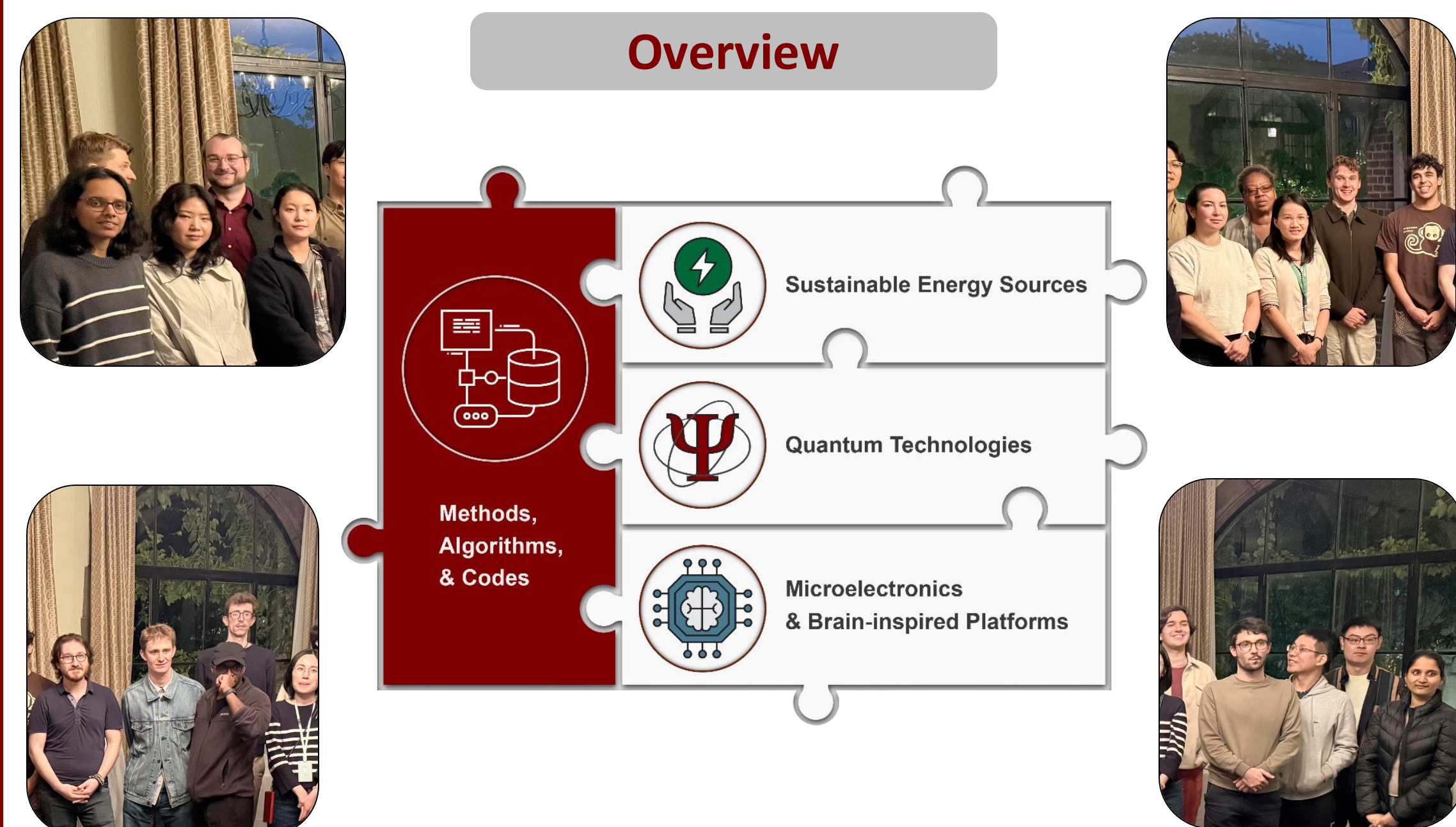


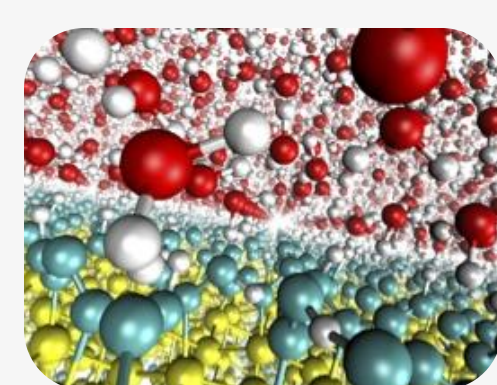
We develop theoretical and computational methods to predict and engineer material and molecular properties from first principles.

Overview

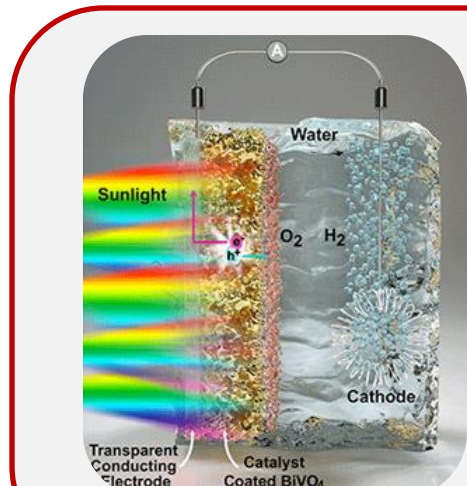


Fundamental Questions Addressed at the Microscopic Scale

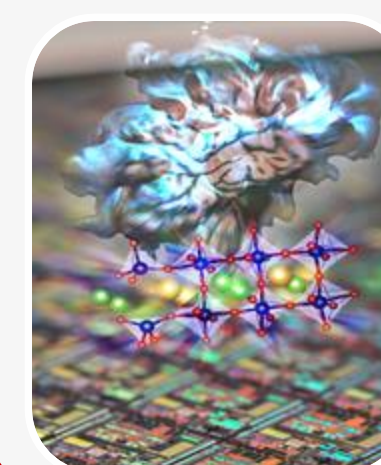
What are the best materials to trigger photo-reactions to generate clean fuel from water?



Can we engineer interfaces to remove organic pollutants from water?



How do we model materials for sustainable energy generation?



Which systems are suitable for energy-efficient neuromorphic platforms and low power electronics?

Engineering Aqueous Interfaces & Solutions

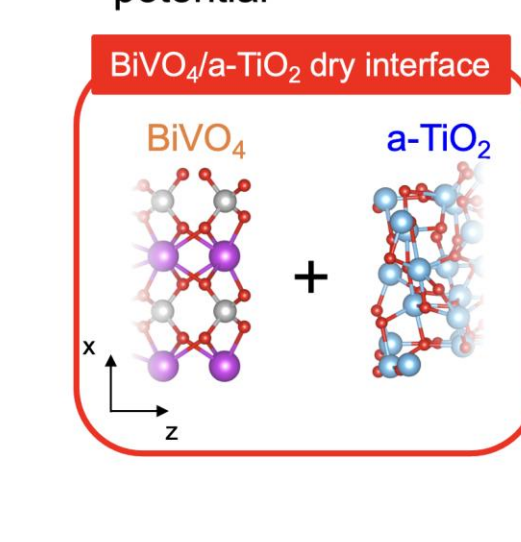
We characterized the atomistic and electronic structure and the vibrational properties of a photocatalytic surface of In_2O_3 ... a promising photoelectrode for the production of hydrogen peroxide – using first principles MD and electronic structure calculations

M. Bousquet, J. Zhan, C. Luo, A. Martinson, F. Gygi, and G. Galli, JPCC 2025

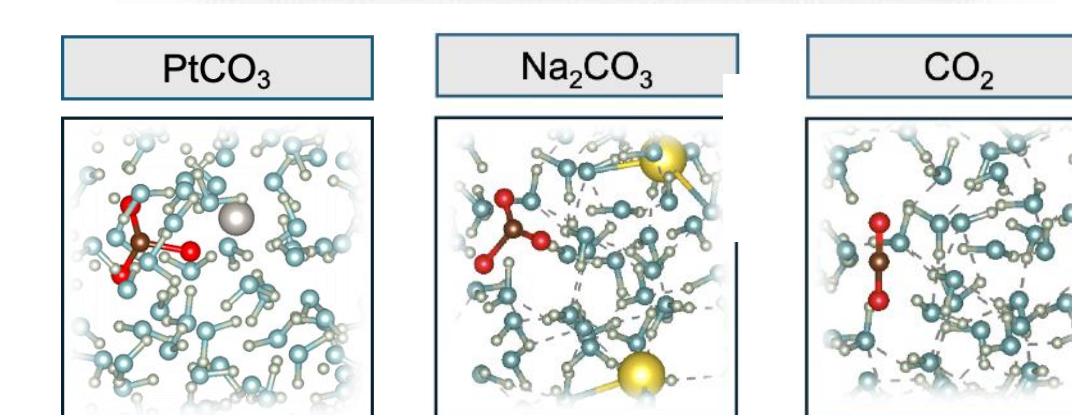
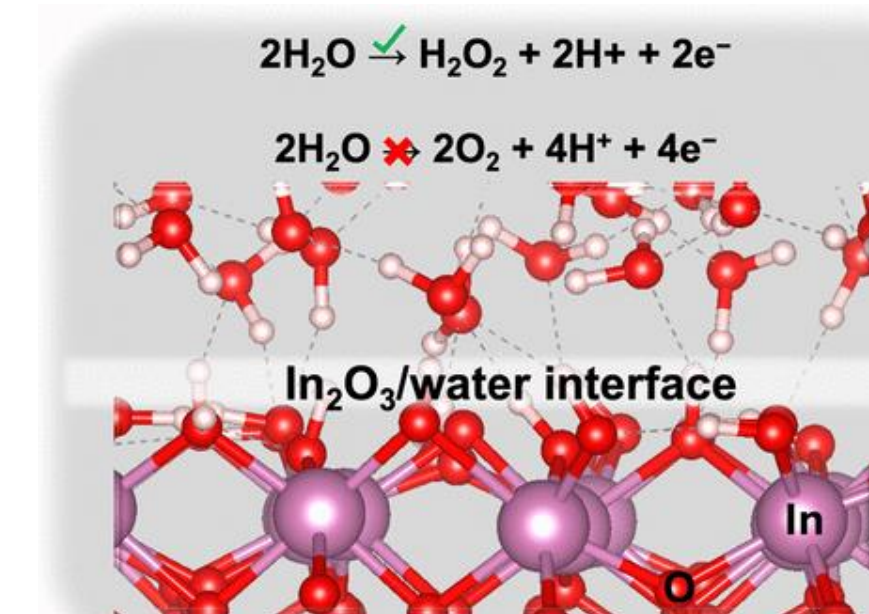
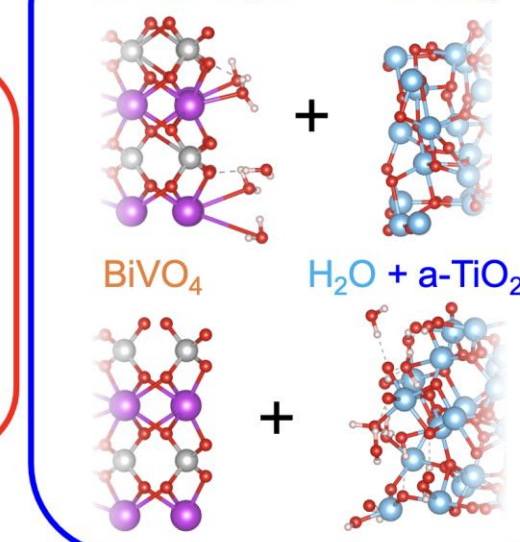
We performed FPMD simulations of aqueous carbon solutions to study how solvation and chemistry are affected by pressure and temperature.

D. Pan, G. Galli, Sci. Adv. 2016 &. Nat. Com. 2020; L. Le, G. Galli, JPCL 2025

➤ $\text{BiVO}_4/\text{a-TiO}_2$ interface models: Deep-MD potential



$\text{BiVO}_4/\text{H}_2\text{O}/\text{a-TiO}_2$ wet interfaces



We investigated interfaces between BiVO_4 , protective layers of TiO_2 and water to understand the effect of interfacial water on the performance of photoelectrodes. Further, we studied the effect of doping bulk BiVO_4 .

D. Han Wi, K. Ishisone, G. Galli, et al JACS 2025, K. Ishisone, Z. Ye, K. Choi, G. Galli Chem. Mater. 2026; D. Seo, V. Somjit et al. JACS 2025

Methods and Code Development

We develop and use methods based on quantum mechanics, and open-source software to understand and predict the properties of solids and molecules at the microscopic scale.

First Principles Molecular Dynamics (FPMD)

Many Body Perturbation Theory (MBPT)

M. Govoni and G. Galli, JCTC 2015, 2018; V. Yu et al. J. Chem Theory Comput. (2024)

Time dependent DFT (TDDFT)

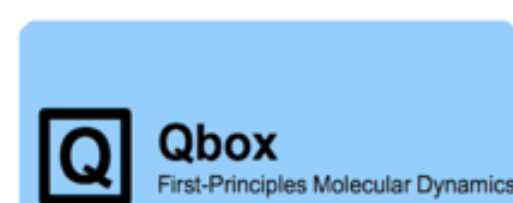
Y. Jin et al. JCTC 2023, J. Zhan and Giulia Galli J. Chem Theory Comput. (2026)

Quantum Embedding Theory (QDET)

M. He, M. Govoni, and G. Galli, npj Comput. Mater. 2020; N. Sheng, C. Vorwerk, M. Govoni, and G. Galli, JCTC 2022; S. Chen, V. Wen-zhe Yu, Y. Jin, M. Govoni, and G. Galli JCTC 2025.

Cluster-Correlation Expansion (CCE)

M. Onizhuk and G. Galli Phys. Rev. Lett. 2024; M. Onizhuk and G. Galli Rev. Mod. Phys. 2025.



Hybrid Density Functionals

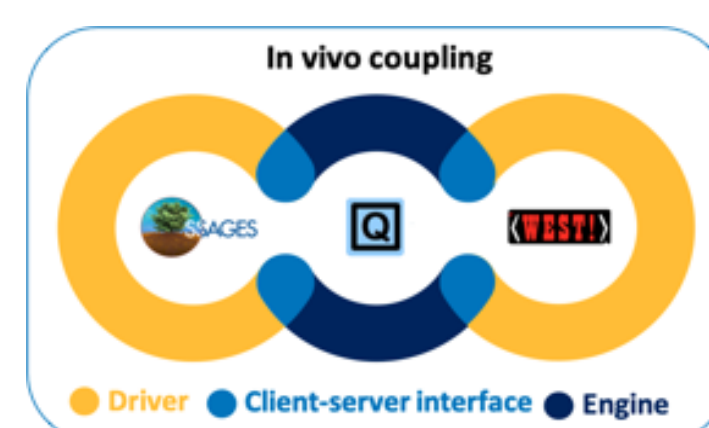
J. Zhan, M. Govoni, and G. Galli, J. Chem. Theory Comput. 2023; J. Zhan, M. Govoni, and G. Galli, Phys. Rev. Mat. 2025, J. Zhan and G. Galli J. Chem. Theory Comput. (2026)

Path Integral Molecular Dynamics (PIMD)

A. Kundu et al. Phys. Rev. Mater. 2021; PNAS 2022; JPCL 2024.

Machine Learned Interatomic Potentials (MLIP)

M. Bousquet et al. arXiv.2607.08617 (2026)



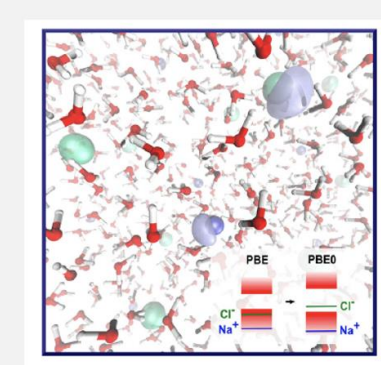
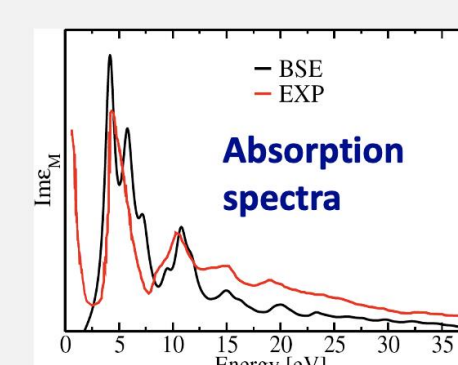
Our code developments are carried out within the **Midwest Integrated Center for Computational Materials (MICCoM)**; we couple codes at different scales and develop strategies for data curation and availability.

Y. Jin et al., J. Chem. Theory Comput. 2023; M. Govoni, J. Whitmer, J. de Pablo, F. Gygi, and G. Galli, npj Comput. Mater. 2021; M. Govoni, M. Munakami, A. Tanik JCPanti, J. H. Skone, H. B. Runesha, F. Giberti, J. de Pablo, and G. Galli, Sci. Data 2019. V. Yu et al. arXiv 2607.14025 (arXiv)

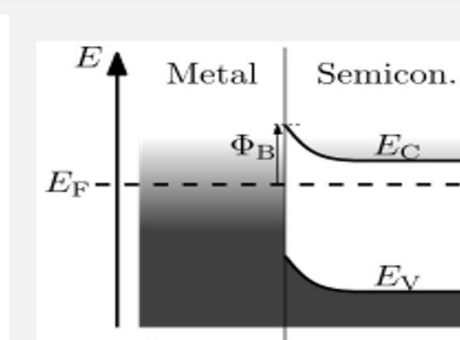
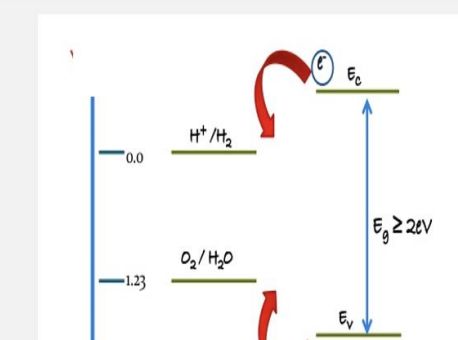
Navigating the puzzle of water photocatalysis

We compute multiple properties of solids, liquids, and interfaces from first principles.

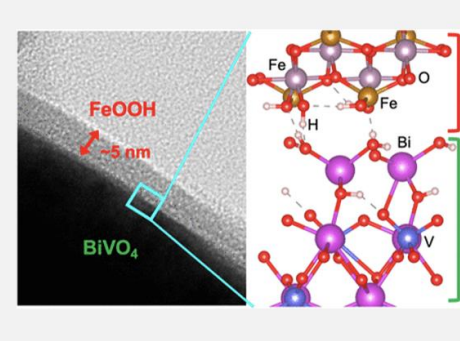
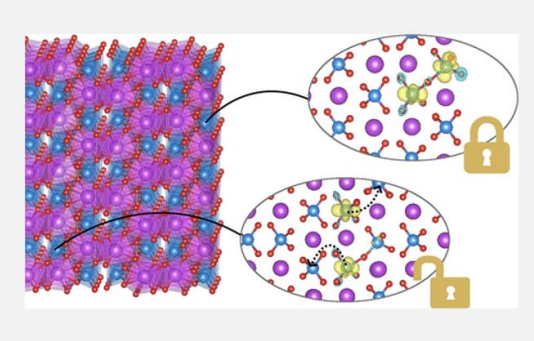
Electronic structure of **photo-absorber** and atomistic model of (salty) **water**



Atomistic models of **solid/liquid interfaces** & their electronic properties (**band offsets** and **Schottky barriers**)



Charge transport @ interfaces, polaronic states and models of **photo-absorber-catalyst** interfaces



Dynamical, defective aqueous interfaces

- Intrinsic properties of materials are insufficient to predict materials for water photo-catalysis
- Defects cannot be ignored; in fact, they may be useful
- Surface & interface morphologies and interfacial water layers are critical
- Electronic properties @ finite T and dynamical fluctuations are key to understand not only charge transport mechanisms but also structural properties and spectroscopic signatures

Water Catalyst Absorber

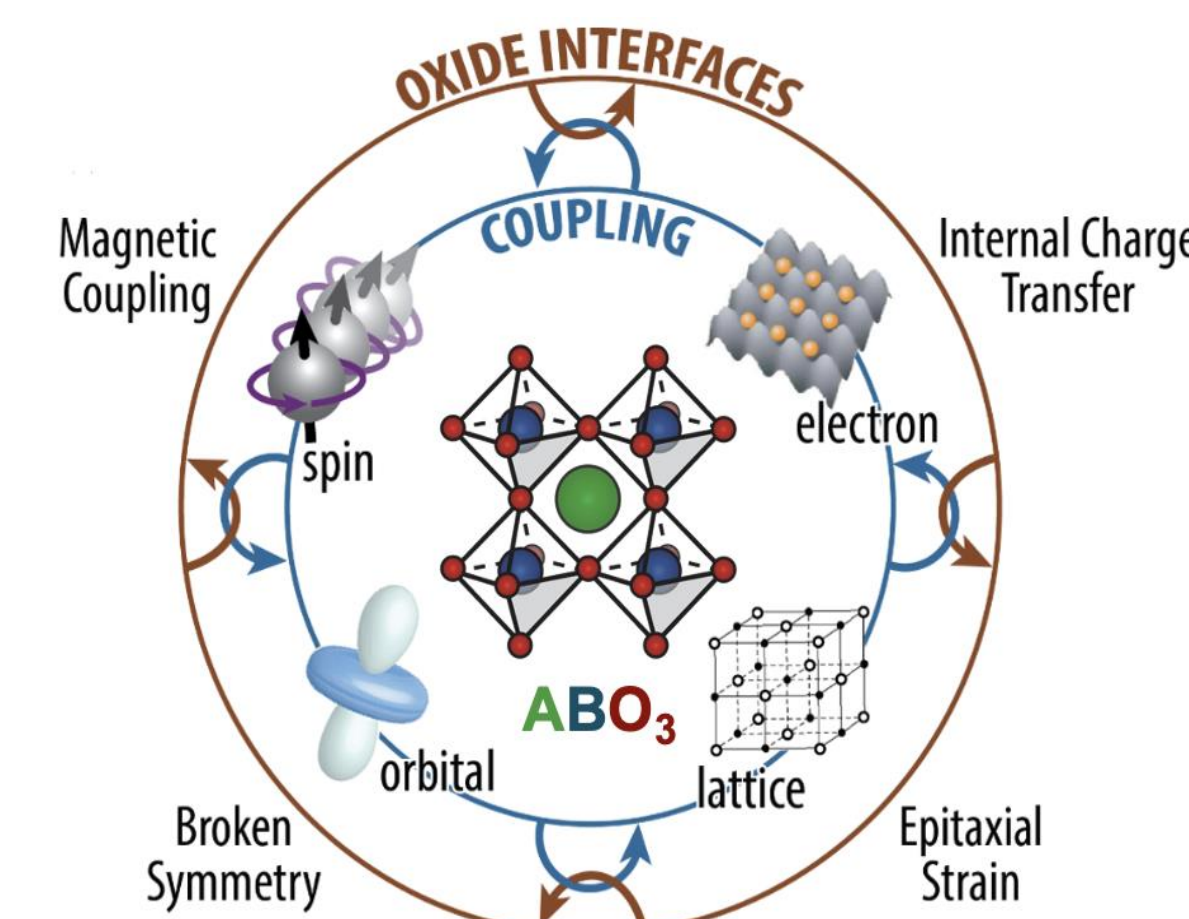
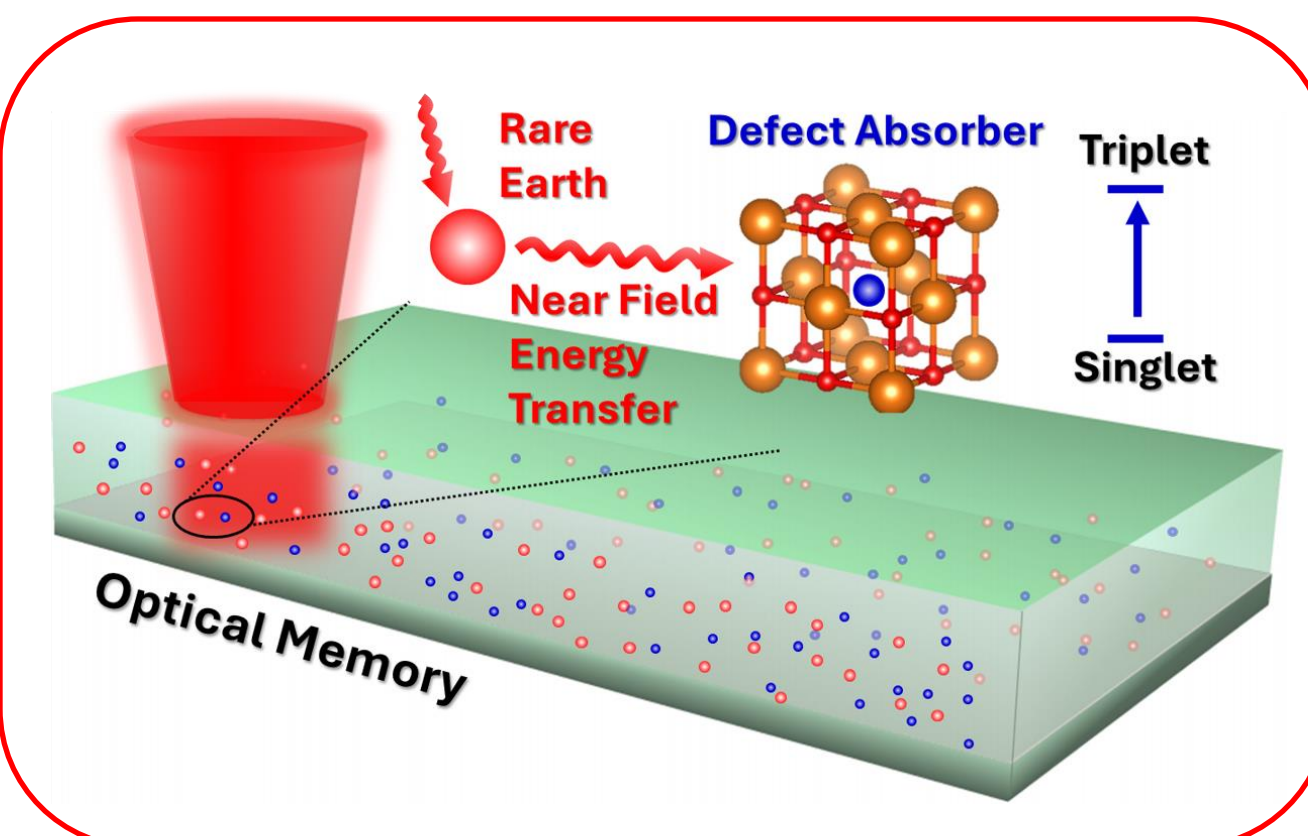
G. Melani et al., ACS Energy Lett. 2024; W. Wang et al., JACS 2023 & JACS 2022; W. Wang, A. Radmilovic, K.-S. Choi, and G. Galli, Acc. Chem. Res. 2021; D. Lee, W. Wang, C. Zhou, X. Tong, M. Liu, G. Galli, and K. S. Choi, Nat. Energy, 2021; W. Wang, P. J. Strohbein, D. Lee, C. Zhou, J. K. Kawasaki, K.-S. Choi, M. Liu, and G. Galli, Chem. Mater. 2020 & Chem. Mater. 2022; M. Bousquet, F. Gygi, G. Galli arXiv. 2607.08617 D. Han Wi, K. Ishisone, G. Galli, et al Journal American Chemical Society (2025), D. Seo, V. Somjit et al. JACS (2025) K. Ishisone, Z. Ye, K. Choi, G. Galli Chem. Mater. (2026)

Saving Energy with Low Power Electronics

In collaboration with experiments, we study **metal-to-insulator transitions (MIT)** in metal oxides for applications in neuromorphic devices, using ab initio simulations.

We develop models to predict the electric bias in driving the metal-to-insulator transition.

S. Zhang and G. Galli, Chem. Mater. 2024; Y. Shin and G. Galli, npj Comput. Mater. 2023; S. Zhang et al., Chem. Mater. 2022; S. Zhang, H. Vo, and G. Galli, Chem. Mater. 2021; H. Vo, S. Zhang, W. Wang, and G. Galli, J. Chem. Phys. 2021; I. Chiu, M. Lee, S. Cheng, S. Zhang et al., Phys. Rev. Mater. 2021; Y. Han, Y. Shin, G. Galli, Chem. Mater. (2026)



We explore defect complexes of RE-native vacancies in oxides for creating **long-lived charged states** suitable for **classical or quantum optical memory applications**.

S. Chattaraj, S. Guha, and G. Galli, Phys. Rev. Research 2024; S. Chattaraj, and G. Galli, Phys. Rev. Research 2025. S. Chattaraj and G. Galli, Phys. Rev. Res. (2025)