Scientists uncover secrets to designing brain-like devices

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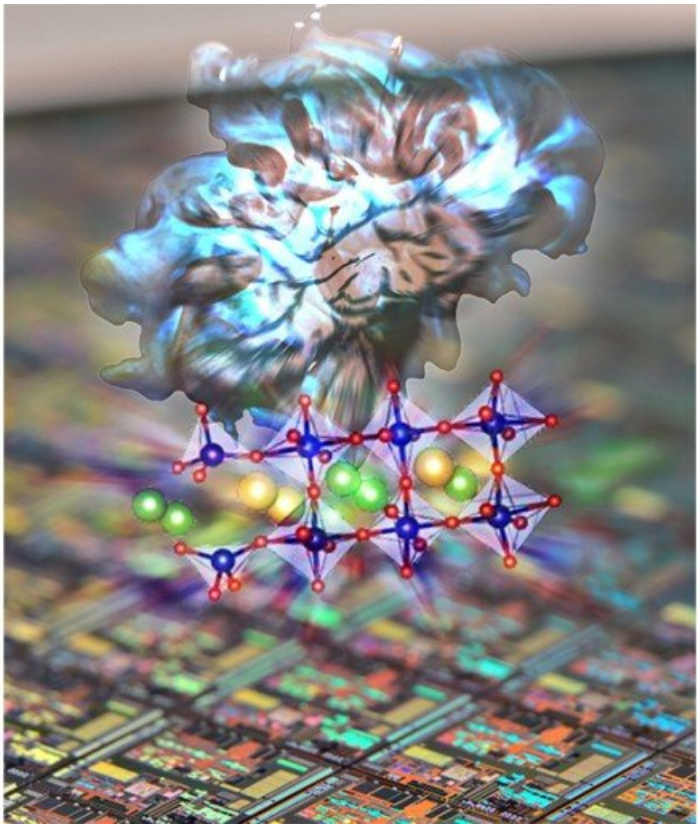

Ball and stick (central) representation of the defective material simulated in the study, for neuromorphic applications. Credit: Illustration by Emmanuel Gygi

Even with decades of unprecedented development in computational power, the human brain still holds many advantages over modern

computing technologies. Our brains are extremely efficient for many cognitive tasks and do not separate memory and computing, unlike standard computer chips.

In the last decade, the new paradigm of neuromorphic computing has emerged, inspired by neural networks of the brain and based on energy-efficient hardware for information processing.

To create devices that mimic what occurs in our brain's neurons and synapses, researchers need to overcome a fundamental molecular engineering challenge: how to design devices that exhibit controllable and energy-efficient transition between different resistive states triggered by incoming stimuli.

In a recent study, scientists at the Pritzker School of Molecular Engineering (PME) at the University of Chicago were able to predict design rules for such devices.

Published November 10 in *npj Computational Materials*, the study predicted new ways of engineering and triggering changes in electronic properties in several classes of transition metal oxides, which could be used to form the basis of neuromorphic computing architectures.

"We used quantum mechanical calculations to unravel the mechanism of the transition, highlighting exactly how it happens at the atomistic scale," said Giulia Galli, Liew Family Professor at Pritzker Molecular Engineering, professor of chemistry, and co-author of the study. "We further devised a model to predict how to trigger the transition, showing good agreement with available measurements."

The impact of defects on electronic properties

The researchers investigated oxide materials that exhibit a change of

electronic properties from a metal—which conducts electricity—to an insulator—which does not allow electricity to pass through—with various concentrations of defects. Defects can be missing atoms or some impurities that substitute for the atoms present in a perfect crystal.

To understand how defects change the state of the material from a metal to an insulator, the authors calculated the electronic structure at different defect concentrations using methods based on quantum mechanics.

"Understanding the intricate interdependency of the charge of these defects, the way atoms rearrange in the material and the way spin properties vary is crucial to controlling and eventually triggering the desired transition," said Shenli Zhang, a UChicago postdoctoral researcher and first author of the paper.

"Compared to traditional semiconductors, the oxide materials we studied require much less energy to switch between two totally different states: from a metal to an insulator," Zhang continued. "This feature makes these materials promising candidates to be used as artificial neurons or artificial synapses for large-scale neuromorphic architectures."

The study, published by Zhang and Galli, was conducted within the Quantum Materials for Energy Efficient Neuromorphic Computing (QMEENC) research center, which is funded by the Department of Energy and led by Prof. Ivan Schuller at UC San Diego.

"Understanding quantum materials will provide the key solutions to many scientific and technological problems, including the reduction of energy consumption in computational devices," said Schuller. "Given the complexity of quantum materials, the Edisonian approach of trial and error is no longer feasible, and quantitative theories are needed."

Such high-level theories are computationally demanding and have been

the target of a long line of work.

"First principles calculations are playing a key role in driving the molecular engineering of neuromorphic computing. It is exciting to see the methods that we have developed for years coming to fruition," said Galli.

More information: Shenli Zhang et al, Understanding the metal-to-insulator transition in La1−xSrxCoO3−δ and its applications for neuromorphic computing, *npj Computational Materials* (2020). DOI: 10.1038/s41524-020-00437-w

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