are then transferred to the plant[9].

Mohr and colleagues' observations raise many questions. The authors considered other interactions integral to the symbiosis, including the bacterial metabolic reactions that fuel nitrogen fixation, and mechanisms by which the seagrass might regulate this process. These include promoting the transport of oxygen through plant roots to support the respiratory demands of the bacteria in the otherwise oxygen-poor environment of the sediments where seagrasses are usually rooted. However, the bacterium's oxygen requirements might need to be balanced by complementary adaptations to prevent inhibition of the oxygen-sensitive nitrogenase enzymes that are needed for nitrogen fixation. The authors also speculate about how this plant–bacterial symbiosis evolved. The next challenge will be to isolate and grow the bacterium for more-detailed physiological study to investigate the symbiosis further. On a larger scale, analysing other broadly distributed tropical and subtropical seagrasses, such as species of *Thalassia*, *Zostera* and *Syringodium*, for the presence of nitrogen-fixing partners would be a logical next step.

As is the case for organisms in many marine ecosystems, seagrasses are under severe threat, and restoration efforts are under way worldwide[10]. Developing a fundamental understanding of the underlying microbial interactions that support seagrass growth will surely help in these efforts.

Douglas G. Capone is in the Department of Biological Sciences, University of Southern California, Los Angeles, California 90089, USA.
e-mail: capone@usc.edu

1. Larkum, A. W. D., Orth, R. J. & Duarte, C. M. (eds) *Seagrasses: Biology, Ecology and Conservation* (Springer, 2006).
2. Lovelock, C. E. & Duarte, C. M. *Biol. Lett.* **15**, 20180781 (2019).
3. Mohr, W. *et al. Nature* **600**, 105–109 (2021).
4. Thies, J. E. in *Principles and Applications of Soil Microbiology* 3rd edn (eds Gentry, T. J., Fuhrmann, J. J.& Zuberer, D. A.) 455–487 (Elsevier, 2021).
5. Zuberer, D. A. in *Principles and Applications of Soil Microbiology* 3rd edn (eds Gentry, T. J., Fuhrmann, J. J.& Zuberer, D. A.) 423–453 (Elsevier, 2021).
6. Larkum, A. W. D., Waycott, M. & Conran, J. G. in *Seagrasses of Australia: Structure, Ecology and Conservation* (eds Larkum, A. W. D., Kendrick, G. A. & Ralph, P. J.) 3–29 (Springer, 2018).
7. Welsh, D. T. *Ecol. Lett.* **3**, 58–71 (2000).
8. Cramer, M. J., Haghshenas, N., Bagwell, C. E., Matsui, G. Y. & Lovell, C. R. *Int. J. Syst. Evol. Microbiol.* **61**, 1053–1060 (2011).
9. Clúa, J., Roda, C., Zanetti, M. E. & Blanco, F. A. *Genes* **9**, 125 (2018).
10. Evans, S. M., Griffin, K. J., Blick, R. A. J., Poore, A. G. B. & Vergés, A. *PLoS ONE* **13**, e0190370 (2018).

Electrocatalysis

Water molecules directed to speed up dissociation

Matthias M. Waegele

A technical feat reveals subtle changes in water structure that can accelerate hydrogen production at an electrode interface. The catalytic process could be developed to help boost supply of this clean fuel. **See p.81**

Electrocatalysis, which accelerates chemical reactions driven by an electric potential at a solid–liquid interface, could be a key contributor to a sustainable global economy because it can convert electrical energy from renewable power sources into green fuels such as hydrogen gas[1]. On page 81, Wang and colleagues[2] describe an important advance in the molecular understanding of how the rate of an electrocatalytic process is rooted in the structure of water at the interface between a solid electrode and an aqueous salt solution (an electrolyte). Their findings could help to improve the reaction selectivity and energy efficiency of electrocatalytic interfaces.

Many of the unique physical–chemical properties of liquid water can be ascribed to the network of weak attractive forces of hydrogen bonding between molecules[3].

Water molecules at an interface formed by liquid water and a gas, solid or another liquid necessarily have fewer hydrogen-bonding partners. Those within one or a few molecular layers from the interface therefore often adopt different structural motifs (geometric arrangements of molecules) from those in the bulk liquid[4,5].

Spectroscopic techniques that probe the stretching of bonds between oxygen and hydrogen, or the vibrations of 'bending' water molecules, have contributed to our understanding of the structure of interfacial water[5,6]. Analysis of these vibrations by infrared or Raman spectroscopy of interfacial water reveals the strength of the hydrogen-bonding network and the presence of specific structural motifs at the interface. Such experiments are technically challenging because
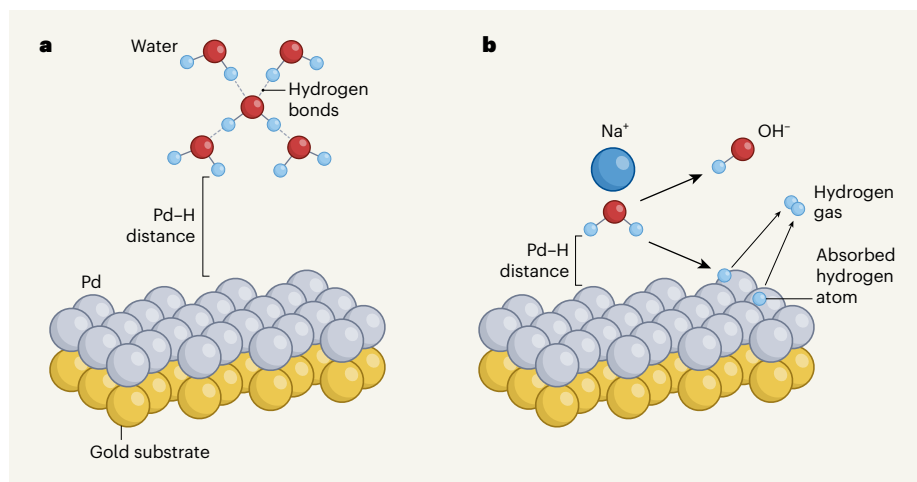
Figure 1 | Catalysis of water dissociation at a palladium electrode. Wang *et al.*[2] studied the structure (geometric arrangement) of water molecules at the surface of an electrode. **a**, At low concentrations of dissolved sodium ions (Na+, not shown) and at relatively positive electrode potentials, a network of water molecules connected by intermolecular hydrogen bonds surrounds the electrode, which comprises a layer of palladium (Pd) atoms on a gold substrate. **b**, At higher concentrations of sodium ions and at relatively negative electrode potentials, hydrated sodium ions (those with associated water molecules) are electrostatically attracted to the electrode, narrowing the distance between Pd atoms and hydrogen atoms in the water molecules. This accelerates electron transfer between the electrode and the water molecules, causing the water to dissociate into hydroxide ions and hydrogen atoms; the hydrogen atoms initially adsorb to palladium atoms, and then combine to form hydrogen molecules (H_2).

they require sophisticated methods capable of selectively probing only a few layers of water at the interface. Furthermore, the interpretation of vibrational spectra is complicated by coupling effects between vibrations in the water molecules themselves[7].

Water molecules at electrolyte–electrode interfaces undergo a reorientation when the surface charge on the electrode changes from positive to negative, or vice versa[8,9]. This reorientation is due to the interaction of electric dipoles of the molecules with the interfacial electric field that arises from the electrode surface charge, which is controlled by the electrode potential. At high potentials, positive or negative ions (cations or anions, respectively) in the electrolyte, whose charge is opposite to that of the net surface charge on the electrode, concentrate in the vicinity of the electrode. This increased concentration of ions is expected to affect the interfacial water structure. However, under potentials at which the electrocatalytic conversion of water to hydrogen occurs, the formation of bubbles of hydrogen gas interferes with spectroscopic measurements, making spectroscopy under reaction conditions highly challenging.

Wang *et al*. have neatly circumvented these difficulties by devising an innovative experimental approach in conjunction with Raman spectroscopy. They used a metal electrode comprising palladium atoms to act as a catalyst that dissociates water into molecular hydrogen (H_2) and hydroxide (OH^-; Fig. 1). As the electrode potential became more negative, they found that the water structure gradually shifted from a relatively disordered to a more ordered state.

The spectroscopic evidence indicates that this transition could be due to weakening of the hydrogen-bonding network, with a loss of water molecules that originally had four hydrogen-bonding partners and a concurrent gain of water molecules associated with sodium cations (Na^+) from the electrolyte; such water molecules form a 'hydration shell' around the ions. Hydrated sodium cations are electrostatically attracted to the negatively charged electrode surface and accumulate at the interface. Intriguingly, the authors found that the population of interfacial water molecules in the hydration shell of sodium ions tracks the rate of hydrogen formation across different single-crystal surfaces of palladium.

For a molecular picture of the more ordered state of interfacial water and its role in the rate of hydrogen formation, Wang *et al*. turned to *ab initio* molecular-dynamics modelling. They found that water in the hydration shell of the sodium ion can more closely approach the electrode surface than can other water molecules. This manifests in a more pronounced shift of the O–H stretching vibration of water associated with a sodium ion when the electrode potential decreases. Their theoretical

modelling indicates that narrowing the physical gap between the hydration shell and the palladium surface aids electron transfer from the electrode to the water, enhancing the rate of water dissociation into molecular hydrogen and hydroxide ions.

The insights derived from this work are relevant to other technologically useful electrocatalytic processes that involve water dissociation, such as the hydrogenation of carbon dioxide to hydrocarbons or

> "The authors have shown that the structure of interfacial water can be systematically tuned."

of nitrogen gas to ammonia. In those reactions, the dissociation of water needs to be carefully controlled to achieve the desired product selectivity. Wang *et al*. have shown that the structure of interfacial water, and, consequently, the dissociation of water, can be systematically tuned by appropriate choice of the electrode's crystal facet and the electrolyte's cation concentration and identity.

Inevitably, some questions remain. For example, how do the dynamics of interfacial water change with decreasing potential? These

dynamics could be crucial in the formation of hydrogen and in electron transfer[10,11]. Investigations are now required to study the extent to which the dynamics of interfacial water at electrocatalytic interfaces can be altered with decreasing electrode potential.

Matthias M. Waegele is in the Department of Chemistry, Merkert Chemistry Center, Boston College, Chestnut Hill, Massachusetts 02467, USA.
e-mail: waegele@bc.edu

1. Katsounaros, I. & Koper, M. T. M. in *Electrochemical Science for a Sustainable Society* (ed. Uosaki, K.) 23–50 (Springer, 2017).
2. Wang, Y.-H. *et al. Nature* **600**, 81–85 (2021).
3. Kumar, R., Schmidt, J. R. & Skinner, J. L. *J. Chem. Phys.* **126**, 204107 (2007).
4. Velasco-Velez, J.-J. *et al. Science* **346**, 831–834 (2014).
5. Tuladhar, A. *et al. J. Am. Chem. Soc.* **142**, 6991–7000 (2020).
6. Gopalakrishnan, S., Liu, D., Allen, H. C., Kuo, M. & Shultz, M. J. *Chem. Rev.* **106**, 1155–1175 (2006).
7. Sovago, M. *et al. Phys. Rev. Lett.* **100**, 173901 (2008).
8. Ataka, K., Yotsuyanagi, T. & Osawa, M. *J. Phys. Chem.* **100**, 10664–10672 (1996).
9. Schultz, Z. D., Shaw, S. K. & Gewirth, A. A. *J. Am. Chem. Soc.* **127**, 15916–15922 (2005).
10. Remsing, R. C., McKendry, I. G., Strongin, D. R., Klein, M. L. & Zdilla, M. J. *J. Phys. Chem. Lett.* **6**, 4804–4808 (2015).
11. Ledezma-Yanez, I. *et al. Nature Energy* **2**, 17031 (2017).

Mathematics

AI aids intuition in mathematical discovery

Christian Stump

Machine-learning tools have been used to assist the part of mathematical research that usually relies on human intuition and creativity — leading to two fundamental results in different areas of mathematics. **See p.70**

Mathematicians have been developing theories by studying examples throughout history. For instance, by looking at a cube and a pyramid, one might realize that the number of vertices, edges and faces are related. A mathematician recognizes such a pattern, extends it to more-general shapes, and then starts to think about why this relationship might hold. Parts of this process involve computations, for which mathematical software has been useful since it first became available in the 1960s. However, human creativity enables mathematicians to instinctively understand where to look for emerging patterns. On page 70, Davies *et al*. now describe a way of using artificial

intelligence (AI) techniques to help with the creative core of the mathematical-research process[1].

The relationship between the properties of convex polyhedra (3D shapes with flat faces, straight edges and vertices that all point outwards) was found centuries ago, and the formula describing this relationship is named after the Swiss mathematician Leonhard Euler. Regardless of the shape, the number of vertices (V) minus the number of edges (E) plus the number of faces (F) is equal to two: $V - E + F = 2$ (Fig. 1). Can you arrive at this formula by studying a few examples of different shapes with a pen and paper? In this case, it's possible, but