

## Sustainability

How to cite: *Angew. Chem. Int. Ed.* **2021**, *60*, 20094–20100

International Edition: doi.org/10.1002/anie.202105324

German Edition: doi.org/10.1002/ange.202105324

# Holistic View on Materials Development: Water Electrolysis as a Case Study

Sebastian Klemenz,\* Andreas Stegmüller, Songhak Yoon, Claudia Felser, Harun Tüysüz,\* and Anke Weidenkaff

catalysis · circular economy · OER · sustainability

**Abstract:** In view of rising ecological awareness, materials development is primarily aimed at improving the performance and efficiency of innovative and more elaborate materials. However, a materials performance figure of merit should include essential aspects of materials: environmental impact, economic constraints, technical feasibility, etc. Thus, we promote the inclusion of sustainability criteria already during the materials design process. With such a holistic design approach, new products may be more likely to meet the circular economy requirements than when traditional development strategies are pursued. Using catalysts for water electrolysis as an example, we present a modelling method based on experimental data to holistically evaluate processes.

The pursuit of performance-enhanced functional materials often leads to increased structural complexity at the atomic, micro- and macroscopic scales. While such materials show increased efficiencies with respect to the primary function, their industrial application can be a long time coming. The

gain in efficiency does not outweigh economic factors and associated risks, such as environmental burdens or supply risk for critical materials. The trend in complexity often contradicts the ideas of a Circular Economy (CE), which is becoming increasingly important for society and industry.

Establishing a functioning CE is a complex task, because it requires not only new and sustainable technologies, but also suitable business models and infrastructure (logistics, processing, and communication facilities) to be implemented. It further requires the consent of participants in the economic system. Thus, thorough planning and anticipatory consideration of environmental, economic, and social implications (the “triple-bottom of sustainability”), psychological aspects, specific technical risks, and product design features are necessary.<sup>[1]</sup> Taking into account these aspects, the definition of “improved materials” shifts from “only” high performance to reflect the actual practicality in real CE applications (Figure 1).

In applied materials science, the classical approach of research and development (R&D) is to tune physico-chemical and structural properties (e.g. electronic properties, element composition) to achieve desired functions. These aspects are usually combined forming a figure of merit for materials performance and price.

In this Viewpoint, we elaborate on the combination of traditional materials development strategies and sustainability assessment for research reaching technology readiness level 3 and higher using the example of catalyst design for water electrolysis.

## Catalyst Development: Shifting the Scale

Water electrolysis for the production of green hydrogen currently is a much discussed technology. Hydrogen is a major base chemical and a promising candidate as a clean fuel of the future. The world demand for H<sub>2</sub> in 2018 was ca. 73 000 Mt and it is rising rapidly.<sup>[2]</sup> The demand for electrolysis power supplying H<sub>2</sub> for the German energy sector is estimated to increase up to 71 GW for the generation of 1420 t h<sup>-1</sup> of H<sub>2</sub> in 2030 and 275 GW in 2050.<sup>[3]</sup> German industrial ammonia synthesis supplied with 100% electrolytic hydrogen would need 27.5 TWh a<sup>-1</sup>.<sup>[4]</sup> Thus, in view of the German and European goal of a climate-neutral energy infrastructure,

[\*] Dr. S. Klemenz, Dr. A. Stegmüller, Dr. S. Yoon, Prof. Dr. A. Weidenkaff  
Fraunhofer-Einrichtung für Wertstoffkreisläufe und Ressourcenstrategie IWKS

Aschaffener Str. 121, 64357 Hanau (Germany)

E-mail: sebastian.klemenz@iwks.fraunhofer.de

Dr. S. Klemenz, Prof. Dr. C. Felser

Solid State Chemistry

Max-Planck-Institut für Chemische Physik fester Stoffe

Nöthnitzerstr. 40, 01187 Dresden (Germany)

Priv.-Doz. Dr. H. Tüysüz

Department of Heterogenous Catalysis

Max-Planck-Institut für Kohlenforschung

Kaiser-Wilhelm-Platz 1, 45470 Mülheim an der Ruhr (Germany)

E-mail: tueysuez@kofo.mpg.de

Prof. Dr. A. Weidenkaff

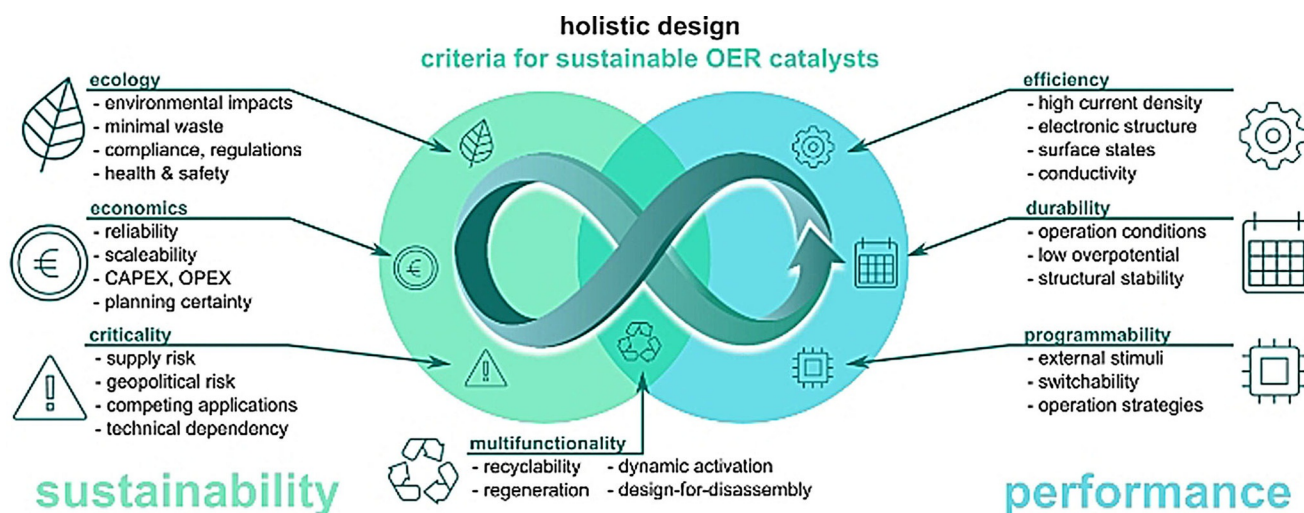
Materials and Resources

Technische Universität Darmstadt

Alarich-Weiss-Straße 2, 64287 Darmstadt (Germany)

Supporting information and the ORCID identification number(s) for the author(s) of this article can be found under:  
<https://doi.org/10.1002/anie.202105324>.

© 2021 The Authors. *Angewandte Chemie International Edition* published by Wiley-VCH GmbH. This is an open access article under the terms of the Creative Commons Attribution Non-Commercial License, which permits use, distribution and reproduction in any medium, provided the original work is properly cited and is not used for commercial purposes.



**Figure 1.** Aspects of sustainability and performance as optimization criteria for OER catalyst development.

the sustainable large-scale production of hydrogen is mandatory.<sup>[5]</sup>



Sebastian Klemenz received his PhD under the supervision of B. Albert at TU Darmstadt in 2017. In the following years, he conducted postdoctoral research at MPI for Chemical Physics of Solids with M. Jansen and C. Felser and at Princeton University with L. Schoop. He became group leader of an Attract Group for Green ICT at Fraunhofer IWKS in 2021.



Andreas Stegmüller studied in Frankfurt, Cambridge, and Marburg and received a PhD in Theoretical Chemistry with R. Tonner for research focussed on surface and interface reactivity from an *ab initio* perspective. Since 2017 he has been developing process modelling methods for multiproperty evaluation in the context of Circular Economy and recycling technology at Fraunhofer IWKS.



Harun Tüysüz gained his PhD in chemistry in the Department of Heterogeneous Catalysis at the Max-Planck-Institute für Kohlenforschung (MPI-KOFO) in 2008 under the supervision of Prof. Ferdi Schüth and then conducted postdoctoral research with Prof. Peidong Yang at the University of California, Berkeley. In 2012 he was appointed head of an independent research group of Heterogeneous Catalysis and Sustainable Energy at the MPI-KOFO. His research group is interested in the design of nanoscale materials for sustainable energy-related catalytic applications. He has received several awards including the DECHEMA Prize 2019 and Forcheurs Jean-Marie Lehn Prize 2020.

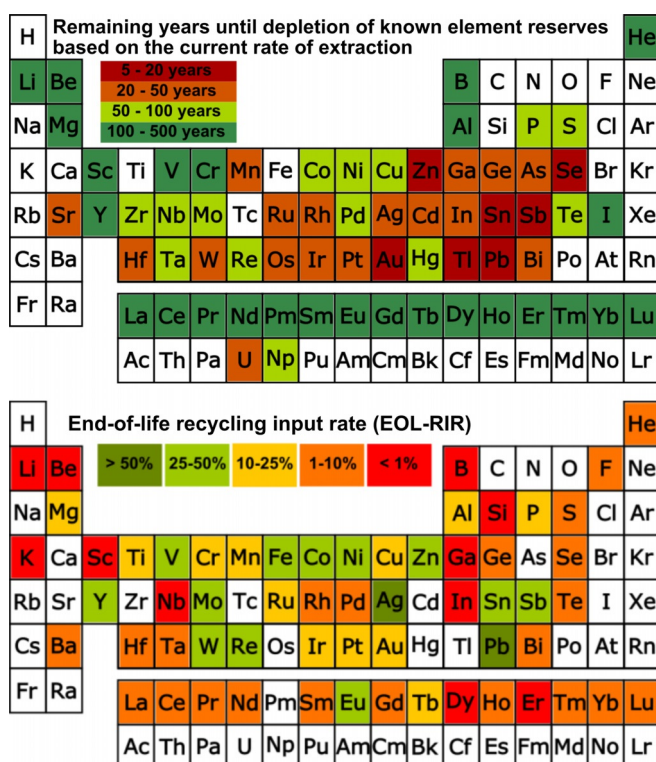
The German government initiative “Wasserstoff-Republik Deutschland”<sup>[6]</sup> put precedence on the challenge of developing methods for green hydrogen production by water electrolysis. The requisite hydrogen evolution (HER) and oxygen evolution reactions (OER) require catalysts to be efficient. A large number of properties are known to influence the performance of OER catalysts, including structural and intrinsic properties as well as the environment of the electrocatalyst.<sup>[7,8]</sup>

While the optimization of these properties is crucial for gaining insights into the physical mechanisms as well as tuning the process yields on the lab scale, for commercial applications further criteria need to be tracked simultaneously. Among these are the production costs, scalability, materials supply, and technical challenges like recyclability as well as the technical compatibility by considering the environmental and geopolitical risks.

So far, commercial water electrolysis has mainly relied on expensive electrode catalysts including the critical platinum group elements. Ir and Ru are used as OER catalysts in most commercial applications.<sup>[8]</sup> The demand for Ir for water electrolysis in Germany by 2030 was estimated with constant loading to be equivalent to one-third of the global Ir production in 2016 (i.e. 2100 of 7100 kg).<sup>[9]</sup> With a fluctuating market price of around 50000 €kg<sup>-1</sup><sup>[10]</sup> and increasing demands in competing applications, the supply situation of Ir (and Ru, Co, rare earths) was ranked as critical by the EU,<sup>[11]</sup> so their usage should be considered in materials design. As shown in Figure 2, the depletion of many elements is further along than we would like to admit.<sup>[12]</sup>

Finding solutions means balancing materials demands while working on closed supply cycles. Thus, efficient materials development should also include intelligent resource management and recycling strategies. In addition to the end-of-life, a holistic approach has to include durability and environmental footprint during operation as well as the catalyst production.

On a global scale, this includes mining, refining, recycling, and transportation. Small gains made by adding materials



**Figure 2.** Periodic tables color coded for the depletion of known elemental (l) and end-of-life recycling input rate (r), respectively, based on data reported elsewhere.<sup>[13]</sup>

complexity might diminish the sustainability or commercial usability of a material, leading to the necessity of lifecycle thinking during development and planning. Including these aspects might change the optimized materials from the most active catalyst to a recyclable material with lower activity, but also lower production cost or supply risk. Such materials are sometimes called *second-best materials*, due to the worse values in traditional figures of merit; however, when viewed holistically, these materials can turn out supreme. Although the holistic view (Figure 1) is not new, mainstream material design has so far changed only marginally.

While clearly performance-driven materials development is crucial to gain understanding of functional mechanisms, we want to stir interest for a parallel way of evaluating materials. This approach is initiated by finding *holistic descriptors* including a many aspects—and developing an appreciation in scientific publishing for second-best materials. Such a descriptor needs an evaluation basis, in this case generalized sustainability assessment and modelling standards.

### Requirements for a Robust Assessment of Sustainability and Performance

To evaluate new technologies—processes, materials, or services—in terms of sustainability, the entire lifecycle needs to be represented. Thus, in *lifecycle management*, highly detailed and consistent models are required to include multiple process steps with features ranging from the global

scale (e.g. supply chains, mining) to the microscopic level (e.g. materials properties, device performance). Naturally, model systems that incorporate these features with the corresponding impact indicators, technical parameters, and materials properties are complex. As it is not feasible for an individual to assess all relevant implications of a product, decisions should be grounded on a multifaceted rationale, which can be provided by comprehensive digital models.<sup>[14]</sup> This is particularly relevant during technology development, while R&D projects accompanied by robust process modeling and multi-criteria evaluation benefit from on-the-fly feedback, supporting, for example, materials or processing choices and, moreover, an increase of mechanistic insight. The criteria for a practical CE extend beyond mere functional performance and include:<sup>[15]</sup>

- 1) reduction of direct environmental (biophysical) impact during production and use (estimated through Life Cycle Assessment (LCA)),
- 2) creation of economic value along all product life stages (e.g. Life Cycle Costing (LCC)),
- 3) social justice in a globalized value chain (e.g. Social LCA),
- 4) awareness and reduction of critical raw materials such as geopolitical risks in production of metals,<sup>[16]</sup> and
- 5) technical aspects such as a) efficient and durable function, b) safe and clean operation, c) the ability to effectively recover high-quality functionality, components, or materials at the end of the first use phase.<sup>[17]</sup>

While conventional LCA and LCC are to some extent standardized procedures, the integration of further impacts or properties into the evaluation is by no means trivial and has not yet been standardized. The assembly of a unique process model inventory reflecting the different impact categories is challenging. Here, we propose an approach going beyond typical *lifecycle sustainability assessment* practices.<sup>[18]</sup> Therein, the model system represents the complete details of the product lifecycle, and is capable of spanning all relevant dimensions of scale and time and integrating various evaluation criteria in parallel. With the model setup proposed, process assessments are performed within identical system boundaries, and the physical accuracy of the model is improved, including fundamental laws such as balance of mass and energy (Figure 3).<sup>[19]</sup>

Figure 3 summarizes the general setup of the proposed comprehensive process modelling. It is based on an accurate bottom-up description of individual processes. The entire system inventory, boundaries, and process chain connectivity are based on input and output flows. Quantitative data included in the process descriptions make it possible to unveil and visualize the relations between flow quantities, properties, impact indicators, and technical process parameters. The implementation (open-source libraries of Python v3.7) allows direct information transfer to/from the model and the application of optimization and decision-making routines.

One major challenge, among others,<sup>[20]</sup> for an extended Life Cycle Sustainability Assessment (LCSA) is the acquisition of sufficient information and data uncertainties in the construction of accurate, complex models.<sup>[21]</sup> For the proposed implementation this can be overcome by making use of

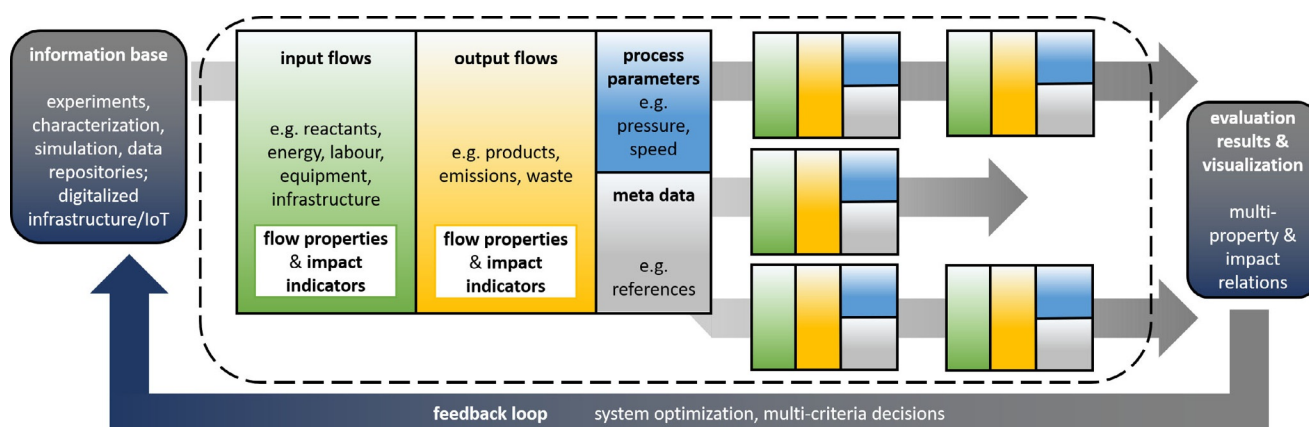


Figure 3. General model system structure for multiproperty evaluation. The data hierarchy per unit process is highlighted.

digitalized hardware, infrastructures and networks, and theoretical computing methods as well as (big) data collections as firsthand information sources. That means, for instance, integrating a) directly measured experimental data, b) results from physics and engineering simulations, c) machine logs or sensor data, as well as d) thirdhand literature information to build LCSA process models,<sup>[22]</sup> preferentially through automated routines (Figure 4). At other levels, machine learning (ML) methods can and should be used to generate insights from large collections of (raw) data as well as to create robust predictive models describing, for example, materials properties, device lifetimes, and the future development of environmental and economic key indicators. Exam-

ple projects and relevant data bases include The Materials Project,<sup>[23]</sup> NoMaD,<sup>[24]</sup> ICSD,<sup>[25]</sup> Topological Materials Database,<sup>[26]</sup> CCDC,<sup>[27]</sup> IMDS<sup>[28]</sup> for automotive applications, Granta,<sup>[29]</sup> IMA,<sup>[30]</sup> and many others.

Similar to other universal model platforms for sustainability assessment,<sup>[31]</sup> in the following example, we show that a consistent data structure and flexible implementation allows efficient interfaces to these various information sources. Frankly, this will become a general requirement for documentation and optimization during product development and R&D. A central platform collecting, storing and distributing data among stakeholders and partners will be the most efficient and least error-prone strategy. In R&D, this interface

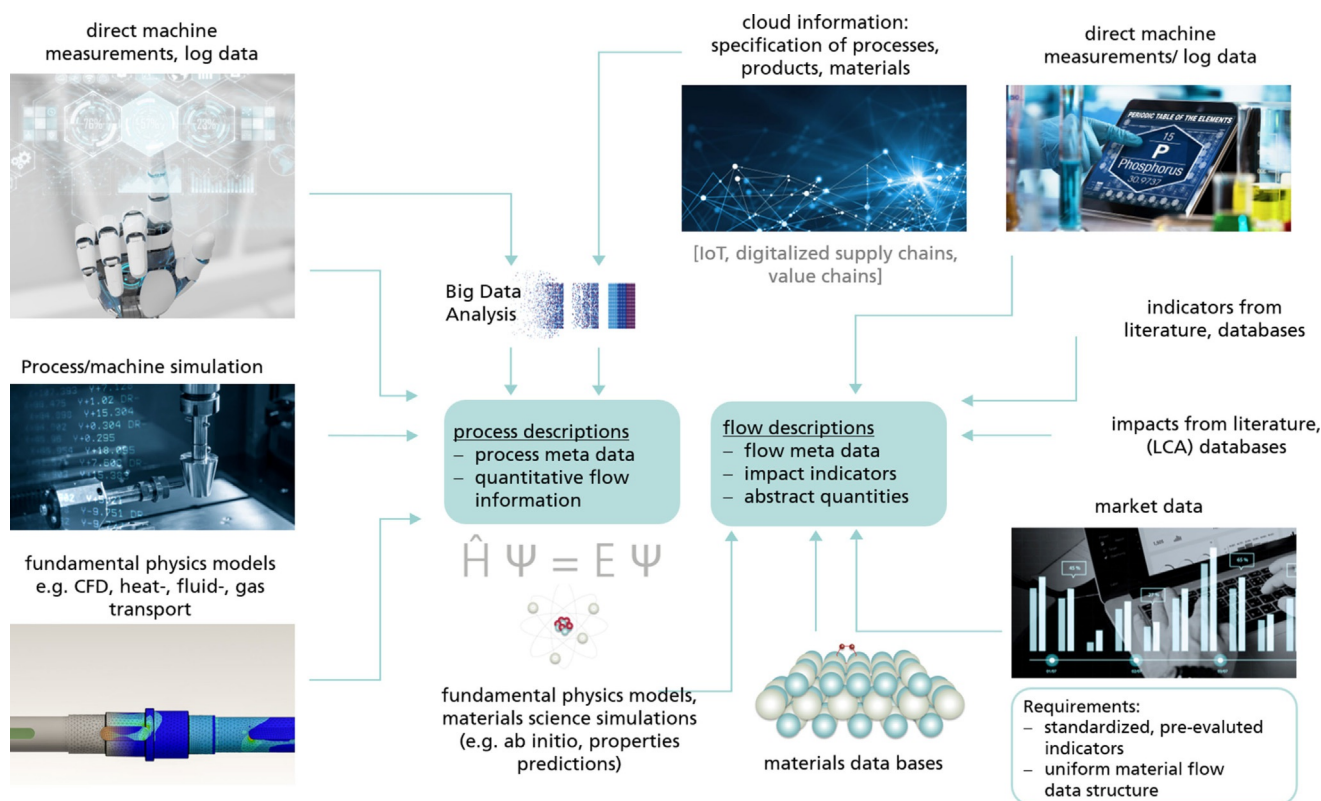
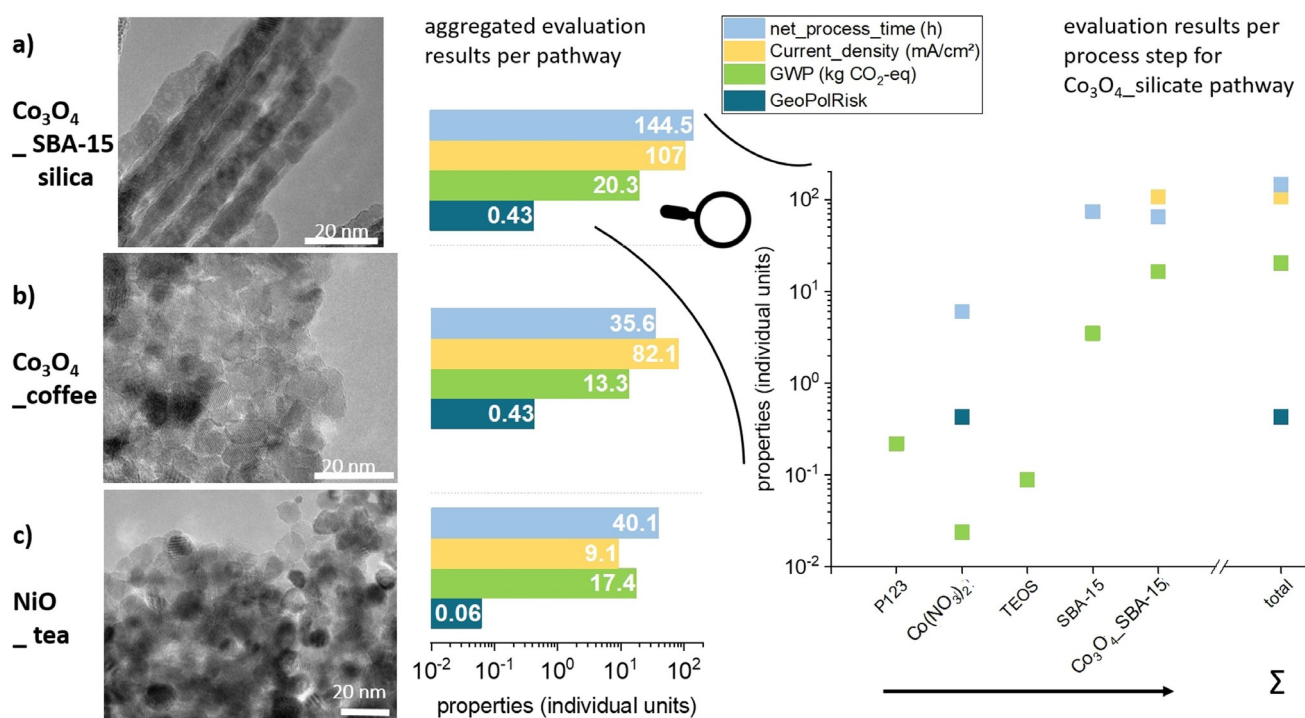


Figure 4. Data acquisition from various sources feeding into comprehensive model systems and supporting R&D work.



**Figure 5.** Multicriteria evaluation results of three alternative catalyst synthesis pathways (a, b, c). Aggregated results on the net process time, the delivered current density at 1.7 V<sub>RHE</sub>, the Global Warming Potential (GWP), and the criticality indicator GeoPolRisk for the full pathways (a, b, and c) are presented (left) next to process-level data for the Co<sub>3</sub>O<sub>4</sub>-SBA-15 silicate pathway (a; right). See SI for data inventory and method details.

can be realized with electronic lab journals or digitally connected experimental hardware. Ideally, the platform is compatible with a generalized data ontology like the Prov-O by W3C.<sup>[32]</sup> By complying to data ontologies, information can be drawn from process digital twins, databases on materials properties, market data, and general statistics sources through property- or indicator-specific queries. With access to such collections, assessments and R&D will benefit even further.<sup>[33]</sup> The proposed implementation will provide interfaces to open-source services using Prov-O in a straightforward fashion.

### Example Assessment of Alternative OER Catalysts

To illustrate the collaboration of experiment and LCA, three alternative synthesis routes of the authors' OER catalyst materials were assessed in a limited model, including criteria to be exemplary for different criteria classes. Co and Ni oxides were prepared via the nanocasting method by using three types of hard templates: mesoporous SBA-15 silica, biomass-based coffee waste, and spent tea leaves.<sup>[34]</sup> Herein, multiple properties were evaluated, including criticality and environmental impacts (Geopolitical Risk<sup>[16]</sup> and Global Warming Potential<sup>[35]</sup>) as well as selected technical process parameters and materials properties. All inventory data were collected through a digital lab journal or directly transferred from the process measurement to the model. The electronic lab journal ELNA<sup>[36]</sup> was used to collect firsthand experimental inventory data. Following the LCA standards,<sup>[37]</sup> environmental impacts were assigned relating to reference

processes and materials where available and otherwise modeled explicitly using process descriptions from the literature. The results are summarized in Figure 5.

SBA-15 silica templated Co<sub>3</sub>O<sub>4</sub> (a), coffee-waste templated Co<sub>3</sub>O<sub>4</sub> (b), and tea-leaves templated NiO (c) deliver current densities of 107.0, 82.1, and 9.1 mA cm<sup>-2</sup> at 1.7 V<sub>RHE</sub>, respectively, for the OER in 1 M KOH electrolyte. Is, consequently, SBA-15 silica templated Co<sub>3</sub>O<sub>4</sub> the *best* OER electrocatalyst since it shows the highest activity? From a performance point of view this can be claimed; however, the synthesis protocol of this catalyst is more complicated and requires an aggregated net process time of above 140 h. The laboratory-scale production (normalized to 500 mg) results in emissions of more than 20 kg CO<sub>2</sub>-eq due to a relatively high energy consumption. On the other hand, switching the SBA-15 silica template to carbon-based coffee waste reduces the catalytic activity by 13 %, but it decreases the process time of the catalyst preparation to 35.6 h and CO<sub>2</sub>-eq emissions to 13.3 kg. Changing the catalyst composition from cobalt oxide to nickel oxide combined with biomass-based templating decreases the efficiency of the catalysts for OER significantly, but it brings the advantage of very low geopolitical risk with Ni instead of Co. From a more holistic point of view—based on selected criteria from four different assessment categories—SBA-15 silica templated Co<sub>3</sub>O<sub>4</sub> should not necessarily be evaluated as the *best* OER electrocatalyst. The carbon footprint and technical efforts during manufacturing of the material are lower for the catalyst in which Co<sub>3</sub>O<sub>4</sub> is templated with coffee waste as opposed to silica.

This example shows that multiproperty evaluation is possible on a unique inventory basis under consideration of

mainly first-hand data. In addition to methodological improvements in digital modelling, this also benefits the development of functional materials, potentially also linking laboratory to commercial scale, accompanied by assessment of both performance and sustainability criteria.

## Conclusion

In application-oriented materials R&D such as catalyst development, there are numerous adjustment screws to reach desired performances. Considering all aspects relevant on the commercial scale is morphing the definition of *best material* away from pure performance criteria. We encourage researchers to 1) build collaborations with life-cycle management experts, scientists, and practical engineers and 2) to collect sufficient experimental and machine data such that they can be included in process modeling and sustainability assessments.

In the long run, implementing standardized information collection, storage, and distribution mechanisms will transform the way we work together. Evaluating and screening these data sets can be automatized, but we will need a sophisticated set of new figures of merit conveying materials properties beyond performance such as environmental, social, and economic impacts. In R&D, there is an urgent need to define these figures for “green materials” and to follow them consistently in developing design strategies for a functioning CE.

## Acknowledgements

We thank Dr. Mingquan Yu for help for the sample preparation and his input. This work was supported by the Fraunhofer Internal Programs under Grant No. Attract 170-600006 and the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) Projektnummer 388390466-TRR 247 within the Collaborative Research Centre/Transregio 247 “Heterogeneous Oxidation Catalysis in the Liquid Phase”. Open access funding enabled and organized by Projekt DEAL.

## Conflict of Interest

The authors declare no conflict of interest.

- 
- [1] a) J. Millward-Hopkins, J. Busch, P. Purnell, O. Zwirner, C. A. Velis, A. Brown, J. Hahladakis, E. Iacovidou, *Sci. Total Environ.* **2018**, *612*, 613; b) C. A. Poveda, M. G. Lipsett, *J. Sustainable Dev.* **2011**, *4*, 36; c) K. Govindan, R. Khodaverdi, A. Jafarian, *J. Cleaner Prod.* **2013**, *47*, 345.
- [2] F. Birol, *The Future of Hydrogen* (IEA), Paris, **2019**.
- [3] C. Hebling, M. Ragwitz, T. Fleiter, U. Groos, D. Härle, A. Held, M. Jahn, N. Müller, T. Pfeifer, P. Plötz, O. Ranzmeyer, A. Schaadt, F. Sensfuß, T. Smolinka, M. Wietschel, *Eine Wasserstoff-Roadmap für Deutschland*, Karlsruhe and Freiburg, **2019**.

- [4] R. Geres, A. Kohn, S. C. Lenz, F. Ausfelder, A. Bazzanella, A. Möller, *Roadmap Chemie 2050*, DECHEMA, Frankfurt, **2019**.
- [5] *Hydrogen Roadmap Europe*, fch.europa.eu, **2019**.
- [6] BMBF, **2020**.
- [7] a) M. Yu, G. Li, C. Fu, E. Liu, K. Manna, E. Budiyanto, Q. Yang, C. Felser, H. Tüysüz, *Angew. Chem. Int. Ed.* **2021**, *60*, 5800; *Angew. Chem.* **2021**, *133*, 5864; b) Z. W. Seh, J. Kibsgaard, C. F. Dickens, I. Chorkendorff, J. K. Nørskov, T. F. Jaramillo, *Science* **2017**, *355*, eaad4998; c) X. Deng, S. Öztürk, C. Weidenthaler, H. Tüysüz, *ACS Appl. Mater. Interfaces* **2017**, *9*, 21225; d) G.-h. Moon, M. Yu, C. K. Chan, H. Tüysüz, *Angew. Chem.* **2019**, *131*, 3529; e) G. Li, Q. Xu, W. Shi, C. Fu, L. Jiao, M. E. Kamminga, M. Yu, H. Tüysüz, N. Kumar, V. Stüb, et al., *Sci. Adv.* **2019**, *5*, eaaw9867; f) M. Yu, G.-H. Moon, R. G. Castillo, S. DeBeer, C. Weidenthaler, H. Tüysüz, *Angew. Chem. Int. Ed.* **2020**, *59*, 16544; *Angew. Chem.* **2020**, *132*, 16687.
- [8] X. Deng, H. Tüysüz, *ACS Catal.* **2014**, *4*, 3701.
- [9] T. Smolinka, N. Wiebe, P. Sterchele, A. Palzer, F. Lehner, M. Jansen, S. Kiemel, R. Miehe, S. Wahren, F. Zimmermann, *IndWEDe. Industrialisierung der Wasserelektrolyse in Deutschland*, Berlin, **2018**.
- [10] Iridium | Precious Metals Management, <https://pmm.umicore.com/en/prices/iridium>, **2020**.
- [11] EU, COM/2020/474 final, **2020**.
- [12] *Element Recovery and Sustainability* (Ed.: A. J. Hunt), RSC, Cambridge, **2013**.
- [13] a) N. Supanchaiyamat, A. J. Hunt, *ChemSusChem* **2019**, *12*, 397; b) G. A. Blengini, F. Mathieux, P. Nuss, L. Talens Peiró, *Towards recycling indicators based on EU flows and raw materials system analysis data*, <https://doi.org/10.2760/092885>, EU, **2018**.
- [14] a) M. A. Reuter, A. van Schaik, *J. Sustainable Metall.* **2015**, *1*, 4; b) N. J. Bartie, A. Abadías Llamas, M. Heibeck, M. Fröhling, O. Volkova, M. A. Reuter, *Miner. Process. Extr. Metall.* **2019**, *131*, 1; c) G. Nicolis, C. Rouvas-Nicolis, *Scholarpedia* **2007**, *2*, 1473.
- [15] M. Niero, X. C. S. Rivera, *Procedia CIRP* **2018**, *69*, 793.
- [16] E. D. Gemechu, G. Sonnemann, S. B. Young, *Int. J. Life Cycle Assess.* **2017**, *22*, 31.
- [17] a) M. D. Bovea, V. Pérez-Belis, *J. Cleaner Prod.* **2012**, *20*, 61; b) E. Franklin-Johnson, F. Figge, L. Canning, *J. Cleaner Prod.* **2016**, *133*, 589; c) G. Moraga, S. Huysveld, F. Mathieux, G. A. Blengini, L. Alaerts, K. van Acker, S. de Meester, J. Dewulf, *Resour. Conserv. Recycl.* **2019**, *146*, 452.
- [18] a) S. Cobo, A. Dominguez-Ramos, A. Irabien, *Resour. Conserv. Recycl.* **2018**, *135*, 279; b) D. Costa, P. Quinteiro, A. C. Dias, *Sci. Total Environ.* **2019**, *686*, 774; c) E. Iacovidou, J. Millward-Hopkins, J. Busch, P. Purnell, C. A. Velis, J. N. Hahladakis, O. Zwirner, A. Brown, *J. Cleaner Prod.* **2017**, *168*, 1279; d) E. Iacovidou, C. A. Velis, P. Purnell, O. Zwirner, A. Brown, J. Hahladakis, J. Millward-Hopkins, P. T. Williams, *J. Cleaner Prod.* **2017**, *166*, 910.
- [19] A. Abadías Llamas, N. J. Bartie, M. Heibeck, M. Stelter, M. A. Reuter, *J. Sustainable Metall.* **2020**, *6*, 34.
- [20] A. Gasparatos, A. Scolobig, *Ecol. Econ.* **2012**, *80*, 1.
- [21] a) M. Saidani, B. Yannou, Y. Leroy, F. Cluzel, *Recycling* **2017**, *2*, 6; b) E. Westkämper, J. Niemann, A. Dauensteiner, *Proc. Ins. Mech. Eng. B* **2001**, *215*, 673; c) M. Thomitzek, N. von Drachenfels, F. Cerdas, C. Herrmann, S. Thiede, *Procedia CIRP* **2019**, *80*, 126.
- [22] J. Hannula, J. R. A. Godinho, A. A. Llamas, S. Luukkanen, M. A. Reuter, *J. Sustainable Metall.* **2020**, *6*, 174.
- [23] Materials Project, <https://materialsproject.org/>, **2020**.
- [24] NOMAD CoE, <https://nomad-coe.eu/>, **2020**.
- [25] Inorganic Crystal Structure Database, <https://www.fiz-karlsruhe.de/de/produkte-und-dienstleistungen/inorganic-crystal-structure-database-icsd>, **2020**.
- [26] Topological Materials Database, <https://www.topologicalquantumchemistry.com/#/>, **2019**.

- [27] Cambridge Structural Database (CSD), <https://www.ccdc.cam.ac.uk/solutions/csd-system/components/csd/>, **2020**.
- [28] International Material Data System, <https://www.mdsystem.com/imdsnt/startpage/index.jsp>, **2020**.
- [29] Granta Design, <https://www.grantadesign.com/de/industry/products/data-products/>, **2020**.
- [30] IMA Dresden, <https://www.ima-dresden.de/>, **2020**.
- [31] a) E. Restrepo, A. N. Løvik, P. Wäger, R. Widmer, R. Lonka, D. B. Müller, *Environ. Sci. Technol.* **2017**, *51*, 1129; b) S. Pauliuk, N. Heeren, M. M. Hasan, D. B. Müller, *J. Ind. Ecol.* **2019**, *23*, 1016; c) R. J. Myers, T. Fishman, B. K. Reck, T. E. Graedel, *J. Ind. Ecol.* **2019**, *23*, 222; d) R. J. Myers, B. K. Reck, T. E. Graedel, *Sci. Data* **2019**, *6*, 84.
- [32] W3C, Prov-O, <https://www.w3.org/TR/prov-o/>.
- [33] K. Pal in *A volume in the Advances in knowledge acquisition, transfer, and management (AKATM) book series* (Eds.: A. Gyamfi, I. Williams), IGI Global, Engineering Science Reference, Hershey, PA, **2019**, pp. 71–102.
- [34] a) M. Yu, C. K. Chan, H. Tüysüz, *ChemSusChem* **2018**, *11*, 605; b) X. Deng, K. Chen, H. Tüysüz, *Chem. Mater.* **2017**, *29*, 40; c) M. Yu, G. Moon, E. Bill, H. Tüysüz, *ACS Appl. Energy Mater.* **2019**, *2*, 1199.
- [35] M. A. J. Huijbregts, Z. J. N. Steinmann, P. M. F. Elshout, G. Stam, F. Verones, M. Vieira, M. Zijp, A. Hollander, R. van Zelm, *Int. J. Life Cycle Assess.* **2017**, *22*, 138.
- [36] M. Franke, J. Weraach, M. Haarländer, *Elektronische Laborbücher in der Max-Planck-Gesellschaft*, MPG e.V., **2017**.
- [37] a) *Environmental Management-Life Cycle Assessment-Principles and Framework*, aISO 14040 **2006**, Geneva; b) M. Finkbeiner, A. Inaba, R. Tan, K. Christiansen, H.-J. Klüppel, *Int. J. Life Cycle Assess.* **2006**, *11*, 80.

Manuscript received: April 19, 2021

Version of record online: July 7, 2021