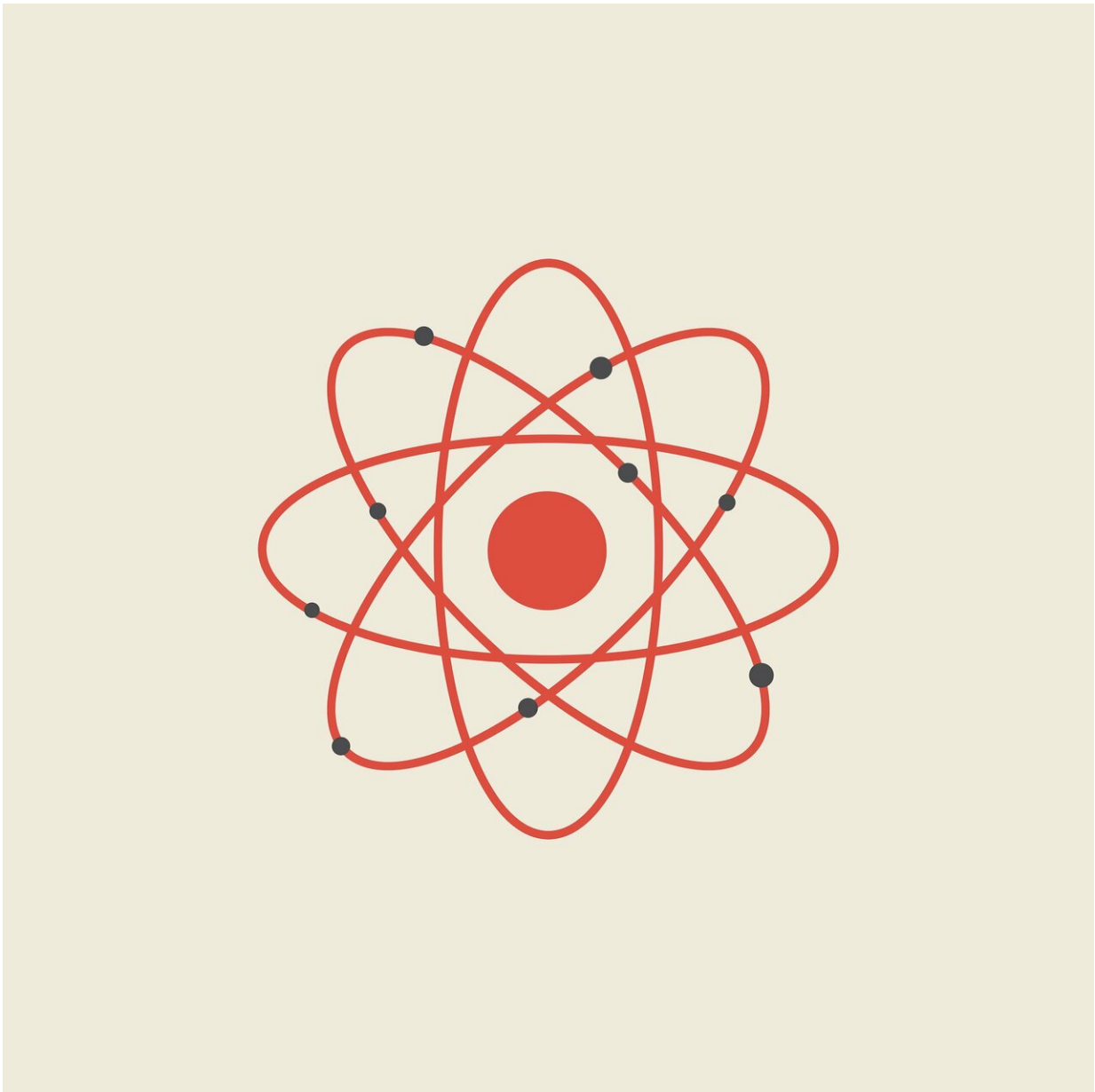


Precision control of complex electrochemical interfaces for separations

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Researchers working within Pacific Northwest National Laboratory's (PNNL's) Separations Science program succeeded in coupling a highly controlled way of modifying surfaces, called ion soft landing, with a PNNL-designed and built electrochemical cell to achieve precise control over the chemical composition of complex interfaces. Once achieved, this allowed them to make atom-by-atom changes to electrodes to study the effect on performance and stability.

The experiments, combined with [theoretical calculations](#) by collaborators in Spain, were published in an *ACS Nano* article titled "Controlling the Activity and Stability of Electrochemical Interfaces Using Atom-by-Atom Metal Substitution of Redox Species." They revealed that substitution of only one to three tungsten atoms by molybdenum atoms in complex metal-atom clusters resulted in a pronounced improvement in their electronic behavior, which controls how efficiently these species accept electrons for separation applications.

In electrochemical devices used for separations, the interfaces are complex. A lot is going on at once as electroactive ions, solvent molecules, and supporting electrolytes interact, exchanging electrons and mass during charge transfer processes. To understand these processes, it is necessary to decouple the different charge transfer and ionic interactions occurring on electrodes. In this study, the researchers did just that, and further, exerted control over the process by tuning electrodes at the atomic level.

"The atomically precise insights obtained from our experiments and theoretical calculations allowed us to develop efficient electrochemical

interfaces using super-active anions that would not have been identified using conventional techniques that sample heterogeneous mixtures," said PNNL chemist Venkateshkumar Prabhakaran, lead author of the study. "This approach can be widely adopted to study electrochemical interfaces in other related technologies, which may assist the nation's future needs in chemical separations, energy generation, and storage."

The researchers are now studying how to modulate the efficiency of separating different ions in solution using well-defined electrodes with precisely controlled-anions and membrane layers. The fundamental insights gained in understanding molecular-level electrochemical interfaces may serve as a foundation for designing superior electrodes for separations, or even energy storage, at the device scale.

More information: Venkateshkumar Prabhakaran et al. Controlling the Activity and Stability of Electrochemical Interfaces Using Atom-by-Atom Metal Substitution of Redox Species, *ACS Nano* (2018). [DOI: 10.1021/acsnano.8b06813](https://doi.org/10.1021/acsnano.8b06813)

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