli".  
Gided tour with information about the cradle of Switzerland.



## Skiing

Free skiing, skipass will be provided  
(depending on the snow condition)



## Sledding

Free sledding from Stockhütte  
(depending on the snow condition)



## Snowwalk

Guided tour  
(depending on the snow condition)







# HISTORY OF SWITZERLAND

## From the beginnings to the present.

**Much of the territory covered by present-day Switzerland is mountainous. For this reason, the Alpine passes have played a significant role in the development of the country, as have the powers that sought to control these important communication and trade routes.**

**The inaccessible mountains with their particular living conditions provided the area with protection and a great deal of freedom because they made it difficult for foreign powers to enforce their control in the longer term. This enabled the population to develop its own traditions and forms of government. This situation also favoured the neutrality that has been in force since 1515 and which has also served the neighboring countries by forming a safety zone between the European states. The state of Switzerland as we know it today only assumed its current form in 1848. Prior to this time there was no real Swiss history as such; rather, it was the history of the various territories that gradually coalesced up until 1848 in order to form modern-day Switzerland.**

From the beginnings to the Romans

The oldest traces of human existence are about 150,000 years old, while the oldest flint tools that have been found are about 100,000 years old. The territory of the present-day Switzerland developed in a similar way to that of the rest of Europe.

Under Roman influence, 58 BC

In 58 BC, the Mittelland-based Helvetians tried to avoid the Germanic incursion from the west and migrate to the south of France. But Caesar sent them back and settled them as a "buffer people".

Switzerland after the Romans

After the departure of the Romans, the Alemanni gradually colonised Switzerland from the north. Western Switzerland was ruled by the Burgundians, while the Alpine regions were dominated by local Gallo-Roman rulers.

The rise of Christianity, 6th century

Initially brought to Switzerland by the Romans, Christianity only really started to spread in the 6th century when the wandering monks from Ireland began establishing monasteries.

Under German rule

Supported by noble families, non-aristocratic landowners, abbots and bishops, the German Emperor Conrad II ruled over large parts of western and central Europe – and united the Swiss territories in 1032.

Switzerland in the late Middle Ages



1291 is traditionally regarded as being the founding year of the Confederation – this was when three rural valley communities banded together in order to be better prepared for attacks from the outside.

In the 14th and 15th centuries they developed a loose federation with rural and urban members. By the end of the 15th century it was strong enough to affect the balance of power in Europe. Various wars were fought in which the Confederates displayed courage and ingenuity, and they gained a reputation as a formidable opponent in combat. The Confederation was enlarged in various ways with some areas joining voluntarily and as equal members while others were more or less forced. The members of the Confederation mainly administered the affairs of their own regions but representatives of each area also met regularly to discuss issues of common interest.

Rise of the Swiss Confederation

The desire for freedom on the part of rebellious miners in their ancestral country prompted the Habsburgs to enforce their claims to power by the force of arms. In the process they suffered heavy losses - while the Confederates grew increasingly confident.

Dissension and the Burgundian Wars

The relationships between the Confederates and other parts of what is now Switzerland were very diverse. At the instigation of Bern and of the French king, the Confederates went to war against the Burgundian duke, Charles the Bold, who suffered a crushing defeat in three battles.

Independence and the end of expansion	Following the success of the Swabian wars the interest of those in central Switzerland now turned towards the south. The Confederates' dreams of having great power finally came to an end with their crushing defeat at Marignano.
Reformation and the 17th century	The 16th century in Western Europe was dominated by the Reformation, a movement which divided western Christianity into two camps. Although the riots and destruction were fought on a religious level, this reflected, above all, the desire for social change and the social tensions that existed primarily between town and country. The 17th century saw three further landmarks in the development of modern-day Switzerland. All came as a result of the 30 Years' War (1618-48). While large parts of Europe were involved in this war, the Confederation remained neutral. An important consequence of the Thirty Years' War was Swiss independence from the Holy Roman Empire, which was formally recognised by the Treaty of Westphalia.
Two Reformers: Zwingli and Calvin	The 16th century was marked by reformations, counter-reformations and religious wars - and also by renewal within the Catholic Church.
Political structure in the 17th century	The rights and freedoms within the Confederation varied greatly depending on the location. There were rural cantons, city cantons, cities dominated by aristocrats, common lordships ruled by bailiffs as well as subject territories.
Thirty Years' War and independence	The Confederation was able to keep out of the Thirty Years' War – had it been involved, it would have led to the collapse of the Confederation due to confessional differences.
Peasant revolts and religious peace	Whereas a currency devaluation led to a peasant uprising, it was the confessional divide that sparked the Villmergen Wars that led to the restoration of a balanced religious peace and an end to Catholic hegemony.
18th and 19th century	In 1798, French troops invaded Switzerland and proclaimed a centralised state. Later, the old cantonal system was restored - albeit in a more centralised form. In 1798, French troops invaded Switzerland and created the centralised Helvetic Republic. For the first time in its history, Switzerland was forced to abandon its neutrality and to provide troops for France. After the Sonderbund War, the foundations for the modern Switzerland were finally laid down with the adoption of the Constitution of 1848. It brought about a more centralised form of government and a single economic area, which put an end to the cantonal rivalries and enabled economic development. Despite this progress, the 19th century was a difficult time for many people in Switzerland. Poverty, hunger and poor job prospects led to a wave of emigration, including to North and South America.
20th century	The 20th century was generally marked by a series of striking developments in the political, economic and social arenas. Domestically there was a shift towards a multi-party system. While at the beginning of the century one party occupied all the positions in the government (Federal Council), there were four parties represented there at the end of the century. Agrarian Switzerland developed into an industrial state with the result that there were more immigrants than emigrants and the standard of living rose significantly. Working conditions and social security steadily improved and there was greater access to a more extensive range of consumer goods. The development of the export sector changed the country's relationship with Europe and the rest of the world. Although Switzerland remained politically neutral – it did not actively participate in either of the two World Wars – neutrality remained the subject of intense debate.



