

# Towards the middle of the century – a Synchrotron Perspective

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# 1. Challenges and expectations

## 1.1. Introduction

*“die Zukunft war früher auch besser“ – “even the future was better in the past” - a famous quote from the Bavarian comedian Karl Valentin from the early 20<sup>th</sup> century might cross peoples mind when reflecting the challenges of the 21<sup>st</sup> century.*

Climate change, sustainable energy supply, environment, bio diversity, clean water, food, and health, seem to confront humankind with almost impossible tasks. In 2019 Frans Timmermans, the Executive Vice-President of the European Commission stated *‘We are in a climate and environmental emergency<sup>1</sup>.*

The atmosphere is warming, 16 of the 17 warmest years on record occurred since 2001 (according to NASA), one 8<sup>th</sup> of all species on the planet are at risk of being lost, 2.2 billion people do not have regular access to clean fresh water<sup>2</sup>, forests disappear<sup>3</sup>, oceans are polluted<sup>4</sup>.

Countless studies have been performed, many reports written, models and calculations published on the topics above, however, while they are certainly the background, they are not the detailed topic of this article, where the focus shall be on intelligent answers, rapid responses and swift action from politics, science and in particular large scale infrastructures.

With the European Green Deal from 2019 the European Union provides a response to major challenges, setting itself the goal of becoming climate-neutral by 2050. With a growth strategy towards a fair and prosperous society, resource efficiency and CO<sub>2</sub> neutrality until 2050, human wellbeing and economic prosperity shall be decoupled from resource use<sup>5</sup>. More than ever, research is seen to be the fundamental ingredient to Europe’s digital and green transformation. Industry process transformation has an amazing potential of saving CO<sub>2</sub>. For example in steel production, responsible for about 6% CO<sub>2</sub> emission worldwide<sup>6</sup>, ULCOS<sup>7</sup> an ultra-low CO<sub>2</sub> steel making project of industries and academia (47 partners, 15 European countries) aimed to reduce CO<sub>2</sub> emissions by 50%. Newly developed industrial processes combined with green electricity will even increase this reduction potential.

With three pillars “Excellent Science”, “Global Challenges and European Industrial Competitiveness”, and “Innovative Europe” all actors from academia to civil society shall be hold responsible; the pillars are underpinned by widening participation and strengthening the European research area. It is worth mentioning that based on the fact that 2/3 of the EU productivity growth over the last decades was

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<sup>1</sup> [https://ec.europa.eu/commission/presscorner/detail/en/IP\\_19\\_6691](https://ec.europa.eu/commission/presscorner/detail/en/IP_19_6691)

<sup>2</sup> UN water report available at UNESDOC Digital library, 2020: The United Nations world water development report 2020: water and climate change - UNESCO Digital Library

<sup>3</sup> Deforestation Report WWF

[deforestation\\_fronts\\_\\_\\_drivers\\_and\\_responses\\_in\\_a\\_changing\\_world\\_\\_\\_full\\_report\\_1.pdf](#) (panda.org)

<sup>4</sup> see also Intergovernmental Panel on Climate Change (IPCC): Special Report on the impacts of global warming of 1.5°C and Intergovernmental Science-Policy Platform on Biodiversity and Ecosystem Services: 2019 Global assessment report on biodiversity and ecosystem services

<sup>5</sup> The International Resource Panel: Global Resources Outlook 2019: Natural Resources for the Future We Want; European Environment Agency: the European environment — state and outlook 2020: knowledge for transition to a sustainable Europe

<sup>6</sup> <https://www.sciencedirect.com/science/article/abs/pii/S1364032115011806>

<sup>7</sup> <https://cordis.europa.eu/project/id/515960/de>

driven by research and innovation investments, that the leverage effect of each Euro invested in R&I will be 11 Euros and more than 300.000 highly skilled jobs will be created in the next two decades<sup>8</sup>

Many national governments preceded or drew level with the European goals as illustrated for example in the German National Hydrogen strategy from 2020<sup>9</sup>, or the Swiss Long-term climate strategy to 2050<sup>10</sup>. An impressive list of national long term strategies including Denmark, Germany, Finland, France, the UK, Japan, Canada, the Netherlands, Norway, Sweden, Spain, South Africa, South Korea, Austria and the United States can be found at the United Nation UNFCCC platform<sup>11</sup>.

What all these strategies have in common is a reliance on science, development and the innovation potential of academics. And justifiable so! With 1.8 million researchers at universities and research centres as well as in industry, Europe is a global scientific powerhouse<sup>12</sup>. Brain circulation, interconnected research infrastructures, European consortia of research facilities, and last but not least an adequate funding situation in many countries allow, that just 7% of the world's population and 24% of global GDP, results in 30% of the world's scientific publications<sup>13</sup>.

So forewarned is forearmed? The solution to the most pressing problems is around the corner by research and innovation? Yes and no. In a remarkable essay<sup>14</sup>, Robert Schlögl, Director of 2 Max-Planck-Institutes in Germany, puts us into the year 2100 looking back to 2050. While cause and effect was common knowledge concerning climate change, desertification, pollution, water scarcity, while photovoltaics, chemical energy conversion, recycling, sustainable agriculture – to just name a few – were highly developed, the use of fossil fuels, ubiquitous plastic, or deforestation did not stop due to the primacy of minimal-costs-maximal-gain. Will the first half of the 21<sup>st</sup> century be judged as the time of hesitancy against better knowledge?

Hesitancy is not an option, when health is concerned. Pandemics require a global effort, which is mirrored at all research facilities worldwide. This is impressively proven by the activities of synchrotrons during the corona pandemic<sup>15</sup>.

## *1.2. The contribution of large scale photons sources<sup>16</sup>*

Large scale facilities are inherently diverse, international, multi- and cross-disciplinary and excellence driven. Their core is the triangle of research, education, and innovation, their goal the advancement of science and knowledge, their focus curiosity and discovery, their strength a scientific community of more than 30,000 researchers using Europe's light sources, their pride some of the brightest minds worldwide, their outcome answers to key challenges and with this of course new questions.

Light sources in Europe and all over the world<sup>17</sup> have developed in a spectacular way, with an impressive research portfolio spanning from physics, chemistry, material research, energy research, biology, medicine, engineering to arts and cultural heritage. A growing user community both in

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<sup>8</sup> J. Guerrier, Horizon Europe: a gateway to the future, DOI:10.26125/v4ne-ag83

<sup>9</sup> [https://www.bmwi.de/Redaktion/EN/Publikationen/Energie/the-national-hydrogen-strategy.pdf?\\_\\_blob=publicationFile&v=6](https://www.bmwi.de/Redaktion/EN/Publikationen/Energie/the-national-hydrogen-strategy.pdf?__blob=publicationFile&v=6)

<sup>10</sup> <https://www.bafu.admin.ch/bafu/en/home/topics/climate/info-specialists/emission-reduction/reduction-targets/2050-target/climate-strategy-2050.html>

<sup>11</sup> <https://unfccc.int/process/the-paris-agreement/long-term-strategies>

<sup>12</sup> Eurostat, <https://ec.europa.eu/eurostat/de/>

<sup>13</sup> CWTS Web of Science

<sup>14</sup> Robert Schlögl in Bunsen-Magazin, page 24

[https://bunsen.de/fileadmin/user\\_upload/media/Publikationen/2021\\_Bunsen-Magazin\\_\\_1\\_.pdf](https://bunsen.de/fileadmin/user_upload/media/Publikationen/2021_Bunsen-Magazin__1_.pdf)

<sup>15</sup> <https://lightsources.org/2021/02/16/lightsource-research-and-sars-cov-2/>

<sup>16</sup> Inevitably, throughout the text, the selection of examples cannot be exhaustive and is thus only illustrative

<sup>17</sup> See [lightsources.org](https://lightsources.org) for an overview as well links to facilities

numbers as in scientific fields makes them crystallization cores for new developments, cooperation and precious instruments to address the grand challenges of the years to come.

In 2017 LEAPS, the League of the European Accelerator based Photon Sources was founded, bringing together 19 European Light Sources<sup>18</sup>, Synchrotrons as well as Free Electron Lasers. A summary of positioning of this consortium towards Horizon Europe missions was lounged in March 2020<sup>19</sup> disclosing a high level of action with regard to the grand challenges.

The versatile and unparalleled properties of synchrotron radiation and the combination of various methods ad loco, facilitate unprecedented measurements otherwise hardly possible or even impossible. Control over photon energy, polarization, space and time resolution, and coherent fraction allowed break through experiments like first real time investigations of magnetization dynamics, or insights into buried layers of working electronic devices such as tandem solar cells.

### *1.3. Some answers of the lightsources to the grand challenges*

A few examples shall illustrate how synchrotrons contribute to addressing and solving major challenges and are given in a by far not exhaustive selection here.

#### **Hydrogen**

Even though the share of renewable energy in final energy consumption increased from 9% in 2005 to 17% in 2018, the EU is still responsible for 10% of global greenhouse gas emissions. Under the Paris Agreement a reduction of emissions by at least 40% by 2030 compared to 1990 shall be a first step toward CO<sub>2</sub> neutrality in 2050<sup>20</sup>, mainly by the elimination of the use of fossil fuels.

Hydrogen, the magic molecule of the up-coming decades? Produced from water in a catalytic electrolysis process, it can be “directly” converted into electricity in fuel cells, used as an energy storage material and finally act as an educt in the production of synthetic fuels. Self-evidently, it has to be produced via carbon-neutral means, such as solar or wind energy.

Transforming abundant or regenerative matter like water and CO<sub>2</sub> from direct air capture into synthetic gases (i.e. hydrogen, methane) or liquids (i.e. methanol) using green electricity is referred to as Power-to-X.

In 60 minutes the sun delivers the energy the whole world needs in one year; 578x578 km<sup>2</sup> of solar panels in the Sahara (3,6% of the area) would satisfy the world’s energy demand<sup>21</sup>. Sunlight, being the most abundant renewable energy source<sup>22</sup>, suffers from limited availability by night, in seasonal cycles, and in less sunny regions of the world.

By solar-to-hydrogen conversion, the production of hydrogen via direct photoelectrochemical water splitting solar energy can be stored and is therefore widely studied. Many studies were and are devoted to understanding and optimizing this process and its catalytic materials<sup>23</sup>, not just a few of them including X-ray based studies at synchrotrons<sup>24</sup>

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<sup>18</sup> <https://leaps-initiative.eu/consortium/>

<sup>19</sup> file:///C:/Users/gfw/Downloads/PostionPaper\_HEmissions\_March2020.pdf

<sup>20</sup> COMMUNICATION FROM THE COMMISSION TO THE EUROPEAN PARLIAMENT 2018, <https://eur-lex.europa.eu/legal-content/EN/TXT/PDF/?uri=CELEX:52018DC0773&from=EN>

<sup>21</sup> BP Statistical Review of World Energy 2018, 67th edition 2018, Weltenergieverbrauch 2017: 157135,25 TWh

<sup>22</sup> Refer to chapter XXX, in this book

<sup>23</sup> Hot Topic: Water Splitting: ChemElectroChem - Chemistry Europe (wiley.com)

<sup>24</sup> <https://doi.org/10.1002/aenm.202003183>

While hydrogen is a perfect candidate for a sustainable energy supply, its storage and transport seemed to limit its practical usefulness. High pressures (300-700 bar) or cryogenic temperatures due to its volumetric storage capacity are major drawbacks for the general and global use. In recent years scientists from the Universität Erlangen-Nürnberg worked on liquid organic hydrogen carriers LOHCs which combine a high hydrogen storage capacity with physicochemical properties similar to diesel fuel. Conventional, already in place storage and transport infrastructures can be used, long-term storage without losses is possible<sup>25</sup>.

Scientific findings<sup>26</sup> including X-ray spectroscopic investigations at the lightsource BESSY II, were one of the puzzle pieces leading to the foundation of Hydrogenious LOHC Technologies GmbH, which offers solutions for a “hydrogen-free hydrogen economy” and became a world leader in LOHC technology<sup>27</sup>

However, water splitting is an energy hungry process. In addition current water electrolyzer technologies only function with either highly alkaline (20–40 wt% KOH) electrolyte obtained from purified freshwater or else purified freshwater alone. Water splitting from sea water, however, might kill two birds with one stone, as the slightly inappropriate proverb goes. Direct use of the vastly more abundant seawater supplies could solve the problematics related to scarce water provision and high fresh water demand, which are severe in many arid areas. Some zones with sea water often have strong solar radiation (United Arab Emirates 340 days a year) and are in the need to replace oil production by more sustainable, future-oriented technologies. Alternatives to fossil fuels will not only be a peace keeping measure in the OPEC (and in particular the MENA)<sup>28</sup> countries, but might be the only way to include these countries in phasing out oil extraction and to join global efforts against climate change (see also chapter 5).

With contributions from synchrotron experiments at BESSY II, scientists have now developed an efficient working alkaline electrolyzer, splitting artificial alkaline seawater, based on nanostructured layers and nanoparticles<sup>29</sup>. Using renewable energy sources like photovoltaics to operate the electrolyzer, the natural day-night cycles even function as a refreshment protocol for the process, which requires catalyst recovery periods resembling day and night changes.

## Batteries

Next to hydrogen, batteries have been identified as one of the major technologies for energy storage. The perfect battery has a high capacity, short charging times, long-term stability (many charge-discharge cycles), is light weight and consists of abundantly available cheap materials.

All these properties can already be fulfilled, yet not in one but “rather 4 different batteries”. Molecular understanding, is required for rational design of new generations of batteries.

All European synchrotrons have accepted the battery challenge as summarized in a joint LEAPS position paper for the European Battery 2030+ Roadmap<sup>30</sup> From novel materials and concepts to battery safety concerns, LEAPS facilities contribute to this important scientific and technological field. A prominent example are Lithium cells, ubiquitously used in electronic devices and electric cars, mobile phones and

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<sup>25</sup> C. Papp, P. Wasserscheid, J. Libuda, H.-P. Steinrück, Chemical Record, <https://doi.org/10.1002/tcr.201402014>

<sup>26</sup> Overview: Hydrogenious LOHC Technologies - Scientific research on LOHC

<sup>27</sup> Hydrogenious LOHC Technologies - Handling hydrogen made easy and Hydrogenious LOHC Technologies - Handling hydrogen as an oil in LOHC

<sup>28</sup> For more political and economic details, please refer to

The Risks and Opportunities of Green Hydrogen Production and Export From the MENA Region to Europe:

<http://library.fes.de/pdf-files/bueros/amman/16998.pdf>

The MENA („Middle East & North Africa“) Hydrogen Alliance, launched in 2020, aims to accelerate the development of value chains for green molecules in the region and brings together private and public sector actors and academia: <https://www.dii-desertenergy.org/mena-hydrogen-alliance/> particularly Chapter 4

<sup>29</sup> P. Strasser, H. Dau et al, Adv. Energy Mater. 2018, 8, 1800338 DOI: 10.1002/aenm.201800338

<sup>30</sup> file:///C:/Users/gfw/Downloads/LEAPS-Battery-Roadmap2030.pdf

little daily things like toothbrushes all the way to airplanes<sup>31</sup> and space crafts<sup>32</sup>. However, explosions of Lithium batteries have attracted much media and legal attention<sup>33</sup>.

At the ESRF, NASA and researchers from University College London have been exploring worst case scenarios when lithium batteries fail<sup>34</sup> and are now able to provide unprecedented insight in failure start and mechanism and a new gold-standard battery safety testing.

In view of environmental issues as well as an increasing demand for storage and flexibility, novel concepts and battery design are indispensable and on the agenda of synchrotron research in the years to come.

## Environment

After only about 100 years of producing plastics, plastic particles are found everywhere – in groundwater, in the oceans, in the air, in the food chain. Just PET (Polyethylenterephthalat, or simply the „bottle plastic“) contributes with 50 million tons of newly produced plastic every year. Its extreme durability and resistance to biodegradation turns from an advantage into a long-term environmental burden. Sustainable production and recovery cycles have to be developed to combat plastic waste. A breakthrough came with the discovery of a bacterium feeding on waste from an industrial PET recycling facility<sup>35</sup>, by production of a PET-digesting enzyme PETase. At DIAMOND light source and BESSY II researchers have determined the precise structure of PETase and have engineered an improved version of it. PETase converts PET to an intermediate product MHET, further decomposed by another enzyme MHETase, into the building blocks or educts of PET. These findings allow for recycling and synthesis of new PET without the addition of crude oil<sup>36</sup>.

## Answers to Corona

The corona virus has shaken Europe and the world to its core and, above all, is a human tragedy. The emergence of the SARS-CoV-2 virus, its spreading around the globe and its adaptability by mutations has unambiguously placed the vulnerability of human society in the spotlight. The speed of propagation of mutant viruses in and by a globalized society calls for a global approach and global solutions. Political barriers such as borders cannot stop a pandemic, therefore national “solo-efforts” are not only shortsighted but might even jeopardize the combat against this and possibly following viruses. If SARS-CoV-2 persists in parts of the world, it will come back to the whole world, most likely as a mutant variant. This unprecedented time pressure, the urgent need of a vaccine in sufficient quantities and availability to all countries and people, brings out the best in cooperative research. All light sources immediately implemented rapid access procedures for Corona-related research to ensure best possible research support. Even during lock-down times, the infrastructures stayed in a so called “warm shutdown” enabling experiments related to SARS-CoV-2 on very short notice<sup>37</sup>. In 2020 every 5 days a much-noticed paper on Corona was published<sup>38</sup>, cooperations between synchrotrons and industry were established or intensified<sup>39</sup>. It goes beyond the scope of this article to mention individual or even break-through results, but it is worth mentioning, that large scale facilities commonly rather compared to “ocean giants” turn into “speed boats” if the situation requires this transition.

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<sup>31</sup> Lithium batteries: safe to fly? | Safety First (airbus.com)

<sup>32</sup> ESA - Nobel-winning lithium-ion batteries powering space

<sup>33</sup> A review of hazards associated with primary lithium and lithium-ion batteries, <https://doi.org/10.1016/j.psep.2011.06.022>

<sup>34</sup> Finegan, D. P, et al, Journal of Power Sources, Volume 417, 31 March 2019, Pages 29-41

<sup>35</sup> S Yoshida et al, Science 2016, DOI: 10.1126/science.aad6359

<sup>36</sup> Austin HP et al. Characterization and engineering of a plastic-degrading aromatic polyesterase. PNAS. DOI:10.1073/pnas.1718804115 (2018) and Palm GJ et al Structure of the plastic-degrading Ideonella sakaiensis MHETase bound to a substrate, Nature Communications (2019) DOI : 10.1038/s41467-019-09326-3

<sup>37</sup> LEAPS facilities research on SARS-CoV-2 and rapid access (leaps-initiative.eu)

<sup>38</sup> <https://lightsources.org/2021/02/16/lightsource-research-and-sars-cov-2/>

<sup>39</sup> For example [https://www.helmholtz-berlin.de/pubbin/news\\_seite?nid=21283;sprache=en;seitenid=76027](https://www.helmholtz-berlin.de/pubbin/news_seite?nid=21283;sprache=en;seitenid=76027) and <https://www.diamond.ac.uk/Home/News/LatestNews/2020/12-05-2020.html>

During the Corona Pandemic in particular the macromolecular or protein crystallography (MX) has shown its incredible potential in medical research from understanding to drug development<sup>32-34</sup>. Protein crystallography has been a workhorse in drug discovery for decades<sup>40</sup> and the implementation of the first MX synchrotron beamline at the ESRF, was the go-ahead for most synchrotrons leading to 90% of X-ray single-crystal structure determinations being from synchrotrons nowadays<sup>41, 42</sup>.

All these examples demonstrate the massive contributions of light sources to solving the challenges of the years and decades to come. However, synchrotrons do not see themselves as self-sufficient, quite the contrary! With many thousands of users from academia and industry, with intense cooperation between research institutions and universities, they form crystallization seeds for multi- and interdisciplinary work and act as hubs for transnational liaison. They live in a mutually stimulating ecosystem with complementary infrastructures. The synergy of light source related methods with techniques based on microscopes, ion and other particle beams, neutrons, lasers and high magnetic fields, made 120 individual research facilities embracing each other to found the consortium ARIE<sup>43</sup> (Analytical Research Infrastructures in Europe), providing infrastructures, services, and know-how to a growing and diverse community of researchers in academia and industry. In a first position paper<sup>44</sup> ARIE, pinpoints its mission and future perspectives toward Europe's major challenges, namely (1) adaptation to climate change, including societal transformation, (2) cancer, (3) climate-neutral and smart cities, (4) healthy oceans, seas, coastal and inland waters, (5) soil health and food. Established in 2020, ARIE became immediately involved in SARS-CoV-2 research, too<sup>45</sup>.

**Science and research being intrinsically international will further intensify all efforts of interdisciplinary, multidisciplinary, cross boundary cooperation – also in an institutionalized way – to help solving the major challenges of the next decades.**

## 2. Curiosity and Basic Research

“wo alle das selbe denken, wird nicht viel gedacht” (Karl Valentin) (were all people think the same, not a lot of thinking takes place)

What is research, what is applied or basic research? Foremost, scientific research is all about is creating knowledge and understanding for the benefit of humanity. The distinction between applied and basic seems to be a bit artificial or as the European Research Council ERC states: “Today the distinction between 'basic' and 'applied' research has become blurred, due to the fact that emerging areas of science and technology often cover substantial elements of both<sup>46</sup>.”

In the previous chapter the emphasis was on the role of science to address the major challenges and most pressing problems of this century. Discoveries to fight climate change or pandemics are urgently needed, a clear aim is defined.

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<sup>40</sup> T. Hogg and R.Hilgenfeld Protein Crystallography in Drug Discovery doi: 10.1016/B0-08-045044-X/00111-5

<sup>41</sup> <http://biosync.sbkb.org>

<sup>42</sup> JR Helliwell and EP Mitchell Synchrotron radiation macromolecular crystallography: science and spin-offs. doi: 10.1107/S205225251402795X

<sup>43</sup> <https://arie-eu.org/>

<sup>44</sup> [https://www.lens-initiative.org/wp-content/uploads/2020/09/ARIE-MISSIONS-PosPaper-FINAL-RELEASE\\_09.2020.pdf](https://www.lens-initiative.org/wp-content/uploads/2020/09/ARIE-MISSIONS-PosPaper-FINAL-RELEASE_09.2020.pdf)

<sup>45</sup> <https://leaps-initiative.eu/analytical-research-infrastructures-of-europe-arie-join-forces-to-face-covid-19-and-other-viral-and-microbial-threats/>

<sup>46</sup> <https://erc.europa.eu/about-erc/mission>

Nowadays we widely use X-rays to tackle these challenges. However, going back 150 years, X-rays were just discovered, not because a programme or a scientific strategy required them – what programme would it have been, not knowing they exist? 20 years of experiments, talent and luck were the ingredients to a technology which is so widely used today. “If we knew what it was we were doing, it would not be called research, would it?” (Albert Einstein).

A wonderful example presented by Daniel Zajfman, President Weizmann Institute of Science, gives the following story <sup>47</sup>:

*“(...) If we would have been sitting here 200 and some years ago ... Well, of course there would be no projectors, no microphone, but also no light. And in any room that we would have been sitting, there would have been a lot of candles. About 200 years ago, actually mostly in the UK but also in Germany, there was a lot of R&D for candles. People were investing a lot of money to get better candles, producing more light, different colors, different perfume. Cheaper ones or expensive ones. A lot of R&D, and there were a lot of discussions. You can read about it. About how one should invest to get a better candle. Then came this gentleman named Michael Faraday and he invented electricity. Now I want to remind you of something. It doesn't matter how much money you're going to invest in developing new candles - you will never get electricity. The solution to your problem is not always where the problem is. (...)”*

X-rays, electricity, the understanding of relativity, the transistor, the giant magneto resistance, synchrotron radiation itself - the list could be endless – triggered scientific revolutions, followed by unprecedented technical innovations. These revolutions have amazingly contributed to the understanding of nature. A remarkable paper in the “Science Family” on Fundamental science behind today's important medicines<sup>48</sup> gives a list of 28 drugs on a multi-billion market, saving millions of lives – 23 of them were found in basic discoveries, i.e. the HIV protease inhibitors<sup>49</sup>. However, it usually takes decades from basic research to products; time the world sometimes simply cannot wait, as Corona currently makes obvious.

Again the question: what really is the difference between basic and applied research? Maybe revolution and evolution? An evolutionary approach based on existing possibilities is indispensable and will create fundamental knowledge on its way. On the other side, a scientific revolution is impossible to predict, but will happen and lead to applications. When, where, in what scientific field is impossible to know, but it will definitely come as long as basic research is funded, access to infrastructure is possible, curiosity and freedom are held in high esteem and knowledge is seen as a cultural value. This perception entails the duty of science and scientists to give an account of their work to the general public, the tax payer financing research to a large extent, but this would be a chapter of its own.

**Two sides of one coin: applied research and basic research. In times of pressing challenges the twin-track approach of is the order of the day.**

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<sup>47</sup> [https://www.helmholtz.de/fileadmin/user\\_upload/Daniel\\_Zajfman\\_Vortrag\\_Berlin\\_180909\\_EN.pdf](https://www.helmholtz.de/fileadmin/user_upload/Daniel_Zajfman_Vortrag_Berlin_180909_EN.pdf)

<sup>48</sup> JM Spector et al, *Science Translational Medicine* 25 Apr 2018, DOI: 10.1126/scitranslmed.aag1787

<sup>49</sup> [https://stm.sciencemag.org/content/scitransmed/suppl/2018/04/23/10.438.eaaq1787.DC1/aag1787\\_SM.pdf](https://stm.sciencemag.org/content/scitransmed/suppl/2018/04/23/10.438.eaaq1787.DC1/aag1787_SM.pdf)

### 3. Synchrotron Facilities in the next decades – up-grades and adaptation

“Kunst ist schön, macht aber viel Arbeit“(Karl Valentin) „Art is beautiful, but requires a lot of work“; same is true for science.

In the previous chapters the need of research to address the most urgent problems of humanity, the contribution of synchrotrons, and the importance of curiosity driven basic science was stroboscopically highlighted. This research is based on the current infrastructure and possibilities.

Already today, synchrotron radiation sources are highly versatile tools serving an increasingly diverse research community from many scientific fields, including physics (e.g., quantum physics in solids, superconductivity, magnetism, topological insulators, clusters, and disordered systems), chemistry (e.g., catalysis and artificial synthesis, real-time investigations of charge transfer), energy research (e.g., materials for energy conversion and storage, solar fuels, and battery research), biology (e.g., bio and bio-mimetic materials, cells, and bacteria), medical and pharmaceutical research (e.g., Corona and other viral diseases, function mechanisms of drugs, dental treatment), materials testing, and cultural heritage investigations. The remarkable success of research at synchrotrons led and leads to a continuous hunt for further options in all domains – spatial, time, energy resolution. The improvements in brightness and the almost explosive progress in new possibilities like in situ or operando experiments, experiments on liquids, biological objects and more, paved the way to a widening of scientific areas and user communities. While physics was predominant in the first decades of synchrotron research many other fields joined and new requirements, wishes for increased options become apparent in an interplay between users and facilities.

Starting from 3 synchrotron facilities in the 1960s, 14 synchrotron sources and 7 Free Electron Lasers in 10 European countries serve more than 24000 users per year today. An ever-increasing demand already leads to a severe oversubscription of many instruments. A detailed landscape analysis of the European light sources including several performance indicators like brilliance, emittance, energy but also the start of their user operation, number of beamlines, publications and user visits, was carried out in 2019<sup>50</sup>.

Almost all European synchrotron facilities have either recently done major up-grades or are planning to do so in the next decade. MAX IV in Sweden has pioneered a novel storage ring design<sup>51</sup> (multi bend achromat MBA) facilitating a factor of 10 increase in both brightness and coherence over existing facilities, followed by the ESRF, who dismantled the existing storage ring and turned it into a revolutionary low-emittance light source<sup>52</sup>, the first-of-a-kind fourth-generation high-energy synchrotron. Both facilities are (back) in user operation. ALBA, BESSY II@HZB, DIAMOND, ELETTRA, PETRA III, and SLS (in alphabetical order) are currently planning up-grades. ALBA, the youngest sibling in this synchrotron family will prepare a careful study for an up-grade in the next few years. BESSY II@HZB is in the process of elaborating a conceptual design report, which will be presented in 2022 for its successor BESSY III@HZB. DIAMOND has published a design report in 2019 proposing a novel implementation of MBA technology with dramatic gain in brightness and coherence as well as additional source points for new beamlines<sup>53</sup>. In its design report from 2020, ELETTRA<sup>54</sup> projects an up-grade towards a 6-bend achromat, also largely increasing the brilliance and coherence of the light

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<sup>50</sup> [https://leaps-initiative.eu/wp-content/uploads/2019/11/LEAPS\\_Landscape\\_Analysis\\_27March2019\\_final.pdf](https://leaps-initiative.eu/wp-content/uploads/2019/11/LEAPS_Landscape_Analysis_27March2019_final.pdf)

<sup>51</sup> Challenge of MAX IV Towards a Multi-Purpose Highly Brilliant Light Source [www.simonleemann.ch/work/pac11/TUOBS4.pdf](http://www.simonleemann.ch/work/pac11/TUOBS4.pdf) and The multi-bend achromat storage rings [doi/pdf/10.1063/1.4952780](https://doi.org/10.1063/1.4952780)

<sup>52</sup> <https://www.esrf.eu/about/upgrade>

<sup>53</sup> <https://www.diamond.ac.uk/Home/About/Vision/Diamond-II.html>

<sup>54</sup> [https://www.elettra.eu/images/Documents/ELETTRA%20Machine/Elettra2/Elettra\\_2.0\\_CDR\\_abridged.pdf](https://www.elettra.eu/images/Documents/ELETTRA%20Machine/Elettra2/Elettra_2.0_CDR_abridged.pdf)

source. PETRA III with the design report (2019) for PETRA IV strives for a MBA storage ring, too<sup>55</sup>; in contrast to all other facilities, however, the unique geometry and the size – before becoming a synchrotron light source, PETRA served as a pre-accelerator for protons and electrons/positrons for the particle accelerator HERA – will make it the most brilliant synchrotron source in the world. In December 2020 just before Christmas, the SLS received the funding for their up-grade programme to SLS 2.0, a MBA storage ring, expected to deliver emittance and brightness improved by up to two orders of magnitude<sup>56</sup>. Just for completion: several non-European Synchrotrons, i.e. APS and ALS in the USA, CLS in Canada, SIRIUS in Brazil, SPring-8 in Japan are in the process of up-grading, too.

No matter how spearheaded and groundbreaking, versatile and manifold science has been in the last decades, research is constantly evolving, and research facilities have to keep up. From the first X-ray image of the wedding ring and hand of Rontgen's wife to atomically resolved X-ray-analysis and tomography, innovation enabled the discoveries and will still pave the way transformative evolutions and revolutions in science and development.

Unpredictable gains in many areas of science, greater capacity and flexibility to accommodate new science drivers and communities are within the range of vision. X-ray performances a 100 times better than today are the first step into a new era of science in many fields.

**Higher Intensities or brightness** allow for unprecedented improvement in spatial resolution for microscopy, imaging, tomography, and diffraction, enabling novel types of experiments, open up the way to a routine-like provision of today's "heroic experiments" and drastically speed up experiments. Better performance, higher accessibility, and higher throughput will be amazingly beneficial for both, the quality and the quantity of experimental results and with this for the depth and the amount of created knowledge.

An important example here is the protein crystallography which is indispensable to understand the molecular background of diseases and plays a crucial role drug development. Its current potential was shown in chapter 1 and the need for extension and enhancement is more than evident.

But enhanced brilliance and flux will also be indispensable in energy research for fast operando investigations of chemical reactions (catalysis), electrode processes (batteries), or non-destructive characterisation of electron transfer in bulk or layered structures (solar cells, catalysts). The dream of spying and eaves dropping any material at work is in reach. Failure analysis of devices from macroscopic to atomic scale like aging of batteries and catalysts as well as basic understanding of materials properties profit greatly from more sensitive and precise identification of chemical species and electronic character during operation. Today in 90% of processes in the chemical industry at least one, often more catalysts are involved. The obligatory ingredient to tailoring catalysts is insight into the basic material properties and reactions often achieved with photon-hungry methods. Micro to nano focus beams, facilitated by high brilliance storage rings, will allow for direct and spectroscopic visibility of functional materials at the local to atomic level. Understanding of nanostructured or heterogeneous materials, where larger synchrotron spot sizes might average over several domains, inhomogeneities or even impurities, becomes accessible, which will boost the comprehension of nano and quantum materials, important in - inter alia- information technology.

**A step change in coherence** will be the enabler for high resolution 3D microscopy in the 10 nm range, a milestone in understanding how the component parts of a system interact with each other to generate higher-order functions and emergent properties of a system. In biology and medicine one could phrase it as "from atoms to bodies", creating a holistic view of molecules, organelles, cells to organisms, which will help for understanding and therewith fighting diseases such as cancer, dementia, viral infections and others. Next to transmission microscopy and imaging, coherent synchrotron

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<sup>55</sup><https://bib-pubdb1.desy.de/record/426140/files/DESY-PETRAIV-Conceptual-Design-Report.pdf>

<sup>56</sup> [SLS 2.0 | sls2-0 | Paul Scherrer Institut \(PSI\)](https://www.psi.ch/en/sls2-0) <https://www.psi.ch/en/sls2-0>

radiation is also the basic ingredient for holography, ptychography, and X-ray photon correlation spectroscopy to advance the understanding of fundamental physics and chemistry of quantum materials and to enable developments of novel functional materials e.g., spintronics, devices based on topological materials or neuromorphic computing

**Time resolution** is the key to investigate dynamic processes, perform operando experiments or follow (chemical) reactions. Adding dynamic information to the view of a static experiment will complete the picture. However, time resolution, spans over more than 20 orders of magnitude, from physical processes like magnetization in the femto-pico second range, chemical reactions often in pico-nano second time scales, to aging i.e. of catalysts or batteries in hours or weeks or hopefully decades. While free electron lasers deliver highest time resolution approaching few femto seconds, synchrotron pulses nowadays are usually in the 10s of pico second range with some exceptions like Femto Second Slicing<sup>57</sup> or low alpha storage ring operation<sup>58</sup>. However, the proposed or recent up-grades suffer from the sacrifice of shortness of the pulses for the benefit of brilliance and coherence. Time resolution in the pico and nanosecond range has to come in by spectroscopic and analytical methods like X-ray photon correlation spectroscopy<sup>59</sup>, while slower processes can easily be followed with fast and efficient detectors.

Going one step beyond the performance of the storage ring itself, the growing scientific community and the expansion of research fields provide their own challenges. Over the last decades the world of light sources became more diverse, a colourful bouquet of research topics, each with an instrumental and scientific challenge of its own. From physics to cultural heritage, from material science to dentistry, from energy to space science, the multitude enriches the eco-system synchrotron greatly. However, the need for additional infrastructure becomes apparent, synchrotron instrumentation has to be adapted or extended in a flexible way, to a manifold of requirements. Sample environment teams – rather new to synchrotrons - support users with design, construction, commissioning, or improvement of dedicated infrastructures, i.e. near ambient pressure modules, customised specimen grips, flow-through cells, liquid jets and more, tailor made for new applications and to the need of the user. The broader variety, the welcoming of non-synchrotron-expert user communities enhances multidisciplinary cooperations and seeds unprecedented networks. “Close to the X-rays” a comprehensive, extensive, and complementary variety of characterization and analysis tools, off line laboratories to enable in-situ materials’ fabrication and characterization have to be made available for parallel use with the synchrotron beam. Higher through put, faster experiments, and shorter beamtimes increase the attractiveness and outreach of synchrotron research even further.

A great step forward in making research at synchrotrons more open and inclusive for everyone is the implementation of remote access to synchrotron infrastructures. Stimulated by SARS-CoV-2 pandemic, solutions for performing experiments without being present on site open a new era in access to synchrotron-based research. Full or partial remote access – expedited by the pandemic situation- was at many beamlines worldwide. It is highly appreciated and gratefully received by the entire user community.

Further developments within this activity like standardized procedures for sample handling, validated protocols for data acquisition, automated data storage and archiving according to FAIR (Findable, Accessible, Interoperable, and Re-usable) data principles are on the agenda of the up-coming years.

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<sup>57</sup>[https://www.helmholtz-berlin.de/forschung/oe/ps/synchrotron-radiation-research/synchrotron/photons/x-ray-pulses/femtospex/index\\_en.html](https://www.helmholtz-berlin.de/forschung/oe/ps/synchrotron-radiation-research/synchrotron/photons/x-ray-pulses/femtospex/index_en.html) and [https://link.springer.com/chapter/10.1007/978-3-540-95946-5\\_39](https://link.springer.com/chapter/10.1007/978-3-540-95946-5_39)

<sup>58</sup><https://accelconf.web.cern.ch/PAC2009/papers/tu5rfp005.pdf> and <https://www.sciencedirect.com/science/article/pii/S016890021631316X?via%3Dihub>

<sup>59</sup> G. Gübel et al, **Correlation spectroscopy with coherent X-rays** [https://doi.org/10.1016/S0925-8388\(03\)00555-3](https://doi.org/10.1016/S0925-8388(03)00555-3)

An opportunity to participate in the experiments remotely is expected to be of increasing demand not only from experienced researchers who are not able to travel due to different reasons, but also from students from academia, new members to the synchrotron community and industry partners. It will lower barriers to make use of large scale facilities, will make experimental time more efficient, allow for attracting and involving newcomers, offers extended training options and creates routes to work simultaneously at different light sources benefiting from their complementarity. It will certainly foster transnational, interdisciplinary cooperation, and more efficient, synergetic use of synchrotrons.

**The cooperation of European research infrastructures, the different characteristics of light sources (i.e. ring energy<sup>60</sup>), and the emphasis on different scientific as well as instrumental and methodological foci are the key for a broad use of synchrotrons. Avoiding the duplication of efforts and a high complementarity as given in the European synchrotron landscape of the future will guarantee for maximising the scientific, economic and societal impact. The concentration of experts, resources, possibilities, and methods in dedicated facilities, guarantees for synergy, knowledge transfer and long-term continuity of know-how.**

#### 4. Synchrotrons in a societal context - Science Diplomacy, Science for peace

„Hoffentlich wird's nicht so schlimm, wie's schon ist.“(Karl Valentin) (Hopefully it will not become as bad as it already is).

##### 4.1. Science for global cooperation

As shown in the previous chapters, humanity is facing unprecedented challenges, which can only be addressed globally. However, a look at the worldwide (science and education) landscape reveals a massive imbalance of possibilities. Inequality, population explosion, poverty, social exclusion and lack of opportunity are strongly interlinked and have one cause in missing educational opportunities starting from primary schools to universities. Research and education are important pillars of sustainable development, gender equality, self-determination, self-empowerment, and with this economic success, participation, and cooperation at eye level. However, in the past decades the formerly so called third world was basically excluded from knowledge circulation; most of the intellectual exchange for example at conferences took arrogantly place in the northern hemisphere.

To solve global problems, intensified transnational cooperation, distribution of knowledge, and most importantly brain circulation are major ingredients. This idea has broken grounds and will be pursued with growing enthusiasm and verve in the next decades.

Noteworthy, online events and conferences, forced by current circumstances arising from the SARS-CoV-2 pandemic, were initially embraced with little enthusiasm. It has, however, brought more light to the issue of worldwide unequal access and opportunities in research and proven to bear some chances with respect to integration and inclusion as virtual settings present a great opportunity to involve and integrate people who might not be able to travel for a manifold of reasons, be it child care,

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<sup>60</sup> <https://lightsources.org/lightsources-of-the-world/>

home care, disabilities or simply the fact that many universities and institutes cannot afford the costs of sending their scientists to conferences in person.

In a LEAPS statement the vision is clearly and unanimously expressed: “A world where European science is a catalyst for solving global challenges, a key driver for competitiveness, a compelling force for closer integration, and an initiative for peace through tighter scientific collaboration<sup>61</sup>.”

#### 4.2. Science for Peace and Prosperity

Often unnoticed by the general public, scientists play an important role when political relations between countries were fraught or even not existent. The list is impressive and considering light sources alone the ability of science to reach across societal divides is tremendous. An idea in 1949 to establish a multinational scientific structure between countries which just fought each other, led 1954 to the foundation of CERN. CERN enabled contacts between nations separated by historical fractures and – to give just one example - paved the way for first Israeli-German contacts. In 1961, between the US and Japan, a first scientific cooperation committee restored the dialogue silenced by World War II; 1972 - USA-USSR - 5 agreements on cooperation in science and technology were signed by Brejnev and Nixon; in the same year the Shanghai Communiqué between China and the US expressed the will to settle differences peacefully and make science an area of cooperation. In 1997 the SESAME (Synchrotron Light for Experimental Science and Application in the Middle East) idea was developed at CERN based on CERN’s collaborations with the Middle East. Under the auspices of UNESCO the project started in 2002 with the founding members Bahrain, Cyprus, Egypt, Iran, Israel, Jordan, Pakistan, the Palestinian National Authority and Turkey, mirroring the strength of hope science shall spread in this region. SESAME opened its doors in 2017<sup>62</sup>.

In the years to come the project “Lightsource for Africa”<sup>63</sup> will be a chance for a more universal and regionally balanced participation in the global economy. Africa will soon become the home to the best part of the world’s youth<sup>64</sup>, these young people will need be part of the economy and developments. Currently, Africa as a whole has 169 scientist per 1 million people (cf. Europe 20 times more), a number that has to increase drastically to achieve economic development through innovation. Crystallization seeds for this development can be an investment in science and technology, international cooperation, and brain circulation at all levels. In the long run, no region or nation can remain a simple ‘user’ of new knowledge but must also become a ‘creator’ of new knowledge. Closing the innovation gap is a necessary role of science and research<sup>65</sup>;

The good news: it is expected that emerging economies will have around 63 million more university students in 2025 than today (2019) and the number worldwide is expected to more than double to 262 million<sup>60</sup>. Cooperation measured by the number of publications with authors from at least 2 countries increased from 8% in 1988 to 23% in 2009. A clear indication that brain circulation rules out the feared effect of brain drain.

An alignment of opportunities and the convergence in living standards are the godparents of a peaceful future and of a way to solve global challenges. Science will play an ever more important role accepting

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<sup>61</sup> [LEAPS-Brochure.pdf \(leaps-initiative.eu\)](#)

<sup>62</sup> Pierre-Bruno Ruffini Science and Diplomacy, A new dimension of international relations, Springer 2017, Chapter 5, ISBN 978-3-319-55103-6

<sup>63</sup> <https://www.africanlightsource.org/>

<sup>64</sup> S.H. Connell et al., Towards an African Light Source, <https://link.springer.com/article/10.1007/s12551-019-00578-3>

<sup>65</sup> <https://unesdoc.unesco.org/ark:/48223/pf0000235406>

its responsibility far beyond the creation of knowledge. The unbeatable advantage is the universal language of science, based on facts and experiments, a language that we can share across cultural and political borders which is truly international and will not fall silent even in situations of deadly hush in politics.

**More than ever before, individual scientists, large scale science facilities and science organization should become ambassadors. They are the facets in the kaleidoscope of scientific facts, global solutions, equal chances, and peaceful coexistence.**

## 5. Summary

„Prognosen sind schwierig, besonders wenn sie die Zukunft betreffen.“(Karl Valentin) „it is very difficult to predict — especially the future“

In this article, the authors tried to cast their net over the role of science and in particular synchrotrons to address the grand challenges of humanity, to provide answers to existential questions like climate change, sustainable energy supply or environment and health. Selected examples demonstrate the potential of research to convincingly and measurably strike new paths.

The other side of the very same coin is curiosity, unpredictably leading to revolutionary developments. In times of pressing challenges the twin-track approach of – sometimes indistinguishable - basic and applied science is the order of the day.

Both will greatly profit from extended instrumental and scientific opportunities, provided by the next generations of synchrotrons. New frontiers can be transcended, unprecedented solutions found, unforeseen developments triggered.

However, there is more to science than knowledge and increasing insight. Science has a responsibility to bring the world closer together for the benefit of all humans, for peace and equal opportunities. Research and synchrotron facilities are aware of their colourful bouquet of responsibilities and accept them with great pleasure.

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