Computational engineering of optoelectronic materials at the atomic scale

Wennie Wang
Assistant Professor
February 2022

wwwennie@che.utexas.edu | https://wangmaterialsgroup.com

The University of Texas at Austin
McKetta Department of Chemical Engineering
Cockrell School of Engineering

My background

Undergraduate

Materials Science & Engineering

MIT

with
Prof. Brian Wardle
Mechanical testing of CNT aerospace composites

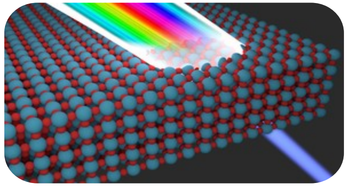
DMSE

Graduate

Materials (Computation)

UC Santa Barbara

with
Prof. Chris G. Van de Walle
Electrochromism in complex oxides



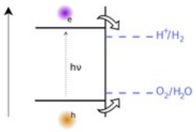
UC SANTA BARBARA MATERIALS

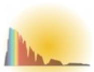
Post-doctoral

Molecular Engineering

University of Chicago

with
Prof. Giulia Galli &
Prof. Kyoung-Shin Choi
Materials optimization for photoelectrochemical water-splitting



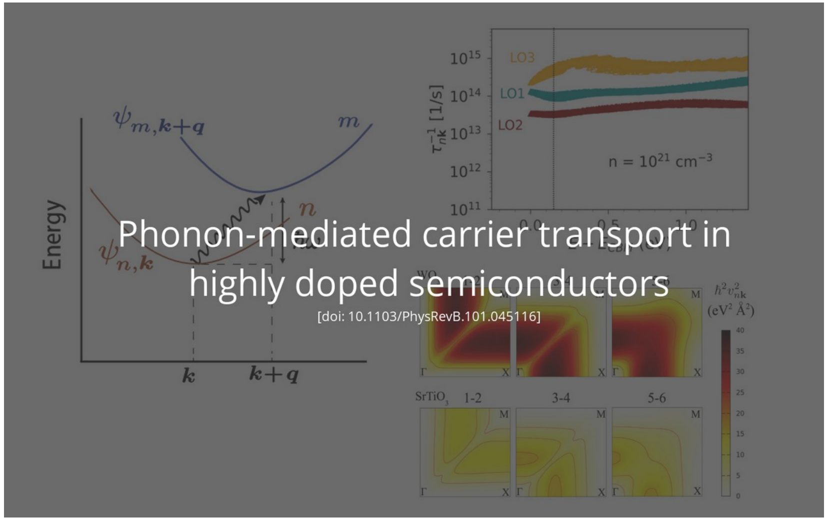


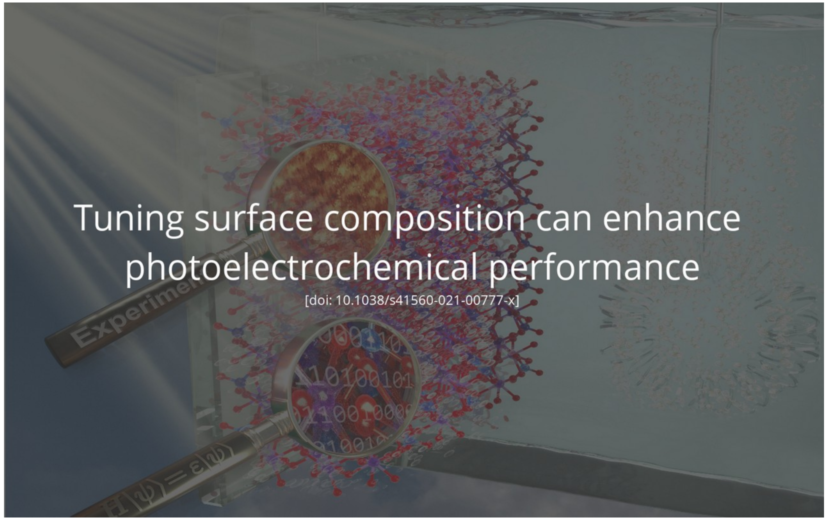
PRITZKER SCHOOL OF MOLECULAR ENGINEERING
THE UNIVERSITY OF CHICAGO

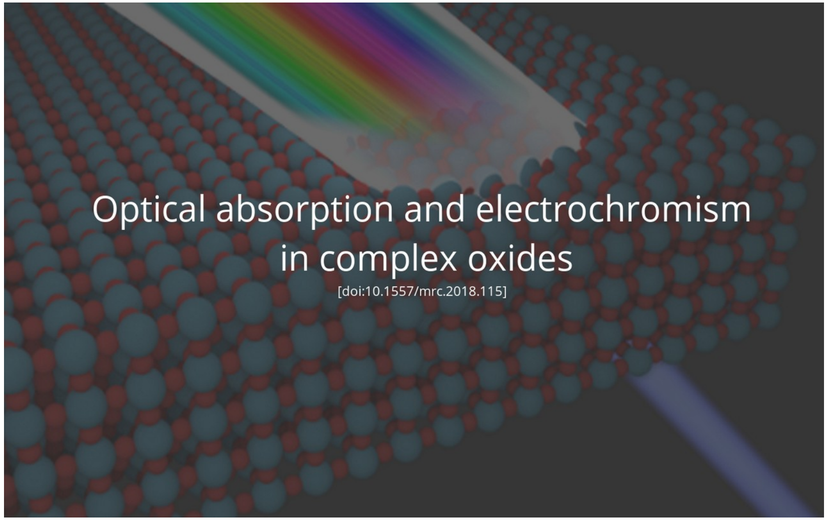
Fall 2022: 2-3 students

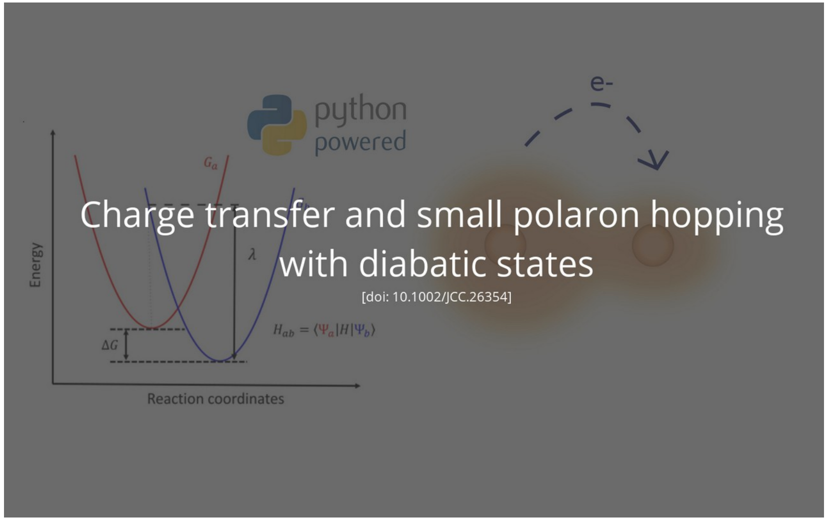
wwwennie@che.utexas.edu | wangmaterialsgroup.com

Past Highlights









Lawrence Livermore National Laboratory

WISCONSIN
UNIVERSITY OF WISCONSIN–MADISON

- Dept. of Materials Science & Engineering
- Dept. of Chemistry

THE UNIVERSITY OF CHICAGO 1890

Argonne NATIONAL LABORATORY

- Pritzker School of Molecular Engineering
- Dept. of Chemistry

MIT

- Dept. of Materials Science & Engineering
- Dept. of Aeronautics & Astronautics
- Metis Design, Inc.

UC DAVIS

BROOKHAVEN NATIONAL LABORATORY

Stony Brook University

UCSB

- Materials Department
- Dept. of Physics
- Dept. of Electrical and Computer Engineering

Fraunhofer

SIEMENS

HZB Helmholtz Zentrum Berlin

wwwennie@che.utexas.edu | wangmaterialsgroup.com

UT Austin and the city

The University of Texas at Austin
McKetta Department of Chemical Engineering
Cockrell School of Engineering

#5	#7	$22M
Undergraduate Chemical Engineering	**Graduate Chemical Engineering**	**Research Expenditures**
U.S. News & World Report	*U.S. News & World Report*	

Academic Areas

- Advanced Materials
- Polymers and Nanotechnology
- Biotechnology
- Energy
- Environmental Engineering
- Modeling and Simulation
- Process Engineering

ODEN INSTITUTE FOR COMPUTATIONAL ENGINEERING & SCIENCES

The University of Texas at Austin
Texas Materials Institute

TACC TEXAS ADVANCED COMPUTING CENTER
Powering Discoveries That Change The World

UT Austin and the city

The University of Texas at Austin
McKetta Department of Chemical Engineering
Cockrell School of Engineering

#5

Undergraduate Chemical Engineering

U.S. News & World Report

#7

Graduate Chemical Engineering

U.S. News & World Report

$22M

Research Expenditures

Academic Areas

- Advanced Materials
- Polymers and Nanotechnology
- Biotechnology
- Energy
- Environmental Engineering
- Modeling and Simulation
- Process Engineering

ODEN INSTITUTE FOR COMPUTATIONAL ENGINEERING & SCIENCES

The University of Texas at Austin
Texas Materials Institute

TACC TEXAS ADVANCED COMPUTING CENTER
Powering Discoveries That Change The World

Chi'Lantro BBQ

Taco More

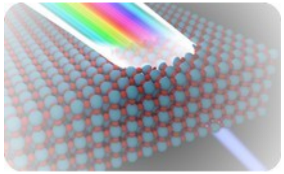
Sway

Images from Natioanal League of Cities (nlc.org) (top) and insider.com (bottom)

Research Philosophy and Methods

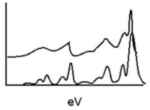
DFT
MD
MBPT
$\hat{H}$ models
.
.
.

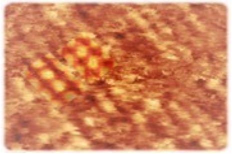
First-principles calculations



Enabled by HPC resources

Experimental collaboration





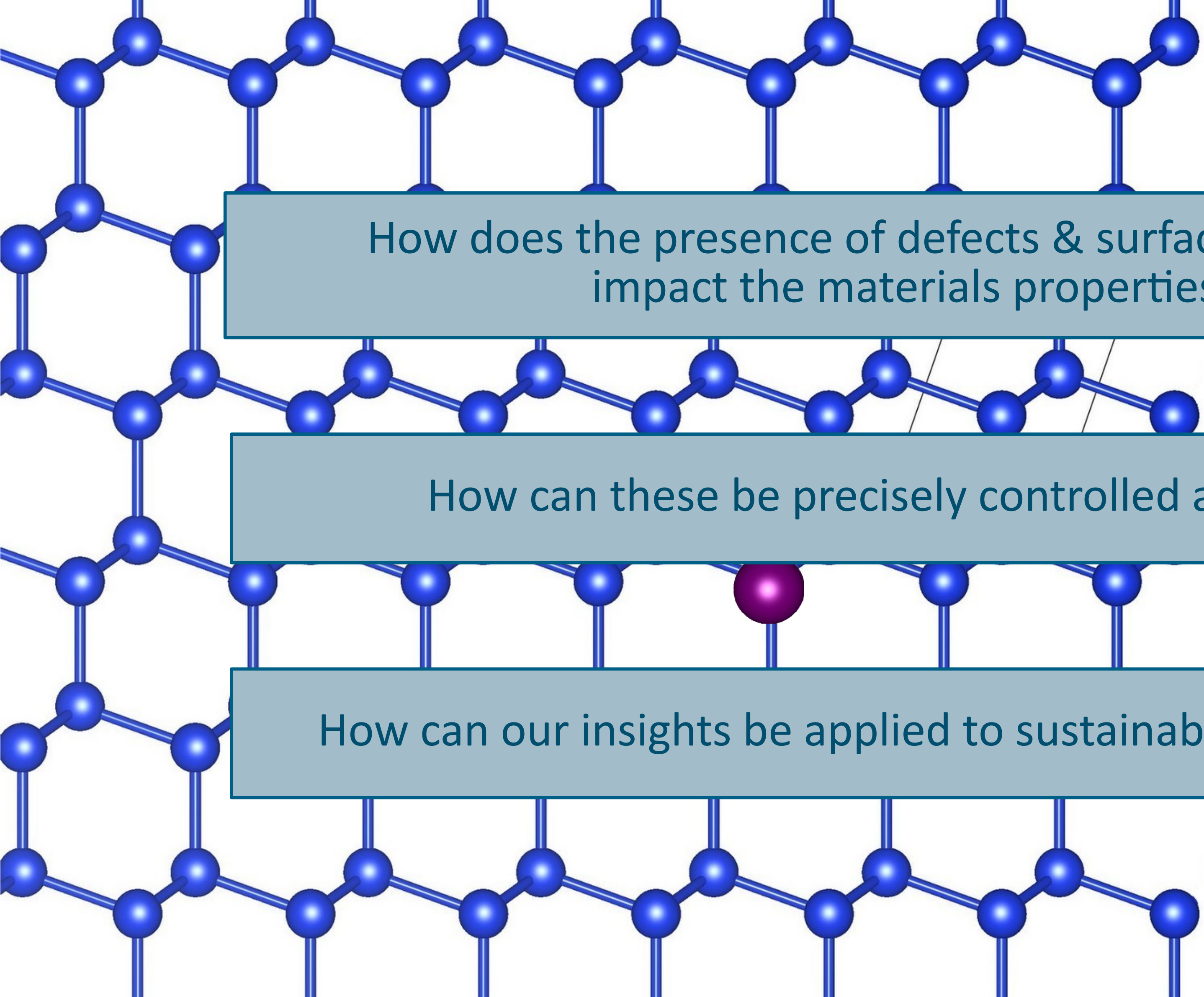
Spectroscopies, microscopies, ...

XPS
STM
XAS
.
.
.

Harnessing Materials Imperfections
for Energy Sustainability

Wang Modern Materials

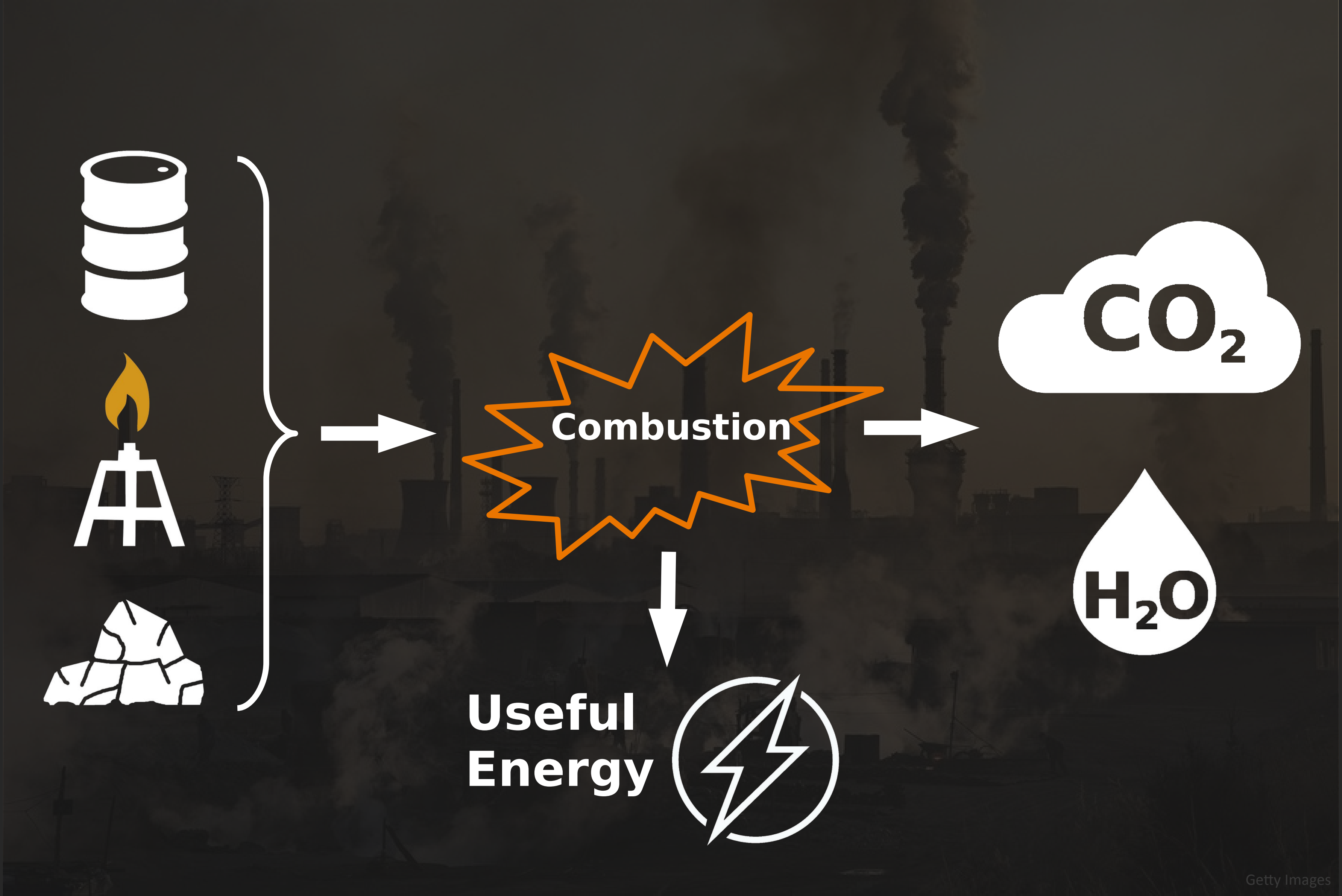
Bird’s eye view

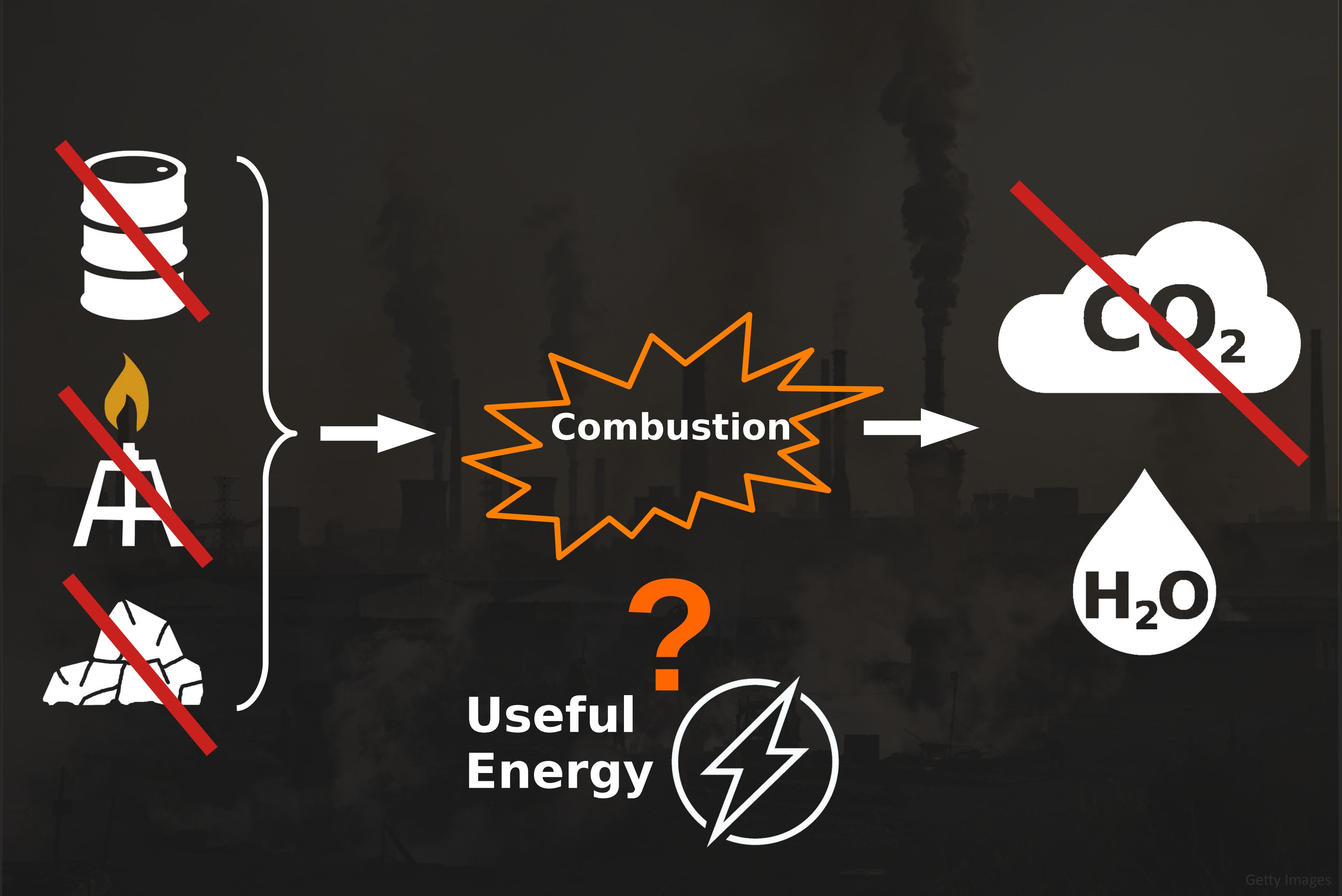


How does the presence of defects & surfaces/interface impact the materials properties?

How can these be precisely controlled and tuned?

How can our insights be applied to sustainable technologies?


Combustion
CO_2
H_2O
Useful Energy
Getty Images



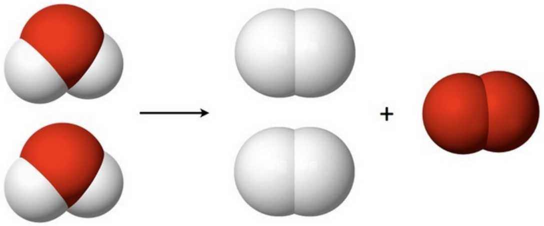
Combustion
CO_2
H_2O
?
Useful
Energy
Getty Images

A closer view: focus topic #1

Electrochemistry: Converting water into useful fuels

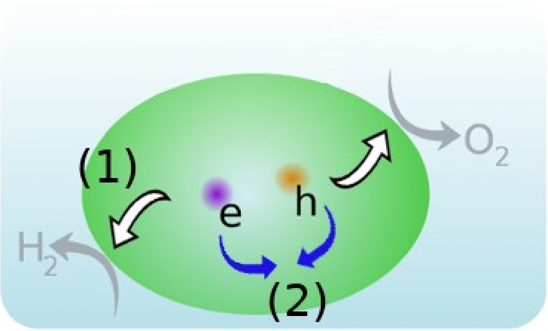
A typical three-electrode setup
An open square cell used for visual clarity

Govindaraju et al. Chem. Mater. 29, 355 (2017)

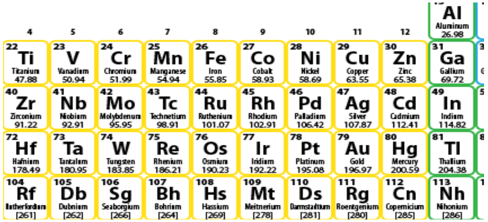


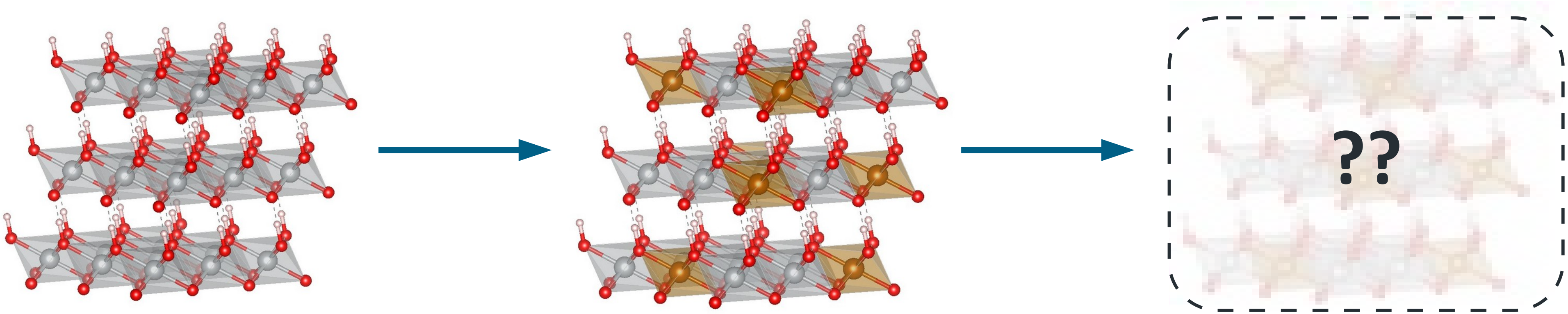
$2H_2O \longrightarrow 2H_2 + O_2$

Scope 1: Mixed transition metal systems for electrocatalysts



Composition-structure-property relationships in
charge transfer and charge transport for metal oxyhydroxides,
one of the most highly active electrocatalyst systems





Amorphization

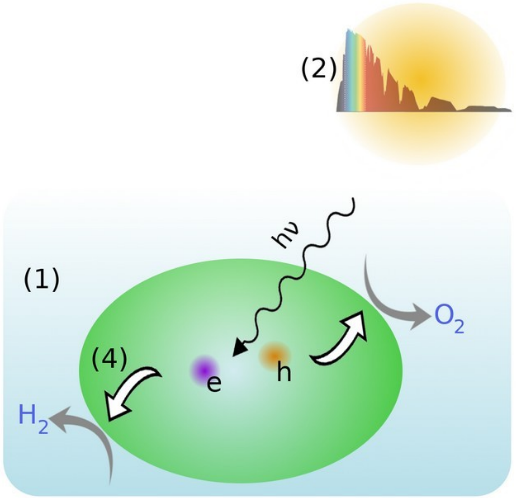
What are the degradation and amorphization mechanisms?

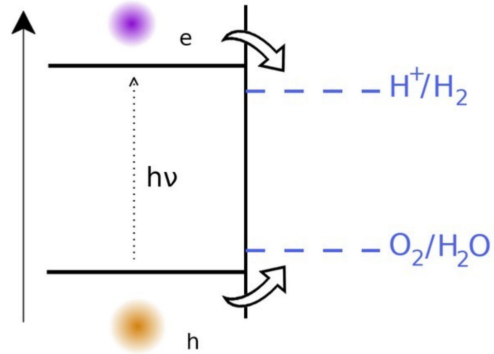
A closer view: focus topic #2

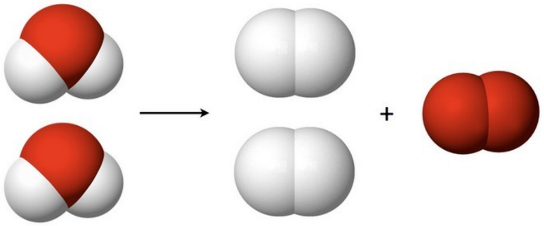
Photoelectrochemistry: Converting water into useful fuels

A typical three-electrode setup
An open square cell used for visual clarity

Govindaraju et al. Chem. Mater. 29, 355 (2017)

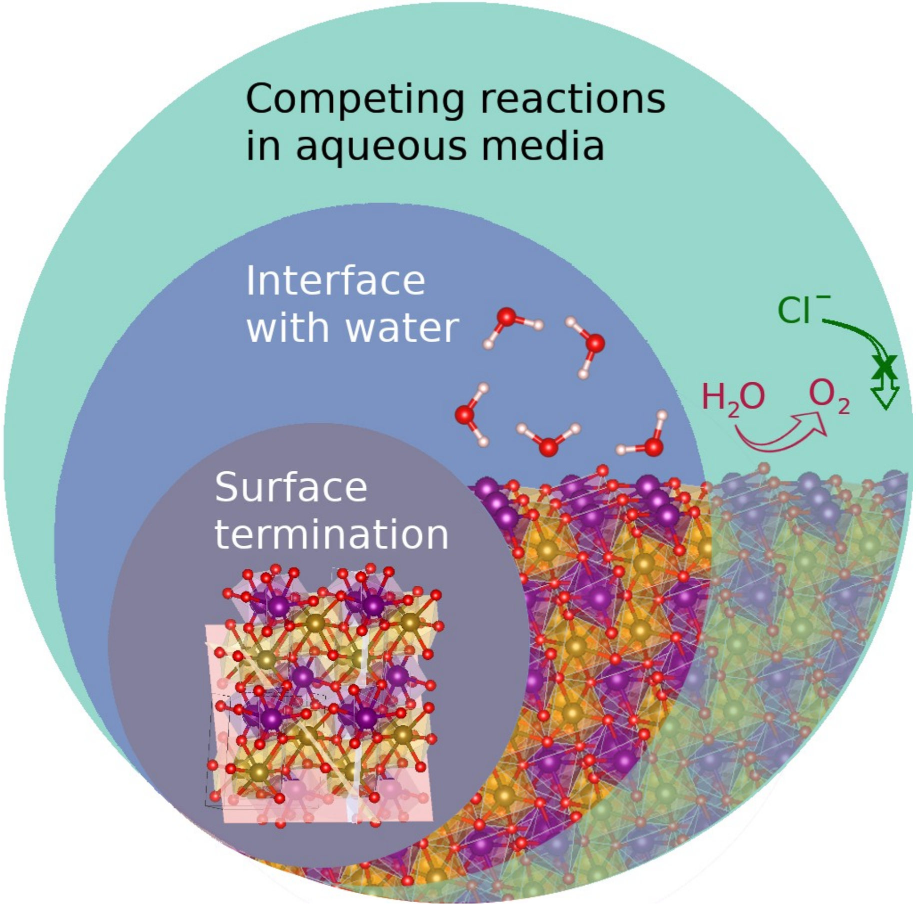






$2H_2O \longrightarrow 2H_2 + O_2$

Scope 2: Chemoselectivity in salty aqueous environments for photoelectrochemical systems

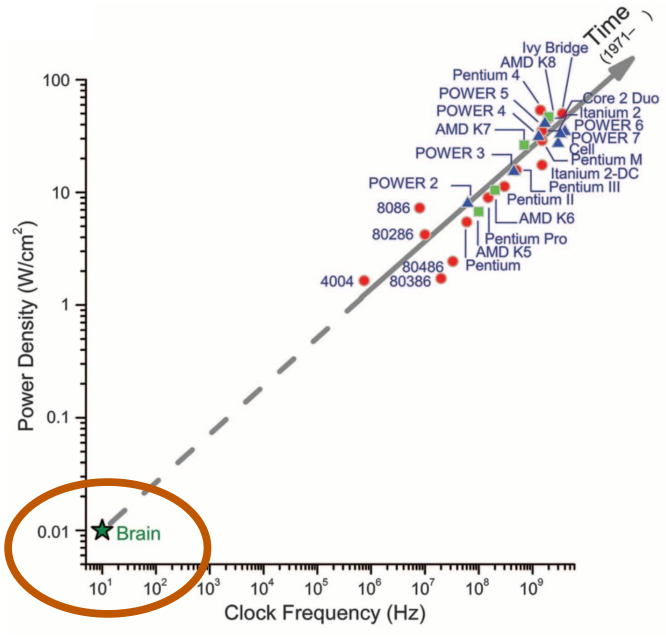


Systematic picture for interfacial interactions of semiconductor surfaces and aqueous environments

- Surface activity in driving water-splitting reactions
- Complications with other ions in solution (seawater conditions)

A closer view: focus topic #3

Neuromorphic computing: A paradigm for efficient computing and AI

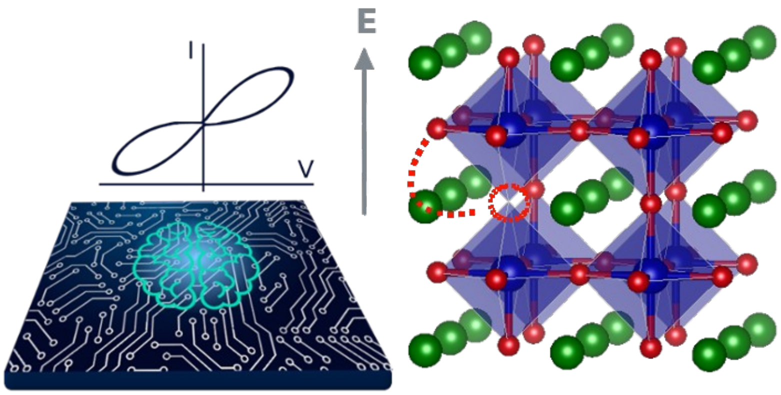


Merolla et al. Science. 345, 668 (2014)

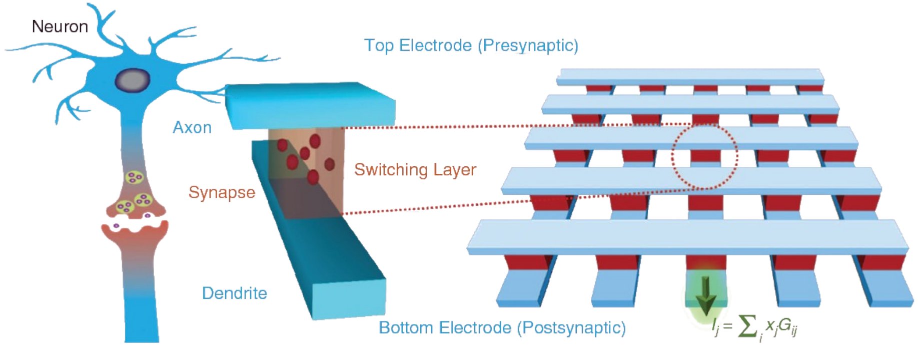
Image credit: Stanford University

Materials engineering for hardware that mimics the computational capabilities of the human brain

Scope 3: Electric fields and oxygen vacancies in perovskites for neuromorphic computing



ABO_3

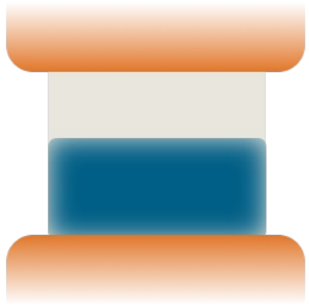


Jeong and Lu. IEEE Nanotechnol. Mag. 12, 6-18 (2018)

Develop computational models for materials platforms based on migration of oxygen vacancies for memristive devices with brain-like computation capabilities

Understanding and identifying (defective) materials with memristive behavior

Conductive filament

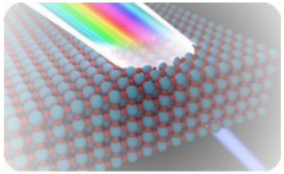


Phase change material

Research Philosophy and Methods

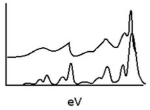
DFT
MD
MBPT
$\hat{H}$ models
.
.
.

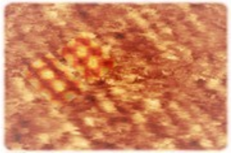
First-principles calculations



Enabled by HPC resources

Experimental collaboration





Spectroscopies, microscopies, ...

XPS
STM
XAS
.
.
.

Harnessing Materials Imperfections for Energy Sustainability

- Establish a **microscopic understanding** of defective systems
- Discover precise and novel ways for **finely tuning and predicting materials properties** for energy sustainability technologies
- Tight coupling with experiment through **spectroscopic fingerprinting**

Thank you!

If any of these are of interest to you....

- **Materials engineering** of inorganic, extended systems in sustainable energy applications
- Prediction of materials properties at the **molecular/atomic scale**
- Numerical simulation (particularly atomistic and molecular simulations)
- **Interdisciplinary/collaborative** work with ChemE, MSE, and solid-state physics

- (Scientific) coding practices
- (High Performance) Supercomputing

Please feel free to reach out!

Wennie Wang

wwwennie@che.utexas.edu

https://wangmaterialsgroup.com

Looking forward to meeting you!
Email, Zoom, etc.

Fall 2022: 2-3 students