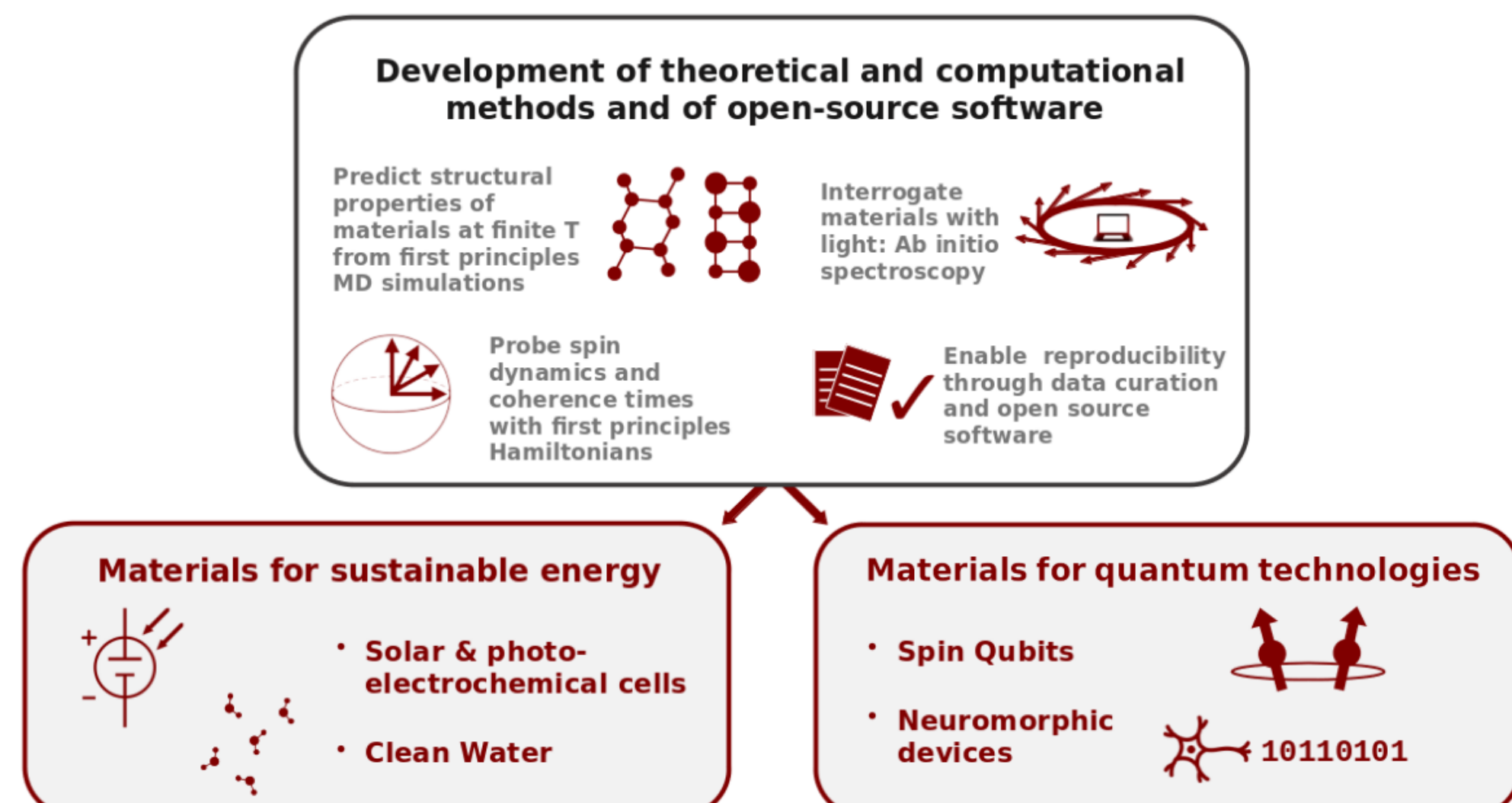


We develop theoretical and computational methods to predict and engineer material and molecular properties from first principles. We focus on problems relevant to the development of sustainable energy sources and quantum technologies.

Research Overview

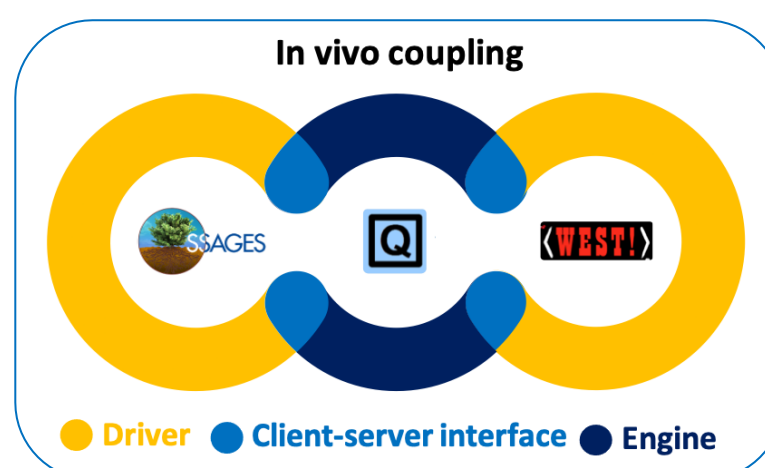


Methods and Code Development

We develop **methods based on quantum mechanics** as well as **open-source software** to understand and predict the properties of molecules and condensed systems at the microscopic scale. We focus on **first principles molecular dynamics (Qbox)**, **many body perturbation theory** methods (WEST), and quantum simulations based on quantum embedding techniques.

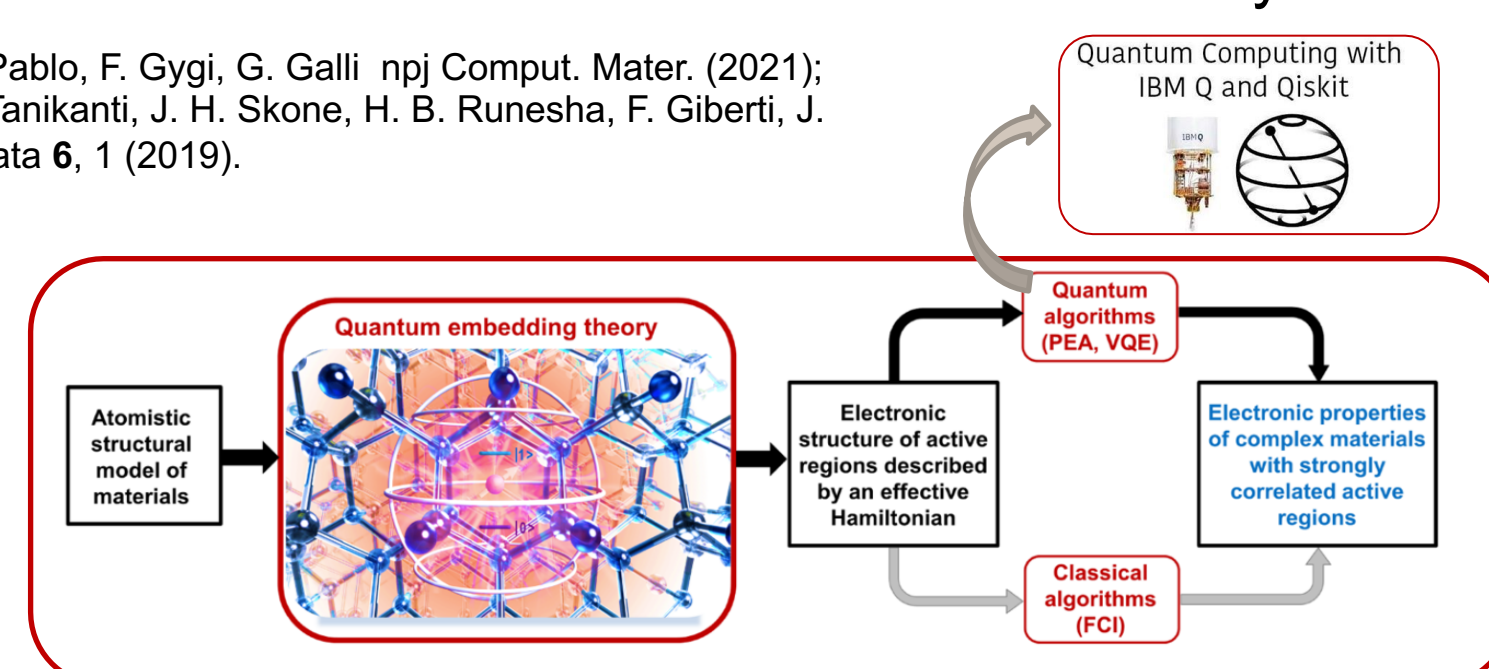


Our methodological developments are carried out within the Midwest Integrated Center for Computational Materials (MICCoM) and include coupling of codes at different scales and the development of strategies for data curation and availability.



M. Govoni, J. Whitmer, J. de Pablo, F. Gygi, G. Galli, npj Comput. Mater. (2021); M. Govoni, M. Munakami, A. Tanikanti, J. H. Skone, H. B. Runesha, F. Giberti, J. de Pablo, and G. Galli, Sci. Data 6, 1 (2019).

H. Ma, M. Govoni, and G. Galli, Npj Comput. Mater. 6, 1 (2020); H. Ma, N. Sheng, M. Govoni, and G. Galli, Phys. Chem. Chem. Phys. 22, 25522 (2020).



We are developing **quantum embedding theories** for the calculation of strongly-correlated electronic states of active regions of materials, with the rest of the system described within density functional theory. Our first demonstrations include calculations on classical and **quantum computers**. We are extending our algorithms to include **machine learning techniques**.

S. Dong, M. Govoni, G. Galli, Chem. Sci. (2021).

Materials to Harvest Sunlight

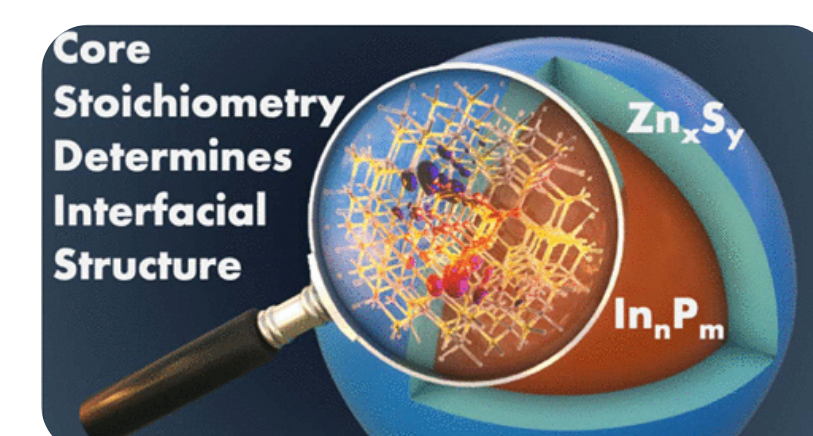
The search for cheap, Earth abundant materials for photo-electrodes for water splitting and carbon dioxide reduction calls for detailed investigations of the efficiency of light absorption in materials and nanostructures. We use simulations based on quantum mechanics to **predict optimal systems for harvesting sun light** and help interpret a growing body of complex measurements. Recently we predicted the best surface composition of commonly used photoelectrodes. Our group collaborate with several experimental groups.

A. E. Lindberg, W. Wang, S. Zhang, G. Galli, and K. S. Choi, ACS Appl. Energy Mater. 3, 8658 (2020); W. Wang, P. J. Strohbeen, D. Lee, C. Zhou, J. K. Kawasaki, K.-S. Choi, M. Liu, and G. Galli, Chem. Mater. 32, 2899 (2020); M. Gerosa, F. Gygi, M. Govoni, and G. Galli, Nat. Mater. 17, 1122 (2018).



Nanostructured Materials for Energy Applications

Nanostructured materials, e.g. semiconductors created by using colloidal nanocrystals as 'artificial atoms' or nanoplatelets, are systems with tunable properties with applications in solar energy conversion, light emission, thermoelectrics, and in electronic devices. We use electronic structure calculations and many body perturbation theory to predict optimal systems harvesting sun light, and materials with desired electronic and thermal transport properties.

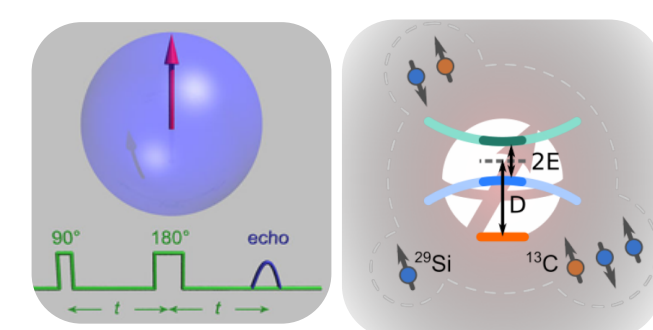
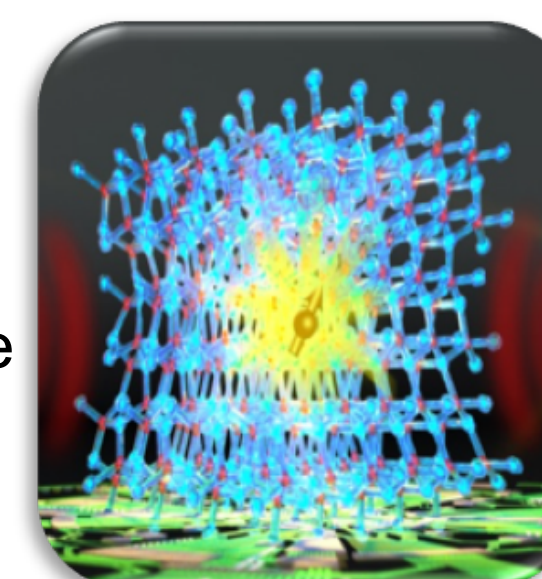


Our studies showed that **interfaces, ligand & matrix engineering** are key to create favorable heterojunctions and to enable charge extraction in nanocomposites: we explained several experiments, e.g. on CdSe nanoplatelets and made predictions that were subsequently verified, e.g. on PbSe/PbS nanoparticles.

S. Mazzotti, A. Greenwood, D. Norris, G. Galli, J. Phys. Chem. C 2021; S. Mazzotti, F. Giberti, and G. Galli, Nano Lett. 19, 3912 (2019); M. Rusishvili, S. Wippermann, D. V. Talapin, and G. Galli, Chem. Mater. 32, 9798 (2020); E. Scalise, V. Srivastava, E. Janke, D. Talapin, G. Galli, and S. Wippermann, Nat. Nanotechnol. 13, 841 (2018).

Spin Qubits for Quantum Information Technologies

Our goal is to understand the electronic structure and quantum coherence dynamics of **spin defects in semiconductors** and predict novel defects as platforms for **quantum information processing**. We work in close collaboration with experimental groups, and we investigate the properties of three- and two-dimensional materials. We are part of the QISpin project, the Chicago MRSEC and the Q-NEXT hub, in addition to the Chicago Quantum Exchange.



We are actively working at developing techniques and software to simulate spin dynamics in qubits and predict coherence times.

M. Onizhuk, K. C. Miao, J. P. Blanton, H. Ma, C. P. Anderson, A. Bourassa, D. D. Awschalom, and G. Galli, PRX Quantum 2, 10311 (2021); A. Bourassa, C. P. Anderson, K. C. Miao, M. Onizhuk, H. Ma, A. L. Crook, H. Abe, J. Ul-Hassan, T. Ohshima, N. T. Son, G. Galli, and D. D. Awschalom, Nat. Mater. 19, 1319 (2020); M. Ye, H. Seo, and G. Galli, Npj Comput. Mater. 5, 1 (2019).

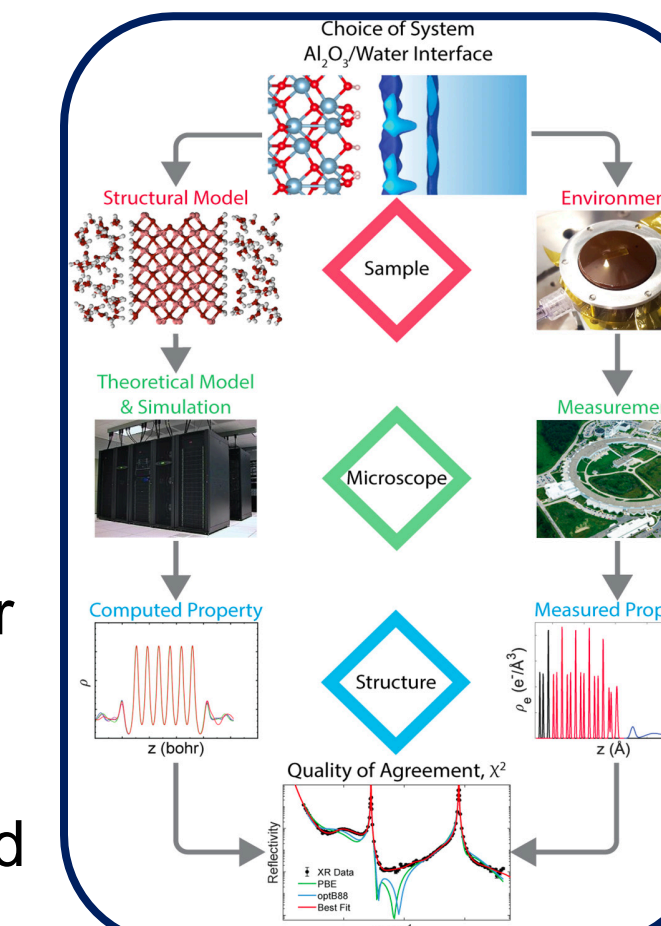
Water and Solutions

We address basic science questions regarding the solvation properties of simple ions in water; we aim at unraveling interactions between water and surfaces, and at predicting spectroscopic properties of aqueous systems, using first principles molecular dynamics (MD). We are part of the Advanced Materials for Energy-Water Systems (AMEWS) Center, headquartered at Argonne National Laboratory.



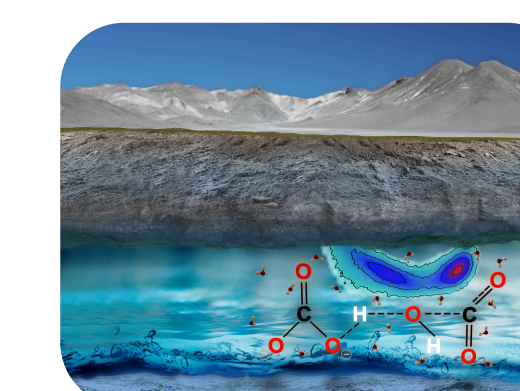
Recently, we developed a validation protocol for solid oxides interfaced with water by comparing high-resolution specular X-ray reflectivity measurements (performed at the ANL Advanced Photon Source) to first principles calculations.

K. J. Harmon, K. Letchworth-Weaver, A. P. Gaiduk, F. Giberti, F. Gygi, M. K. Y. Chan, P. Fenter, and G. Galli, Phys. Rev. Mater. 4, 113805 (2020); V. Rozsa, T. A. Pham, and G. Galli, J. Chem. Phys. 152, 124501 (2020); V. Rozsa, T. A. Pham, and G. Galli, J. Phys. Chem. B 125, 124501 (2021).



Materials in Extreme Environments

We are studying carbon and water bearing solids and fluids under pressure, to improve our understanding of the physical and chemical behavior of carbon and water at extreme conditions, as found in the deep interiors of Earth and other planets.

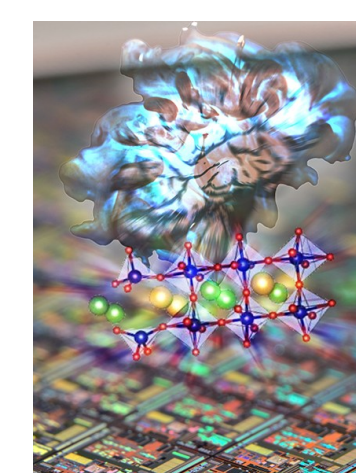


We are also investigating how tweaking and modifying chemical bonds with temperature and pressure may lead to the discovery of new materials and novel properties.

C. Zhang, F. Giberti, E. Sevgen, J. J. de Pablo, F. Gygi, and G. Galli, Nat. Commun. 11, 1 (2020); D. Pan and G. Galli, Nat. Commun. 11, 1 (2020); V. Rozsa, D. Pan, F. Giberti, and G. Galli, Proc. Natl. Acad. Sci. U. S. A. 115, 6952 (2018).



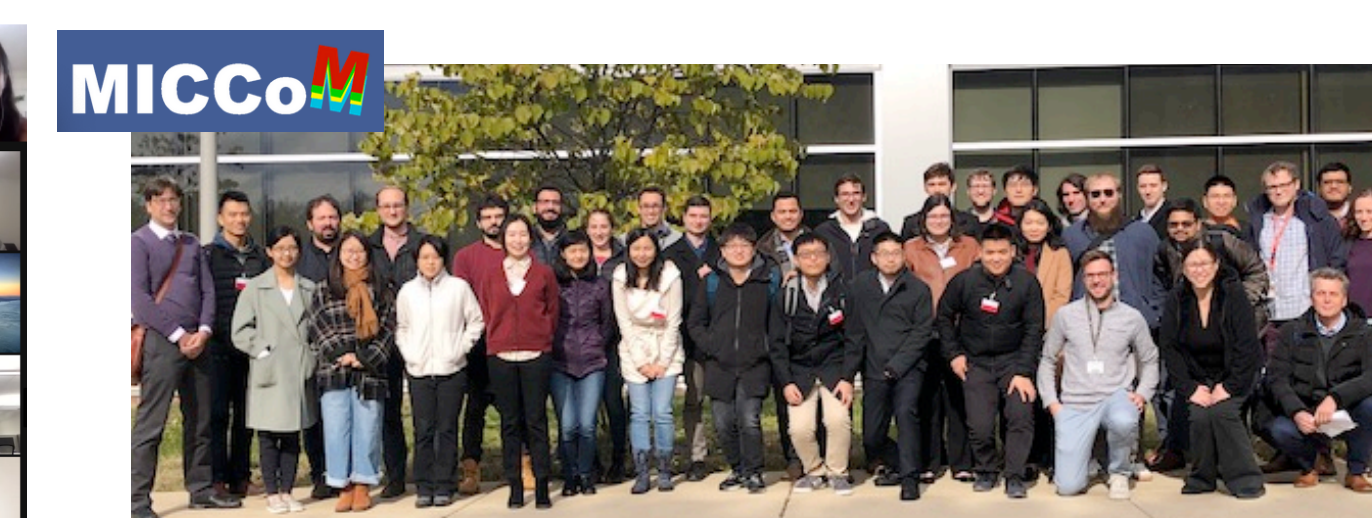
Materials for Neuromorphic Devices



The emerging paradigm of neuromorphic computing is inspired by neural networks of the brain and based on energy-efficient hardware for information processing. We study the properties of **promising transition metal oxides for neuromorphic applications** using first principles, electronic structure calculations, and we develop models to predict the electric bias and the effect of structural distortions in driving metal to insulator transitions.

S. Zhang and G. Galli, Npj Comput. Mater. 6, 1 (2020).

<https://galligroup.uchicago.edu/People/people.php>



<http://miccom-center.org/>