## Towards an Expanded Palette of Materials and Mechanisms for Neuromorphic Computing

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The metal-insulator transitions of electron correlated transition metal oxides provide an attractive vector for achieving large conductance switching with minimal energy dissipation. However, given the sparse and disconnected current knowledge of neuromorphic materials, a fundamental understanding of descriptors of neuromorphic function formulated in terms of intrinsic material properties, and the influence of atomistic defects on mesoscale domain evolution in the presence of external applied fields is currently lacking. Using VO<sub>2</sub> and  $M_xV_2O_5$  compounds as model systems, I will detail our efforts to develop a systematic understanding of how compositional modifications through substitutional or interstitial doping alter transformation characteristics such as the transition temperature, magnitude of switching, energy dissipation, and hysteresis.

The inclusion of dopant atoms strongly modifies the free energy landscapes in terms of relative phase stabilities, transformation barriers, and pathways; thereby profoundly altering the coupling of lattice, electronic, and spin degrees of freedom in a non-trivial manner. I will particularly focus on the three distinct mechanisms: (a) discovery of diffusive dopants that provide a distinctive new way to alter the dynamics of electronic transitions; (b) cation shuttling and polaron oscillation as a means of engendering metal—insulator transitions; and (c) lattice-anharmonicity-driven mechanisms in compounds with stereochemically active lone pairs.



**Figure 1:** An inverse design approach to identifying mechanisms and materials for neuromorphic computing.

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## **Brief Bio**

Sarbajit Banerjee, FRSC, FInstP, is the Davidson Chair Professor of Chemistry, Professor of Materials Science and Engineering, and Chancellor EDGES Fellow at Texas A&M University. He serves as Associate Director of Reconfigurable Electronic Materials Inspired by Nonlinear Neuron Dynamics (REMIND), a Department of Energy EFRC. He is a graduate of St. Stephen's College (B.Sc.) and the State University of New York at Stony Brook (Ph.D.). He was a post-doctoral research scientist at the Nanoscale Science and Engineering Center at Columbia University prior to starting his independent career at the State University of New York at Buffalo in 2007 where he founded and served as the Co-Director of the New York State Center of Excellence in Materials Informatics. At SUNY-Buffalo, he was promoted to the rank of Associate Professor in 2012. In 2014, Prof. Banerjee moved to Texas A&M University as a Professor of Chemistry and Materials Science and Engineering and was named to the Davidson Chair in 2020. Recent distinctions include a NASA Innovative Advanced Concepts Fellowship in 2021, two separate Special Creativity Extension Awards from the National Science Foundation (2020 and 2021), the O'Donnell Award from The Academy of Medicine, Engineering, and Science of Texas (2021), and the 2021 Stanley C. Israel Southwest Regional Award for Advancing Diversity in the Chemical Sciences from the American Chemical Society.