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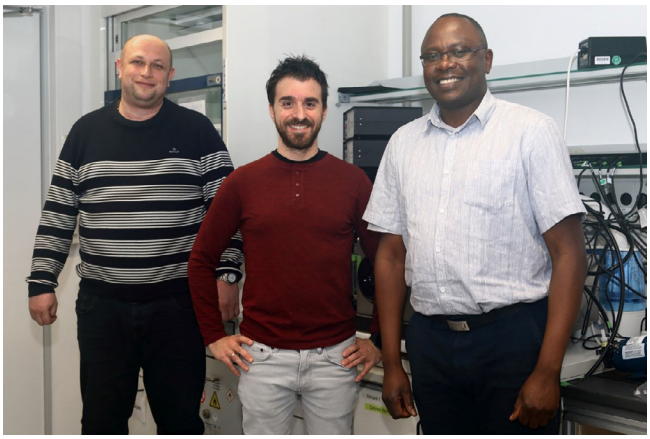
Electrocatalysis Beyond 2020: How to Tune the Preexponential Frequency Factor

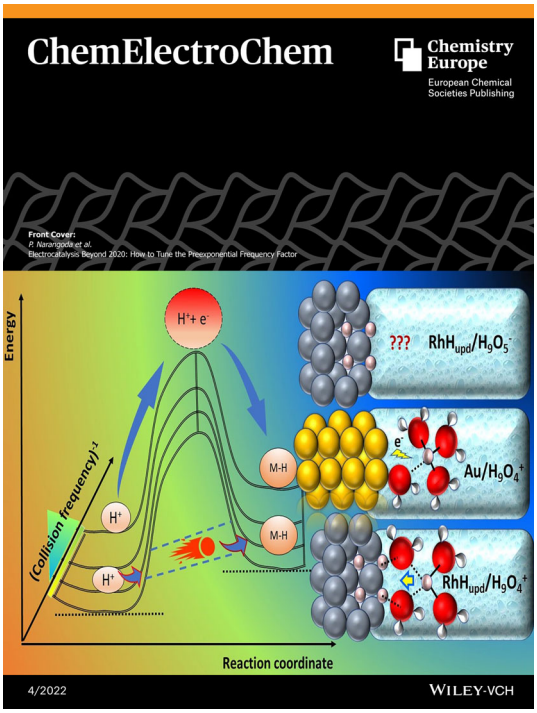


From left to right: Dr. Aleksandar R. Zeradjanin (Scientific Staff and coordinator of activities in the area of Physical Electrochemistry), Dr. Ioannis Spanos (Head of Electrochemistry Group and coordinator of activities in area of Analytical Electrochemistry), Dr. Justus Masa (Scientific Staff and coordinator of activities in the area of Material's Electrochemistry).

Invited for this month's cover picture are Dr. Aleksandar R. Zeradjanin and colleagues, from the Max Planck Institute for Chemical Energy Conversion, Mülheim an der Ruhr, Germany. This cover is part of the Special Collection dedicated to the 65th birthday of Prof. Wolfgang Schuhmann. The cover picture shows how metals with more destabilized interfacial water molecules could behave as efficient electrocatalysts for hydrogen evolution reaction (HER) where high reaction rate, despite of relatively high activation energy, is possible to achieve via high values of preexponential factor by proton tunnelling. While destabilization of the proton's solvation sphere in acidic electrolytes is intuitive, in alkaline media this proceeds via a more complex mechanism. Read the full text of the Article at 10.1002/celc.202101278.

What is the most significant result of this study?

The most significant result is that for the first time, after many decades, we now know the answer to one of the most essential questions in electrocatalysis, that is: does activation energy predominantly control reaction rate as widely accepted? For the example of HER on Rh in alkaline electrolyte, we observed that high reaction rate is achieved on a metal that has a substantial activation barrier, but at which the preexponential frequency factor (exceptionally high number of collisions) compensates for the high activation barrier. We predicted the possibility of this outcome in the past despite literature suggesting that reducing activation energy by tuning the adsorption energetics of reaction intermediates is the ultimate approach to enhance electrocatalyst activity.



What was the biggest surprise (on the way to the results presented in this paper)?

The biggest surprise was when we discovered that after 70 years of conceptual shaping of hydrogen electrocatalysis and more than 100 years of experimental research, there was practically no thorough systematic investigation of high- tempera-

ture hydrogen electrochemistry covering a significant number of samples/electrocatalysts. That required lot of patience and dedication of the main experimentalist (Dr. Praveen Narangoda, postdoctoral researcher) and in-depth analysis that was possible due to strong interaction inside our Electrochemistry Group (see the group photo and description).

Is your current research mainly curiosity driven (fundamental) or rather applied?

We believe that research is always curiosity driven. It is fascinating to search for answers on real-life problems in fundamental science. That is the mentality of our Electrochemistry Group as well as that of the founding and managing director of our institute Prof. Robert Schlögl. The Electrochemistry group was initiated as a part of the Department of Heterogeneous Reactions with the ambition to establish strong ties with the Department of Inorganic Spectroscopy as well as the Department of Molecular Catalysis, to essentially link the departments through dedicated expertise and infrastructure in Electrochemistry. Our essential motive is to discover how to further accelerate key electrocatalytic reactions related to electrochemical energy conversion and storage. On that road, it is necessary to complement the existing paradigm of electrocatalysis based on the Sabatier principle and adsorption energies, with more realistic concepts. For that we developed a roadmap that we follow, without excluding serendipity. We strongly believe that our efforts will open some important new fundamental research avenues relevant for electrocatalyst design.

What was the inspiration for the cover design?

Inspiration for the cover design (what is probably not obvious…) comes from the Lord of the Rings, where Fellowship of the Ring initially used high pass Redhorn Gate to cross Caradhras in the Misty Mountain, but then after facing insurmountable difficulties, they decide instead of crossing the mountaintop to go through the mountain tunnels, through unknown territory, Mines of Moria.

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COVER PROFILE

"After a century of electrocatalysis based on tuning of activation barrier by modifying adsorption energies of intermediates, awareness is developed about the possibility to achieve very high reaction rate via high values of preexponential factor despite of high activation barrier. From the dissection of the rate law we concluded that there are overall eight parameters that contribute to reaction rate and on that basis new structure-activity relations are required where each of these parameters will be correlated to some property of material or property of the electrode/electrolyte interface…" Learn more about the story behind the research featured on the front cover in this issue's Cover Profile. Read the corresponding Article at 10.1002/celc.202101278.

*P. Narangoda, I. Spanos, J. Masa, R. Schlögl, A. R. Zeradjanin**

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