Researchers propose a common yardstick to the efficiency of molecular electrocatalysts

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PNNL scientists suggest a consistent and accurate approach to compare the performance of molecular catalytic reactions using overpotential.

(Phys.org) —In an invited *ACS Catalysis* Viewpoint paper, scientists at Pacific Northwest National Laboratory proposed a way to measure and report the energy efficiency of molecular electrocatalysts, small molecules that quickly convert electrical energy into chemical bonds or break those bonds to release energy. The definition and process they

propose is designed to clear up inconsistencies in describing and reporting overpotential, a measure of the catalyst's efficiency. By adhering to a set of uniform procedures and metrics, researchers can consistently compare one catalyst to another.

In chemical reactions, a catalyst is like a matchmaker, fanning the marriage proposal flames without actually walking down the aisle. Increased interest in fuels made from renewable energy has ignited the discovery and testing of many new efficient, robust and effective catalysts. Propelled by the desire to replace expensive and rare metal catalysts with less expensive and abundant sources, researchers are also looking for catalysts that are fast and efficient. Researchers use the measure of overpotential as a way to quantify the catalyst's energy efficiency. In the competitive bid to find this catalytic brass ring, researchers have used different metrics to determine and report the overpotentials of their catalysts. The Viewpoint presented by Dr. Aaron M. Appel and Dr. Monte L. Helm at PNNL offers a clear and consistent path for the determination of overpotential, allowing an easy and consistent apples-to-apples comparison.

The idea of finding a consistent and accurate way to compare the performance of molecular catalytic reactions intrigued the PNNL team. The scientists are researchers at the Center for Molecular Electrocatalysis (a DOE-funded Energy Frontier Research Center) led by PNNL. After working to compare many different catalysts through the literature, they noted that there was no easy way to view catalysts' performance without a consistent and uniform measure of efficiency. Overpotential is one such measure, yet they found various methods and approaches for describing and measuring overpotential that did not enable an "apples to apples" comparison. Even conversion of previous measurements into a common system proved out of reach.

Noting the inconsistencies in the way overpotential has been reported,

the researchers set about finding metrics that allowed the scientific community to easily compare different catalysts. They discussed and analyzed options and arrived at the recommendations they present in this article. Their innovative idea for a common language or description of overpotential can be used in future research in this fast-growing field. Their Viewpoint paper describes the method to determine and measure potential and overpotential, in an accurate and consistent way that works within and across all catalyst families.

The researchers have adopted this process in their research and continue to build consensus on this method in their research community.

More information: Appel A, and M Helm. 2014. "Determining the Overpotential for a Molecular Electrocatalyst." *ACS Catalysis* 4(2):630-633. DOI: 10.1021/cs401013v

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