

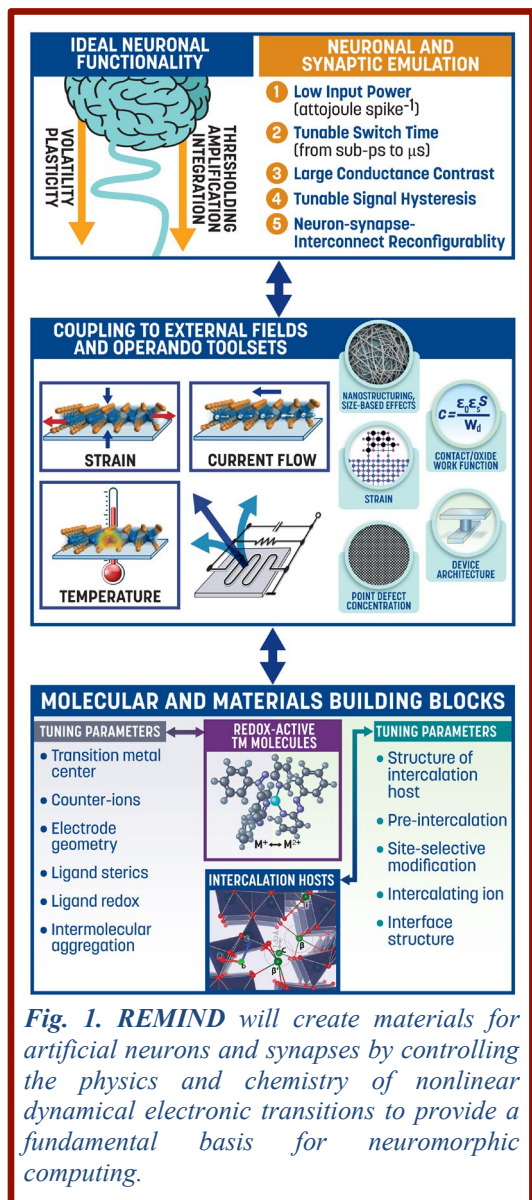
Reconfigurable Electronic Materials Inspired by Nonlinear Neuron Dynamics (REMIND)

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Mission Statement: To establish foundational scientific knowledge underpinning the function of massively reconfigurable computing architectures that approach fundamental limits of energy efficiency and speed, enabling real-time learning and embedded intelligence emulative of specific neuronal and synaptic functions of the human brain.



The current paradigm of developing computational devices and architectures invokes forward design, which leverages the well-defined properties of silicon and its interfaces with metals and dielectrics to tune electrical conductance *via* well-established mechanisms. **REMIND's** goal is to connect dynamical material properties and underlying electrochemical transformations to discover and exploit new mechanisms, materials, and interfaces that can emulate specific neuronal and synaptic functions of the human brain. We will design and realize reconfigurable neuron- and synapse-like materials based on crystalline transition metal oxide intercalation hosts and thin films of self-assembled redox-active coordination complexes with precisely programmable redox cascades. We will flip the current paradigm by blending inverse and forward design and connecting dynamical material properties and underlying transformations to discover and exploit new materials, mechanisms, and interfaces that are required to emulate specific neuronal and synaptic functions (**Fig. 1**).

REMIND comes at a watershed moment for computing. Transmitting, storing, and processing data already account for approximately 10% of global energy use. Fifty zettabytes of data were collected in 2020, and that very large number (a zettabyte is 10²¹ bytes) is expected to grow a million-fold by 2040. The microelectronics industry is encountering roadblocks directly traceable to fundamental physical constraints of present computing paradigms. This upward trajectory of data has just begun in earnest, Moore's Law scaling has stalled, and the efficiency of transistors has not improved in the past few generations, thus setting the stage for a crisis in computing and the global information economy.

REMIND's goals are to: (1) Identify fundamental neuromorphic conductance switching mechanisms that enable 4 to 5 orders of magnitude improvements in speed and energy efficiency of neuromorphic analog computing over scaled digital CMOS. (2) Develop experimental tools to interrogate form and function,

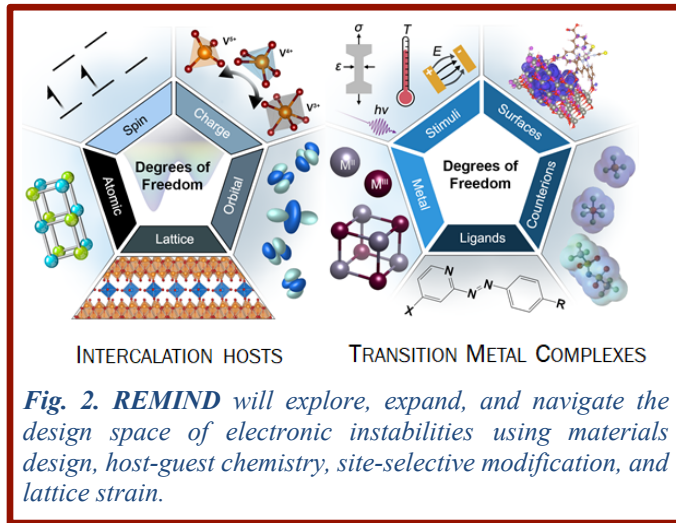


Fig. 2. REMIND will explore, expand, and navigate the design space of electronic instabilities using materials design, host-guest chemistry, site-selective modification, and lattice strain.

bridging length, time, and energy scales, to predict the cumulative nonlinear electrically-triggered response of (a) microscopic elements and (b) nontrivial ensembles of such elements interfaced within physical networks. (3) Create inverse design rules that work backwards from neuronal/synaptic function to material/interfacial properties (Fig. 1). (4) Tailor conductance switching and reconfigurability across two material classes that exhibit low-entropy transformations: (a) intercalation hosts and (b) transition-metal coordination complexes, using materials design, host-guest chemistry, site-selective modification, and lattice strain

(Fig. 2) to establish rules for decoupling transformation characteristics such as conductance differential, threshold voltage, sharpness of the transition, and hysteresis. (5) Demonstrate *in situ* device reconfiguration by tuning material properties, thereby enabling small-scale networks that can explore the ultimate limits of speed and energy consumption.

REMIND's materials chemistry focus areas investigate low-entropy electrochemical transformations in intercalation hosts and thin films of redox-active molecular complexes as a means of neuronal and synaptic emulation (Fig. 2). Our multidisciplinary team will leverage DOE national user facilities to research new molecules, materials, interfaces, and circuit elements by integrating operando toolsets for interrogating the dynamics of electronic and atomistic structure, scale-bridging modeling that captures discontinuous changes in electronic properties, and machine learning and artificial intelligence frameworks mapping desired neuronal and synaptic function to the structure and composition of molecules and materials.

Success will be a new scientific foundation for neuron- and synapse-like materials that enable intelligent and energy-efficient information processing inspired by living systems. The knowledge gained will pave the way to computing architectures with unprecedented efficiency, speed, and reconfigurability; "reboot" the microelectronics industry; and through enablement of real-time AI, will lay the foundations for a new era of atom-precise transformative manufacturing.

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