Sustainable Materials from First Principles

Galli Group

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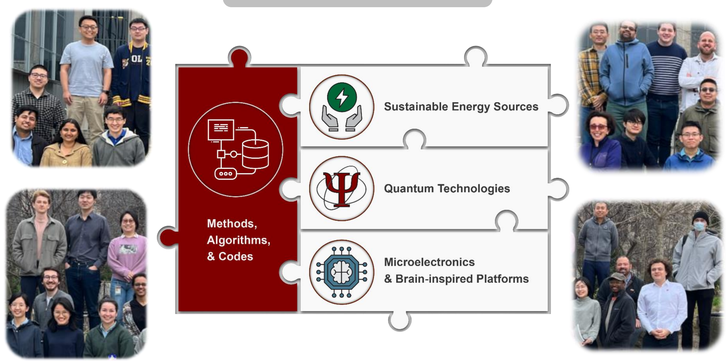
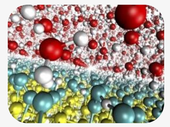
We develop theoretical and computational methods to predict and engineer material and molecular properties from first principles.

Overview

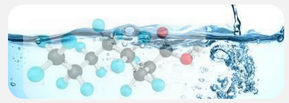


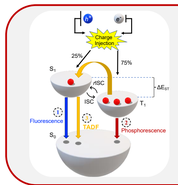
Fundamental Questions Addressed at the Microscopic Scale

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

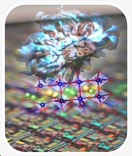


Can we engineer membranes to **remove** organic **pollutants from water?**





How do we design efficient **all organic** light emitting diodes (**OLEDs**) and **solar cells**?

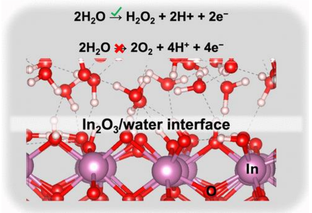


Which systems are suitable for energy-efficient **neuromorphic platforms** and **low power electronics**?

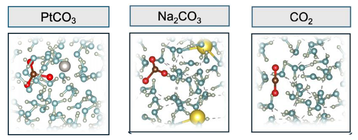
Engineering Aqueous Interfaces & Solutions

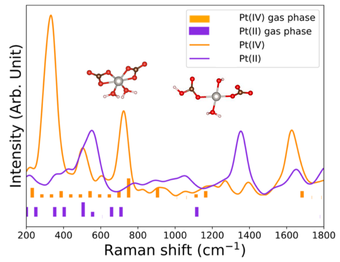
We characterized the atomistic and electronic structure and the vibrational properties of a photocatalytic surface of In_2O_3 – a promising photoelectrode for the production of hydrogen peroxide – using first principles MD and electronic structure calculations

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



We performed FPMD simulations of aqueous carbon solutions with different cations to study the changes in solvation and chemistry as a function of pressure and temperature; we also investigated how these changes affect the deposition of metals (e.g. Pt) in the Earth and the deep carbon cycle.





D. Pan, G. Galli. Sci. Adv. 2016; D. Pan, G. Gali. Nat. Com. 2020; L. Le, G. Galli. JPCL 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. 2024 (submitted).

Time dependent DFT (TDDFT)

Y. Jin et al. JCTC 2023.

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.

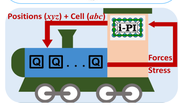
Qbox First-Principles Molecular Dynamics

WEST!

pycce

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.



Path Integral Molecular Dynamics (PIMD)

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

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.

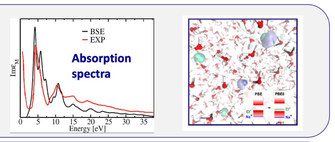
Y. Jin et al., J. Chem. Theory Comput. 2023; M. Govoni, J. Whitmer, J. de Pablo, F. Gygi, and G. Galli, npj Comput. Mater. 2021; M. Govoni, M. Munakami, A. Tanikanti, J. H. Skone, H. B. Runesha, F. Giberti, J. de Pablo, and G. Galli, Sci. Data 2019.

Navigating the puzzle of water photocatalysis

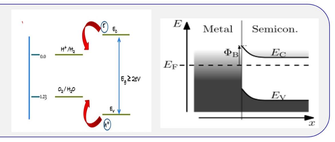
We compute **multiple properties of solids, liquids , and interfaces** from first principles.

Water
Catalyst
Absorber

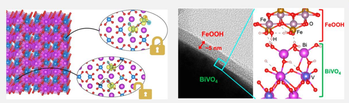
Electronic structure of **photo-absorber** and atomistic model of (salty) **water**



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



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; A. E. Lindberg, W. Wang, S. Zhang, G. Galli, and K. S. Choi, ACS Appl. Energy Mater. 2020; W. Wang, P. J. Strohbeen, D. Lee, C. Zhou, J. K. Kawasaki, K.-S. Choi, M. Liu, and G. Galli, Chem. Mater. 2020 & Chem. Mater. 2022; M. Gerosa, F. Gygi, M. Govoni, and G. Galli, Nat. Mater. 2018. D. Han Wi*, K. Ishisone*, Z. Xi, Z. Ye, D. Seo, J. Zhan, X. Tong, M. Liu, G. Galli, and K. S. Choi JACS 2025.

Dynamical, defective aqueous interfaces

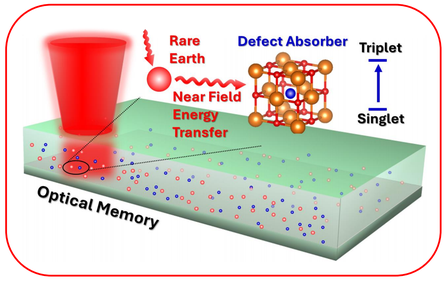
- Intrinsic properties of materials are insufficient to predict materials for water photo-catalysis
- Defects cannot be ignored; in fact, they may be useful
- Surface & interface morphologies and interfacial water layers are critical
- Electronic properties @ finite T and dynamical fluctuations are key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

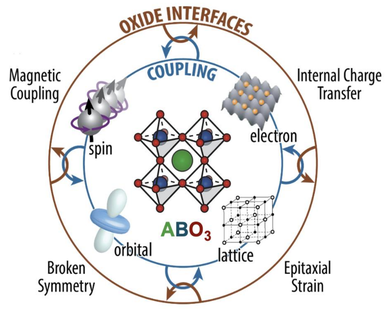
Saving Energy with Low Power Electronics

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; S. Zhang and G. Galli, npj Comput. Mater. 2020.





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.

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AMEWS ADVANCED MATERIALS FOR ENERGY-WATER SYSTEMS

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