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Concept of a Public Outreach Project on PCET Reactions

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Abstract

Reactions involving proton-coupled electron-transfer (PCET) steps are of enormous relevance for processes in biology and chemical industry. Furthermore, PCET is the key to enable and optimize the most important reactions for the transition to a sustainable future: Electrochemical nitrogen fixation and CO_2 reduction involves PCET and therefore its detailed understanding as well as the development of optimized catalysts (both heterogenous and homogenous) is the overarching goal of a proposed collaborative research center (CRC) based in Göttingen with participating institutions from all over Germany.
However, despite the relevance of PCET for processes that are already taught in school e.g., photosynthesis[1] and water electrolysis, the importance of coupled proton and electron transfer for these processes is rarely known and not explicitly mentioned. In this contribution, we will present our science outreach strategy to make basic principles as well as recent results from fundamental research on PCET more visible to the public. Our outreach measures include teaching materials and educational offers targeting both school students and the general public. They will consist of a "PCET portfolio" with curricular valid teaching materials ranging from fundamental concepts and tools ("How to read a Pourbaix diagram?") to adapted experiments and literature[2] closely related to the actual research (e.g., electrochemical functionalization of hydrocarbons[3]). Targeting the general public, we develop exhibitions for science museums and public events in a close collaboration with participating researchers. In addition, impressions from lab work, recent publications and the daily life of young researchers will be shared via social media.
Overall, apart from communicating scientific content and to transfer knowledge about PCET, we aim to strengthen the appreciation of fundamental research and to show how interdisciplinary and collaborative research works. The latter is predominantly targeting young people to help them in their vocational orientation and motivate them to become the scientists of tomorrow.

Keywords: *Science Outreach, PCET, Science Exhibition*

1. Introduction

The coupled transfer of protons and electrons is a common phenomenon observed in various reactions with fundamental importance for nature and industry. Its understanding is crucial for the development and optimization of reaction pathways and tailored catalysts to enable a transition to a more sustainable society and industry Such processes make use of reactions which can be described as the "grand challenges" of sustainable chemistry:

$$2\ H^+ + 2\ e^- \rightleftharpoons H_2 \qquad \text{(eq. 1)}$$

$$2\ H_2O \rightleftharpoons H_2O_2 + 2\ H^+ + 2\ e^- \rightleftharpoons O_2 + 4\ H^+ + 4\ e^- \qquad \text{(eq. 2)}$$

$$N_2 + 6\ H^+ + 6\ e^- \rightleftharpoons 2\ NH_3 \qquad \text{(eq. 3)}$$

$$CO_2 + 2\ H^+ + 2\ e^- \rightleftharpoons CO + H_2O \qquad \text{(eq. 4)}$$

$$R_3C{-}H + H{-}X \rightleftharpoons R_3C{-}X + 2\ H^+ + 2\ e^- \qquad \text{(eq. 5)}$$

The immediate importance of water splitting with the associated reactions of hydrogen reduction and oxygen oxidation (eq. 1) is well known even in the general public as it offers a great potential for the storage of electrical energy from renewable sources (like e.g., wind or solar generators). Less

commonly known are the other reactions mentioned, like the electrosynthesis of hydrogen peroxide as a safe and environmentally friendly oxidizing agent.
The next two reactions (eq. 2 and 3) describe the use of relatively inert atmospheric gases for the synthesis of building blocks important for the production of fuels, fertilizers and a variety of chemical compounds. In the case of carbon dioxide reduction (eq. 4), this also to decrease the emission of the most prominent greenhouse gas or in combination with direct-air-capture the active lowering of atmospheric carbon dioxide levels. The selective C-X bond cleavage (X = O, N, C) and the reversed process of C-H-activation described in eq. 5 focusses on converting biopolymers from renewable feedstock to valuable chemical products.
Despite the described importance, the term “proton-coupled electron transfer” was not very well defined in the scientific literature for a long time[4]. In general, when transferring both, an electron and a proton, the transfer can either be concerted or consecutively with major differences in the underlying mechanisms. Therefore, some authors coined the term electron-proton transfer (EPT) exclusively for the concerted pathway and propose the use of “proton-coupled electron transfer” (PCET) for the more general class of reactions[5]. We will follow the latter definition to broaden the scope to an even wider range of reactions with profound educational potential. More importantly, this is also consistent with the use of this term in the particular Collaborative Research Center (CRC) described below.

2. The CRC 1633 - “Pushing electrons with protons”

The overarching research goal of the CRC is to unify physicochemical models about the three main classes of catalysts (homogenous and heterogeneous as well as enzymatic catalysts) for specific reactions and/or substrates. Catalysis plays such an important role for the mentioned processes, as the substrates like nitrogen, carbon dioxide and C-H-bonds are very inert in nature and need to be activated to overcome electrochemical overpotentials. The central approach of the CRC is to understand PCET at the atomic scale which will enable the optimization of existing solutions for the target reactions and develop new ones. This fundamental research is only possible with the interdisciplinary work of chemists with expertise in organic synthesis, electrochemistry, homo- and heterogenous catalysis, biochemists and experts on surface science, theory and computational chemistry. The framework for such a comprehensive research effort is given by the DFG (Deutsche Forschungsgemeinschaft, *German Research Foundation*) which provides funding for these large interdisciplinary projects called “Collaborative Research Centers” (CRC). In case of CRC 1633, 28 principal investigators from seven universities and research institutions in Germany are granted a funding for a four year period, ensuring the success of this project which then can apply to be extended for two additional funding phases of four years each.
The CRC is subdivided into 16 projects researching on various aspects of PCET regarding the “grand challenges” mentioned before, jointly lead by experts from the respective fields. These projects are organized in the form of both “working groups” representing the research goals (I: The PCET site, II: Enabling PCET Catalysis, III: Beyond Catalyst Design) and “project groups” reflecting the type of reaction and catalysis investigated (A: Molecular PCET, B: Biological PCET, C: Interfacial PCET).
The CRC steering committee highly acknowledges the value of public outreach for both, communicating importance and basics of PCET science in an appropriate way to various target groups as well as fostering the appreciation for (fundamental) research in general. Therefore, a dedicated outreach project is funded as an integral part of the CRC. The outreach project closely cooperates with the scientific projects with the help of a science outreach advisory board comprised of three scientists representing their respective project group.

3. Outreach approach and strategy

To reflect the interdisciplinary structure of the CRC itself, the public outreach project is jointly sustained by experts in physics and chemistry education, respectively.
The public outreach project will act as an important link between the CRC, the involved researchers, and the obtained results on the one hand and the society as a whole on the other hand. Crucial for its success is the intense and coordinated collaboration between research groups and the departments of chemistry and physics education to develop and implement attractive outreach activities which provide insights into scientific processes. These activities will be developed for the interested general public and implemented on science fairs and local events.
However, to make the understanding for and appreciation of science in general and this CRC in particular more sustainable, we focus on schools and school students as a central target group. By connecting fundamental research to concepts and phenomena reflected in chemistry and physics

curricula, CRC related research can be widely distributed to a large audience of young people in the age of 16 to 19 who are not only the next generation of society but can also be motivated to become the scientists of tomorrow.
The planned public outreach activities will be developed in jointly supervised bachelor and master theses and in workshops with PhD students. They will be designed with respect to preconceptions of the selected target group, applicable educational standards, the learning environment and expectations of the audience, respectively. The science outreach advisory board will support the public outreach team in identifying topics suitable and relevant for outreach measures. These include research questions of general interest in the context of sustainability and scientific results reported in recent publications from CRC researchers. They will be selected with scientific advice from the involved project concerning the possibility to develop adapted and simplified experiments and other materials while preserving scientific correctness.

Figure 1. Examples from previous public outreach projects for formal education (Course at the XLAB, left) and the interested public (exhibition at a science fair, right).

3.1 Educational offers for schools and school students

Although PCET reactions play an important role in nature, science, technology and the everyday life, their relevance is rarely known in the society and also in the formal education sector they are only implicitly addressed at best. Important processes like the respiratory chain, photosynthesis[1] as well as electrolysis and fuel cells are integral parts of school curricula but the involved chemical reactions are in most cases not categorized as PCET. Therefore, the projects in this section focusses on educational offers developed according to educational guidelines connecting PCET reactions in general and CRC related research in particular to subjects covered in the curricula and to implement corresponding materials and concepts for the formal education sector. Apart from promoting scientific knowledge about PCET, further main objectives of these offers are to provide insights into scientific processes and to support students in their vocational orientation. To ensure a widespread dissemination of the respective offers, this science outreach project will make use of established structures like the cooperation with contractual partner schools, school laboratories and regular events on study orientation. To ensure a successful communication of scientific concepts, methods and results we will evaluate and optimize accessibility and comprehensibility of the developed materials using qualitative and quantitative methods of educational research as well as eye-tracking techniques.
The developed educational materials like experiments, information texts, digital materials and adapted primary literature (APL) are compiled into an expandable PCET portfolio which will be available free of charge as an open educational resource (OER). To foster widespread use, we will conduct further teacher trainings at the end of the funding period, where the participants are introduced into how these materials relate to curricular standards and they can be used in upper secondary education.
Additionally, courses at the student laboratory ‘XLAB – Experimental Laboratory for Young People’ as extracurricular activities will provide school students with more advanced experiments not readily

viable for the use in most high schools. Several of these courses will be combined to a science camp aiming at highly motivated school students with ambitions to study chemistry or physics.

3.2 Offers for the interested public

Apart from the formal education sector, the focus in this project lies on enhancing the communication between science and the interested public. In order to raise the interest and the appreciation of science in the public's eye and to contribute to a scientific literate society, opportunities for an exchange between scientists and the general public will be created. To achieve this, we will provide insights into the often complex scientific system, increase transparency of the structural organization of scientific institutions, explain interdisciplinary research and the relevance of fundamental research for sustainable developments like a fossil-free future. For this purpose, we will utilize existing and established outreach structures and events at the University and explore new formats and ways for public outreach communication, both on-site and online. These include for example the science fair 'IdeenExpo' with approx. 425.000 visitors, the Göttingen Night of Science with approx. 25.000 visitors and social media channels with relevant posts about science and beyond called "Protons, Papers, PhD: Young Scientists in CRC 1633". The planned activities for these events and formats will be developed, organized and implemented in close cooperation with scientific and educational personnel through recurring joint workshops, a collaboration with the public relations department as well as the "Forum Wissen".

3.3 First steps

The CRC is going to start in April 2024 and will be accompanied with the public outreach activities right from the beginning: The general importance of PCET and the potential of fundamental research in this field for a more sustainable future will be presented at local science communication events like 'Science goes City' (May) in Göttingen and the 'IdeenExpo' fair in Hannover (June). Simultaneously, the screening process to identify suitable subject matter for developing the first building blocks of the PCET portfolio will take place in close collaboration with the science outreach advisory board and the steering committee. Starting from general concepts, methods and terminologies in PCET science will be adapted into teaching materials for school students. This includes an already ongoing thesis focusing on the construction and use of Pourbaix diagrams as a valuable tool to visualize the pH-dependence of redox potentials in various redox systems.

4. Summary

Our approach to identify and select suitable topics, develop corresponding activities and materials as well as disseminate them to the respective target groups can be summarized in figure 2.

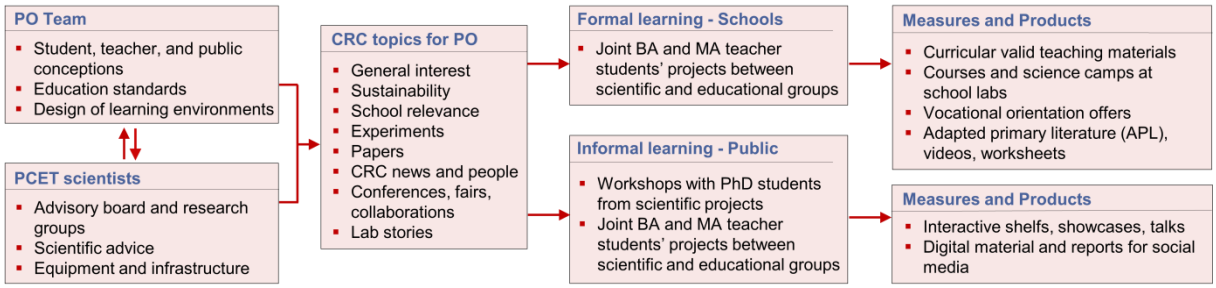

Figure 2. Schematic diagram on the development and dissemination of public outreach measures.

The unique potential of PCET to connect complex fundamental research with apparently simple reactions offers various opportunities to facilitate a dialogue between academia and the rest of the society represented by the interested public, teachers and school students.

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