Nano-confinement may be key to improving hydrogen production

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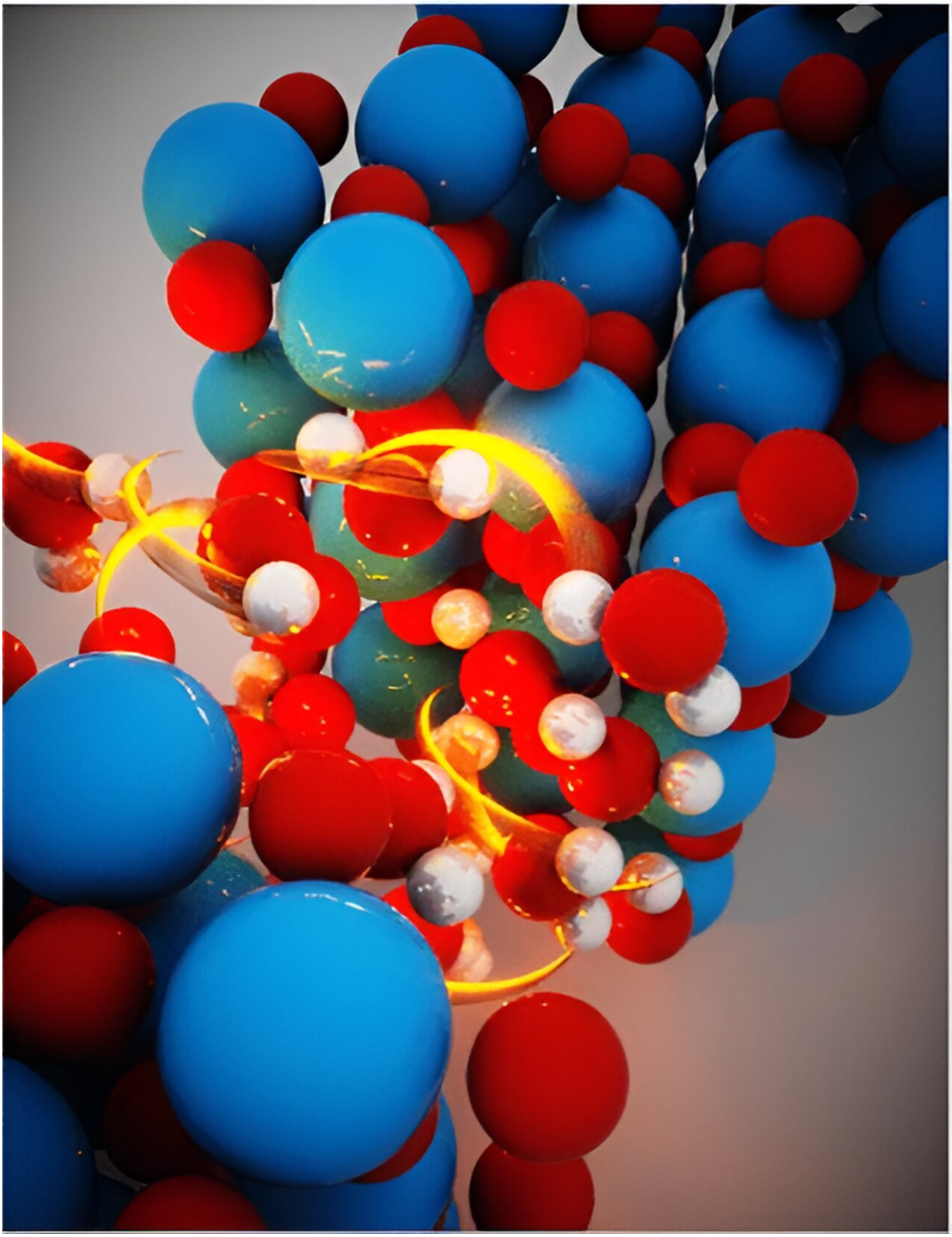

Credit: *ACS Applied Materials & Interfaces* (2024). DOI:

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Researchers at Lawrence Livermore National Laboratory (LLNL) have discovered a new mechanism that can boost the efficiency of hydrogen production through water splitting.

This research, published in *ACS Applied Materials & Interfaces*, was featured on the journal cover and provides new insights into the behavior of water reactivity and proton transfer under extreme confinement, suggesting potential strategies to enhance the performance of electrocatalysts for hydrogen production, while protecting the catalyst from degradation.

Hydrogen production via photoelectrochemical water splitting has long been considered a "Holy Grail" of electrochemistry. A key for the widespread deployment of this technology is the development of an active, durable, yet affordable electrocatalytic system.

Together with Columbia University and the University of California, Irvine, LLNL scientists have developed a new strategy to improve the balance between activity and durability of electrocatalysts by encapsulating the catalyst with ultrathin and porous titanium dioxide layers.

The Columbia team led by Daniel Esposito had previously reported that the nanoporous oxides covering platinum nano particles could improve the durability of the system without compromising the catalytic activity, contrary to the commonly held view: covering the catalyst surface will severely compromise the catalytic activity. The nanoporous structure also appears to improve the selectivity by favoring water splitting reactions over competing processes.

In their study, LLNL scientists used advanced molecular dynamics (MD) simulations with a machine learning potential derived from first-principles calculations. This platform enables the exploration of the potential energy surface and and reaction kinetics with extraordinary accuracy at scales beyond the reach of conventional first-principles approach. The simulations revealed that water confined within nanopores smaller than 0.5 nanometers shows significantly altered reactivity and proton transfer mechanisms. In particular, the team observed that confinement lowers the activation energy for proton transport.

"Our findings demonstrate that in extremely confined environments, the activation energy for water dissociation is reduced, leading to more frequent proton transfer events and rapid proton transport," said Hyuna Kwon, a materials scientist in LLNL's Quantum Simulations Group and Laboratory for Energy Applications for the Future (LEAF). "This insight could pave the way for optimizing porous oxides to improve the efficiency of hydrogen production systems by tuning the porosity and surface chemistry of the oxides.

"Our study therefore represents collective efforts of three DOE centers and underscores LLNL's commitment on improving the renewable hydrogen production technologies," Kwon said.

Other LLNL co-authors on the paper include Marcos Calegari Andrade, Tuan Anh Pham and Tadashi Ogitsu.

More information: Hyuna Kwon et al, Confinement Effects on Proton Transfer in TiO_2 Nanopores from Machine Learning Potential Molecular Dynamics Simulations, *ACS Applied Materials & Interfaces* (2024). DOI: 10.1021/acsami.4c02339

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