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EDITORIAL

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Physical chemistry of the energy transition

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Climate change is no longer a distant possibility but a daily reality all over the world. Global warming in concert with increasing atmospheric CO_2 concentrations are steadily progressing with not the slightest sign of reduced effects. Future CO_2 concentrations in the atmosphere are a cumulative result of past, current and future human emissions. When considering the decades long residence time of CO_2 in the atmosphere, it is very unlikely that the political target to limit warming to 2° will be met; if true, global warming will become an even more serious issue. Active removal of atmospheric CO_2 (*e.g.* direct air capture) is still only a futuristic option, considering the scale (Gt per a in CO_2) of needed removal.

It is thus critical that we stop debating and now evolve our energy systems from linear ones into circular structures. Sadly, it took way too long to convince all the stakeholders how this can be accomplished without reducing our necessary energy consumption – there is enormous waste in the current system resulting from the fact that the cost of environmental CO_2 damage is not built into the price.

Energy systems of the future will use free electrons generated through solar energy as their basis, a vast resource on a planet whose land surface area receives 4500 TWa per a, which can potentially be converted to electricity. Compare this to the current total energy demand of about 20 TWa per a. But problems remain to be solved, before a ''drop-in'' solution of renewable electricity for fossil power can be achieved. Solar energy is volatile and the best locations for its production (*e.g.* deserts, stormy coasts, *etc.*) are far from where energy is needed. Furthermore, electrical storage in batteries is only a local solution useful for short-time volatility. There is a better way.

The solution is to ''liquify sunshine'' by chemically converting primary solar electricity to molecular energy carriers, which can be thought of as ''chemical batteries''. The concrete tasks involve developing optimal CO_2 neutral technologies that can both convert solar electrons into chemical bonds and recover the stored energy, effectively discharging these ''chemical batteries''. This concept mirrors the natural carbon cycle of life, but uses high performance conversion chemistry capable of serving the energy density requirements of human activity.

The resistance of some stakeholders to this approach is still substantial and is partly justified by an efficiency argument. A circular molecule-based conversion process is indeed less energy-efficient than the immediate and direct use of renewable electricity, at least for the case where an electro-mechanical or thermal energy application is desired. In order to serve the ultimate goal of minimizing the climate change produced by human energy consumption, this system energy efficiency is, of course, relevant. Hence, we have to see that the process design serves the system needs best, bearing in mind that although we lose up to 80% of the initial solar energy, it is available in great excess. Following this logic, we must design double-functioning energy systems combining the local use of solar electricity whenever possible, with molecular energy carriers being made from dedicated sources of renewable electricity in remote locations.

Understanding and developing the means for charging and discharging of these chemical batteries is a central task – one could say THE central task – of physical chemistry. The ''value chain'' begins with water splitting to produce green hydrogen, which is a suitable energy carrier for selected applications

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with, however, unfortunate physicochemical properties. For a more general system service, the hydrogen must be converted in a second refinement step to derivatives (*e.g.* ammonia) that exhibit a transport and usage profile similar to the present fossil energy carriers. In this way, we can de-fossilize those parts of our energy systems that are hard to electrify in the short term. This model also has the advantage that existing infrastructure and applications will need only minimal changes. The derivative molecules are important, since they can store energy for an unlimited time and in large amounts. They allow energy to be a commodity within global trade and enable the supply of sustainable energy to those regions without a potent energy distribution infrastructure.

The basic science and technology for all of this is catalysis in the form of electrocatalysis, forming the interface between free electrons and bound electrons and as thermal catalysis for producing the derivative molecules. Sorption and washing processes will also be needed to clean and condition the feed streams for catalysis and to close the carbon circle. These tasks all fall within the core competence of physical chemistry and it is thus absolutely fair to say that physical chemistry is the enabling science for sustainable energy systems, and therefore, for mitigating climate change.

Although much is deliberated in project announcements to start the changeover in our energy systems, it is not understood sufficiently well that an enormous amount of science and technology is still needed in order to realize the value chain of liquid sunshine in the dimension required. It is estimated that the EU as a 10% contributor to the global energy demand despite its efforts in the ''Green Deal'' still has to de-fossilize 13 600 TW h per a of primary energy consumption. Even if we optimistically assume that 80% of this can be electrified and saved through increased efficiencies, we would still need 80 Mt per a hydrogen or 600 Mt per a ammonia production to reach this goal. Compare this to the current world production of ammonia (150 Mt per a). Clearly, enormous efforts are needed that will likely take much more time than foreseen by our political planners.

Physical chemistry offers us enormous potential for improvements through rational design of catalytic processes based upon optimized catalysts and engineering solutions within the systemic context of internationally integrated production and use of energy carriers. The Bunsen-Tagung 2023 that was held in Berlin from June 5th to 7th 2023 was dedicated to the ''Physical Chemistry of the Energy Transition'' and exactly addressed the severe issues summarized above. Bringing together over 500 scientists active in physics, chemistry, material science, engineering, theoretical modeling and various other disciplines clearly showed the diversity of the field and provided the necessary platform to discuss the newest results for the various facets of physical chemistry related to energy transformation and storage.

The conference showed that many tools for the design task exist in basic science both on the theoretical and on the experimental side. However, we lack the broad-based use of advanced methodologies in *operando* experimentation, data-centric meaningful testing and advanced theories bridging the material gap. Only if we can convince all stakeholders from academia, industry, politics and funders to now really make a concerted effort in bringing to bear our conceptual tools, will we be able to deliver the promise of ''technology leadership''. It must be founded on a robust knowledge base rather than on empirical accidental developments. The time to act is now!