Sustainable Materials from First Principles

Galli Group

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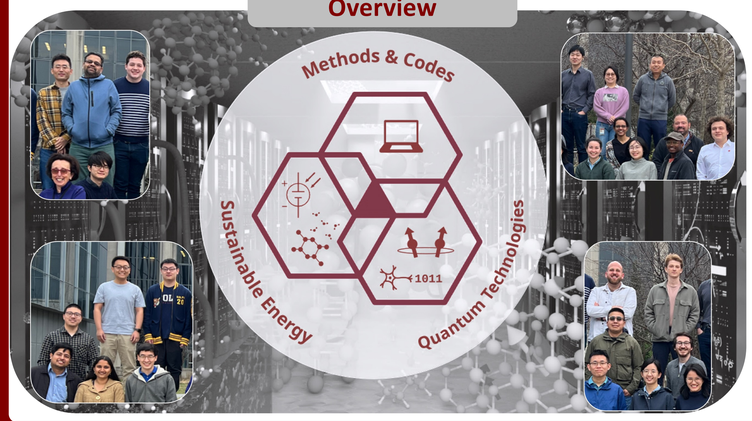
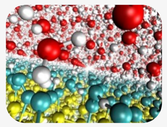
We develop theoretical and computational methods to predict and engineer material and molecular properties from first principles.

Overview

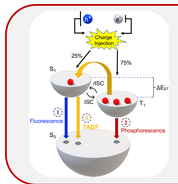


Fundamental Questions Addressed at the Microscopic Scale

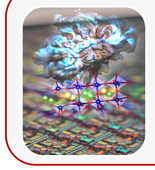
What are the best materials to trigger photo-reactions to **generate clean fuel** from water?



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



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

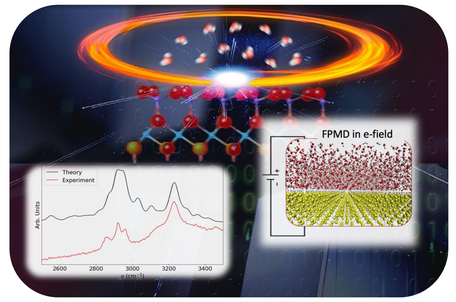


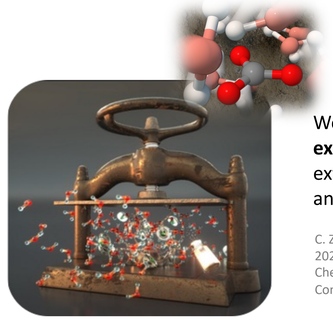
Which systems are suitable for energy-efficient **neuromorphic platforms** and **low power electronics**?

Engineering Aqueous Interfaces

We investigate **atomistic structures, interfacial currents, and interfacial vibrational & absorption spectra** using FPMD coupled with MBPT. We study salts and pollutants in water.

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. 2020; Z. Ye, A. Prominski, B. Tian and G. Galli, PNAS 2021; Z. Ye, F. Gygi and G. Galli, JPCL 2024.





We study carbon and **water** bearing solids and fluids **under extreme pressure and temperature** with FPMD and how extreme conditions lead to the discovery of new materials and/or novel properties.

C. Zhang et al., J. Phys. Chem. B 2023; Z. Ye*, C. Zhang*, and G. Galli, Faraday Discuss. 2022; V. Rozsa and G. Galli, J. Phys. Chem. B 2021; V. Rozsa, T. A. Pham, and G. Galli, J. Chem. Phys. 2020; C. Zhang, F. Giberti, E. Sevgen, J. J. de Pablo, F. Gygi, and G. Galli, Nat. Commun. 2020.

Methods and Code Development

We develop 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.

Cluster-Correlation Expansion (CCE)

M. Onizhuk and G. Galli 2024 (submitted).

Qbox
First-Principles Molecular Dynamics

WEST!

pycce

Hybrid Density Functionals

J. Zhan, M. Govoni, and G. Galli, J. Chem. Theory Comput. 2023.

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.

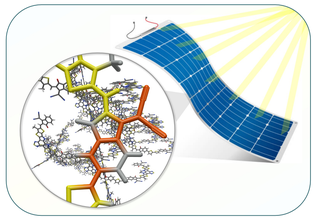
Y. Jin et al., J. Chem. Theory Comput. 2023; M. Govoni, J. Whitmer, J. de Pablo, F. Gygi, and G. Galli, npj Comput. Mater. 2021; M. Govoni, M. Munakami, A. Tanikanti, J. H. Skone, H. B. Runesha, F. Giberti, J. de Pablo, and G. Galli, Sci. Data 2019.

Harvesting Sunlight

OLED and Organic Solar Cells

Using ab initio, we predicted how the **optoelectronic properties of polymers (PSMAs) used in organic solar cells** can be substantially improved.

We predicted the properties of **thermally activated delayed fluorescence** compounds in an **all-organic emitter** for OLED design.

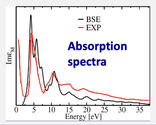


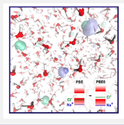
D. Sorbelli et al., J. Mater. Chem A 2024; Y. Wu, Y. Yuan, D. Sorbelli et al., Nat. Comm. 2024; A. Kundu and G. Galli, J. Phys. Chem. Lett. 2024; T. Francese, A. Kundu, F. Gygi, and G. Galli, Phys. Chem. Chem. Phys. 2022.

Navigating the Puzzle of Water Photocatalysis

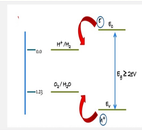
We compute **multiple properties of solids, liquids , and interfaces** from first principles.

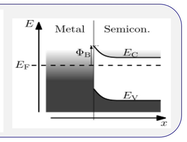
Electronic structure of **photo-absorber** and atomistic model of (salty) **water**



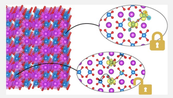


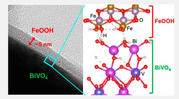
Atomistic models of **solid/liquid interfaces** & their electronic properties (**band offsets** and **Schottky barriers**)





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





Water
Catalyst
Absorber

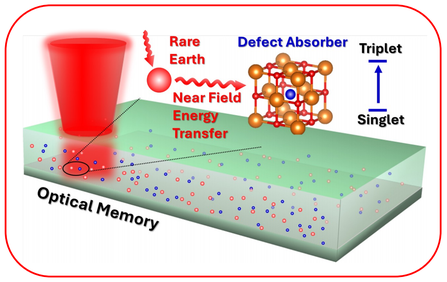
G. Melani et al., ACS Energy Lett. 2024; W. Wang et al., JACS 2023 & JACS 2022; W. Wang, A. Radmilovic, K-S. Choi, and G. Galli, Acc. Chem. Res. 2021; D. Lee, W. Wang, C. Zhou, X. Tong, M. Liu, G. Galli, and K. S. Choi, Nat. Energy, 2021; A. E. Lindberg, W. Wang, S. Zhang, G. Galli, and K. S. Choi, ACS 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.

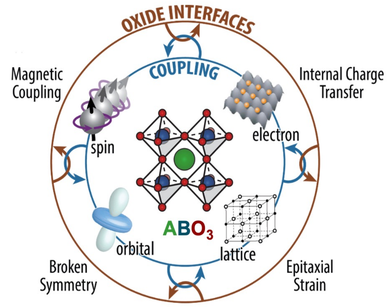
Saving Energy with Low Power Electronics

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.

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