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Institute of Functional Materials for Sustainability: Current and Future Directions

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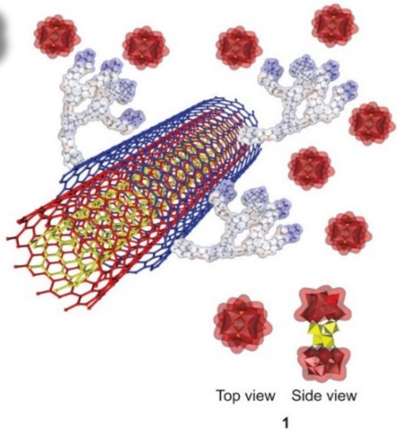
My background

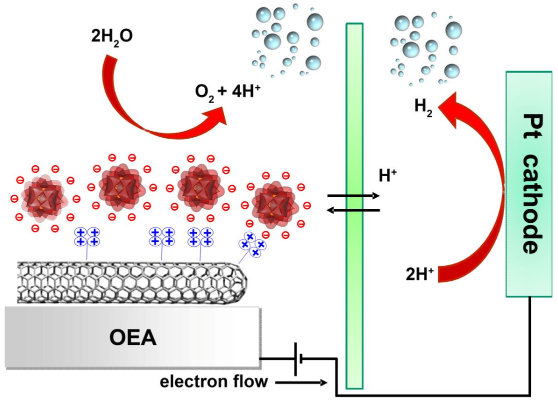
Catalytic nanointerfaces

Electrocatalysts for water oxidation

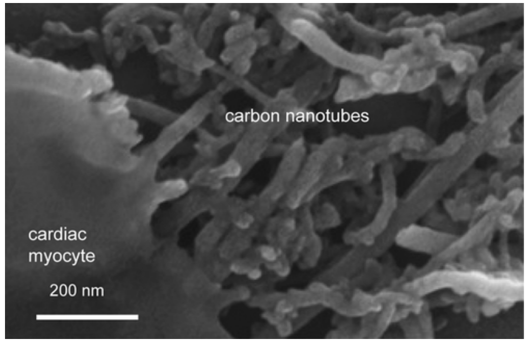
Nat. Chem. **2010**, ChemComm **2011**, Pure Appl. Chem. **2011**, ChemSusChem **2011**; EES **2012**, ACS Nano **2013**, PD2010A000162

POM@CNTs-based anode





TIME

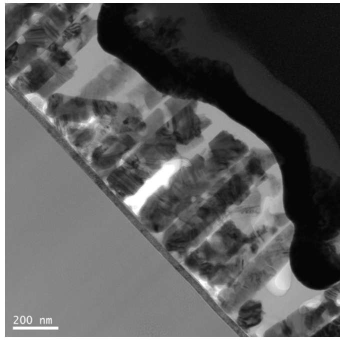


Gene delivery and tissue repairing

JACS **2009**, FASEB J **2010**, ChemComm **2010**, J. Mat. Chem. **2011**; ACIE **2012**; Bioconjugate Chem. **2015**; J Neurosci **2010**, Small **2011**, ACS Nano **2012**, NanoLett **2012**, ACS Nano 2013, Plos One **2013**, Nanolett **2013**, PCT/US2012/028930

Cardiac cell interacting with CNTs

Bioactive nanointerfaces



Hybrid and totally organic light absorbers

Adv. Mater. **2013**, ACIE **2013**, Adv. Energy. Mater. **2014**, ACIE **2015**, J. Phys. Chem. Lett. **2016**

CdSe/Pedot:PSS solar cell

Organic/inorganic interfaces

Energy Problem and Climate Change

climate.nasa.gov

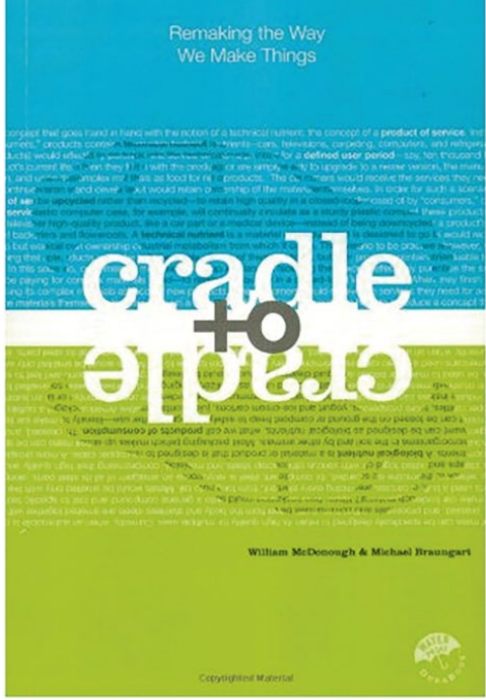
United Nations sustainable development goal 7: Affordable and clean energy

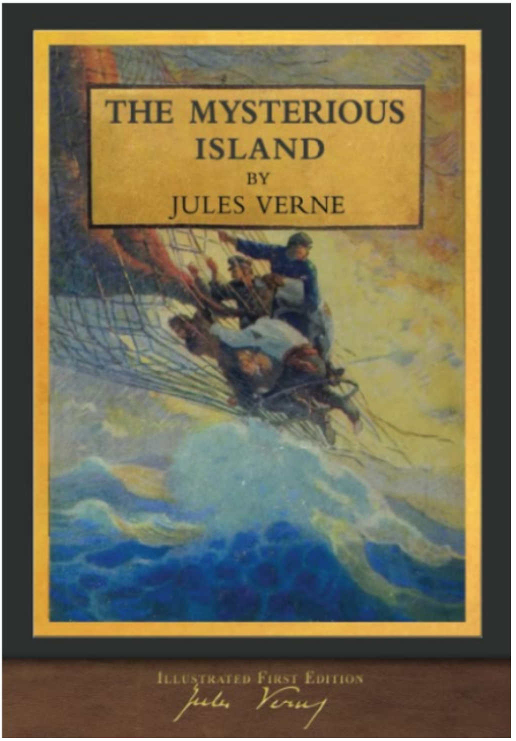
SUSTAINABLE DEVELOPMENT GOALS
17 GOALS TO TRANSFORM OUR WORLD

By 2030:

- increase share of renewable energy in the global energy mix
- enhance international cooperation to facilitate access to clean energy research and technology

Towards a More Sustainable Future





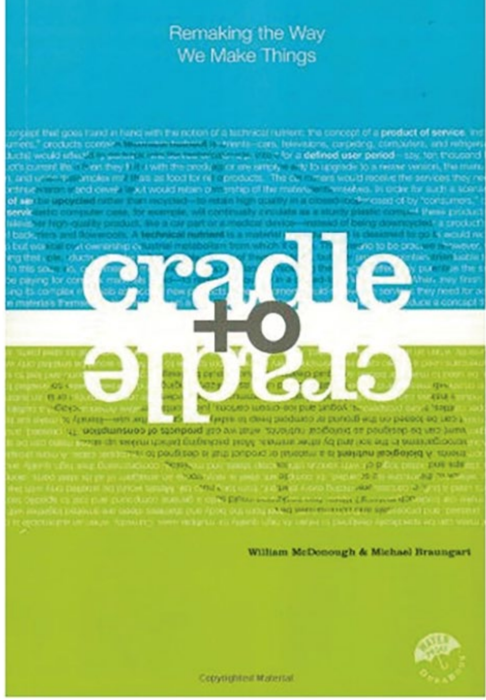
"Imagine that you have been given the assignment of designing the Industrial Revolution -- retrospectively. With respect to its negative consequences, the assignment would have to read something like this:

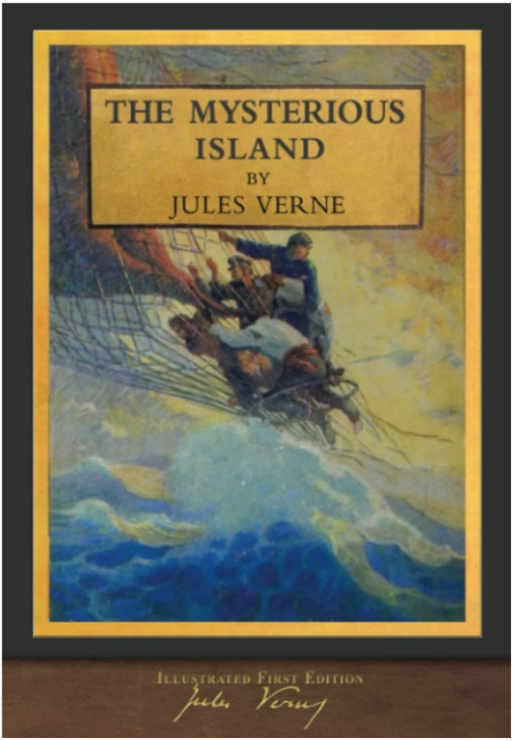
Design a system of production that

• puts billion of pounds of toxic material into the air, water, and soil every year
• produces some materials so dangerous they will require constant vigilance by future generations
• results in gigantic amounts of waste
• puts valuable materials in holes all over the planet, where they can never be retrieved
• requires thousands of complex regulations not to keep people and natural systems safe, but rather to keep them from being poisoned too quickly
• measures productivity by how few people are working
• creates prosperity by digging up or cutting down natural resources and then burying or burning them
• erodes the diversity of species and cultural practices.

Of course, the industrialists, engineers, investors, and other minds behind the Industrial Revolution never intended such consequences. In fact, the Industrial Revolution as a whole was not really designed." – 2002

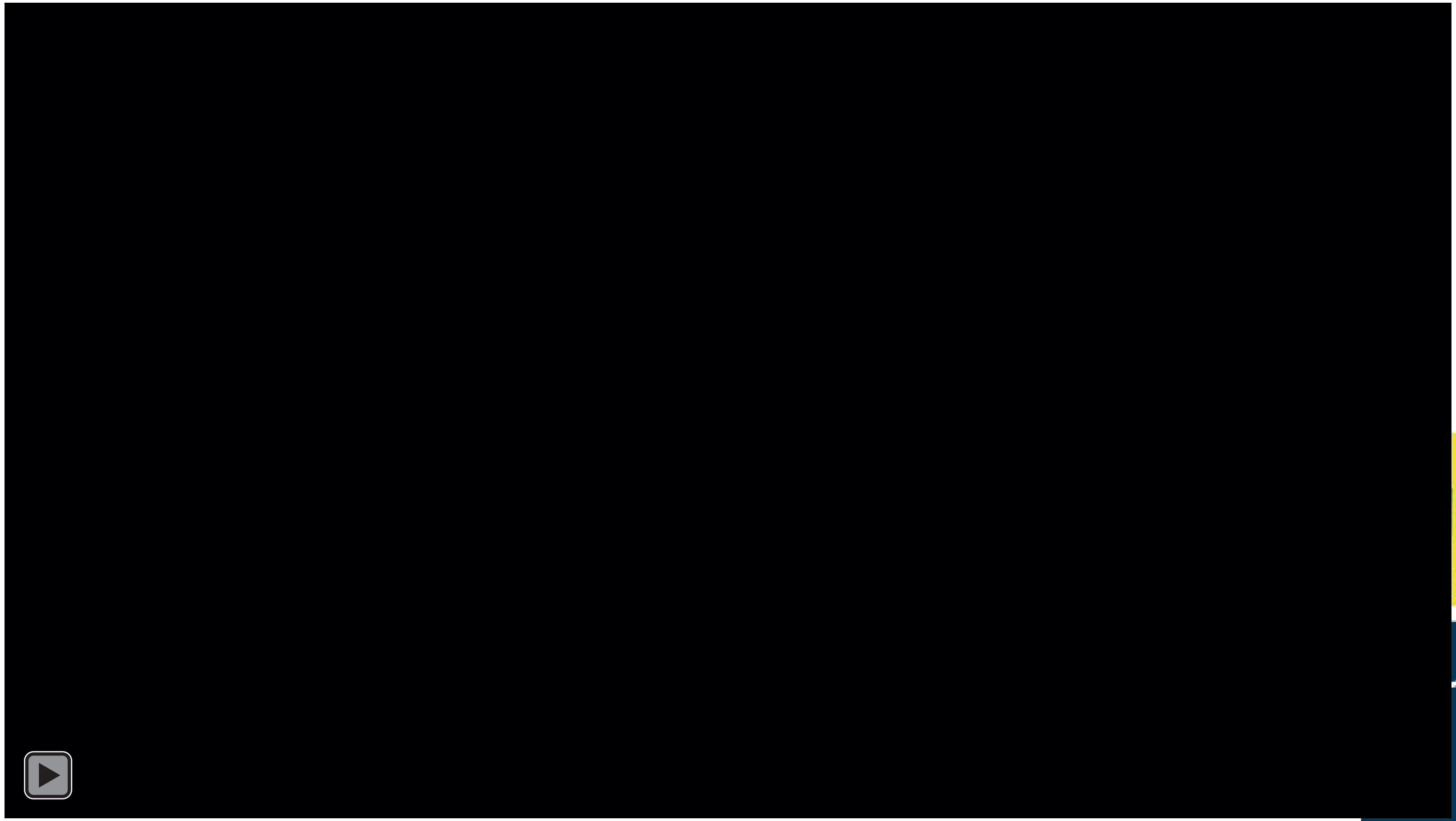
Towards a More Sustainable Future





“water will one day be employed as fuel, that hydrogen and oxygen which constitute it, used singly or together, will furnish an inexhaustible source of heat and light, of an intensity of which coal is not capable” – 1875

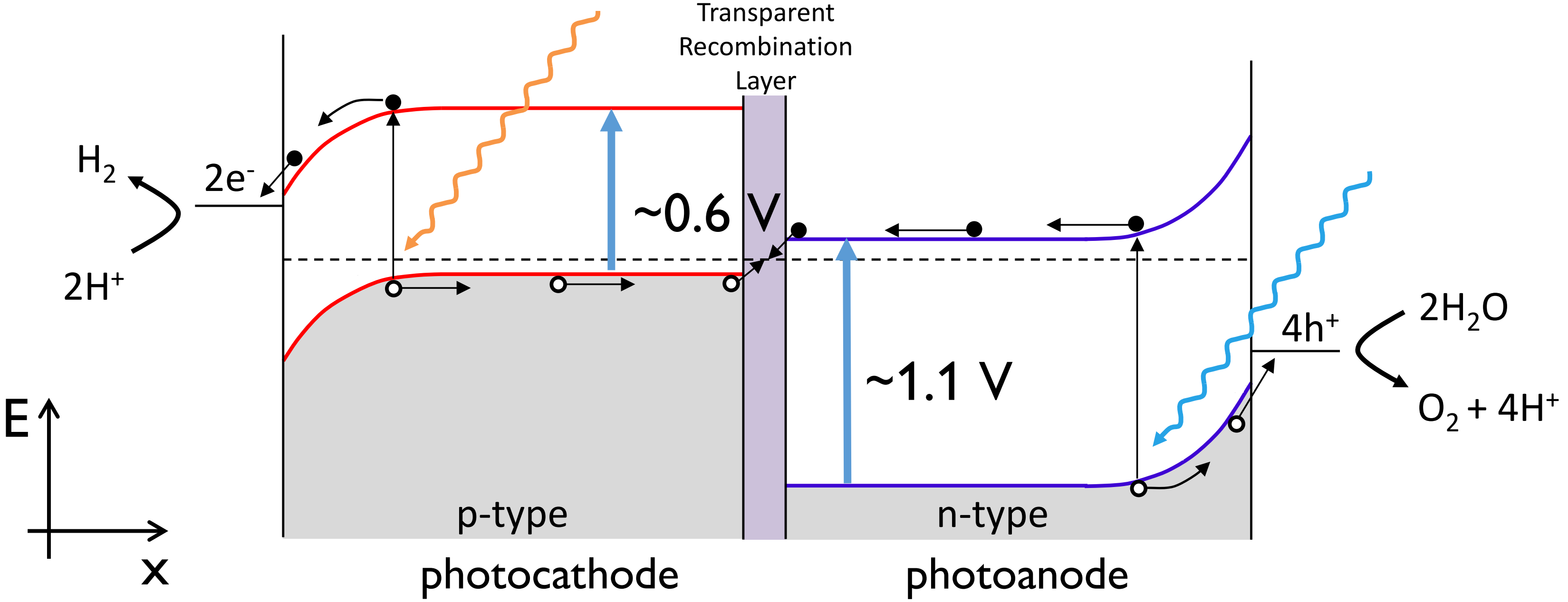
Towards a New Concept of Functional Interfaces



JCAP
JOINT CENTER FOR
ARTIFICIAL PHOTOSYNTHESIS
BERKELEY LAB

Walczak, Sharp *et al*. Adv. Energy Mater. 2017

Artificial Photosynthesis



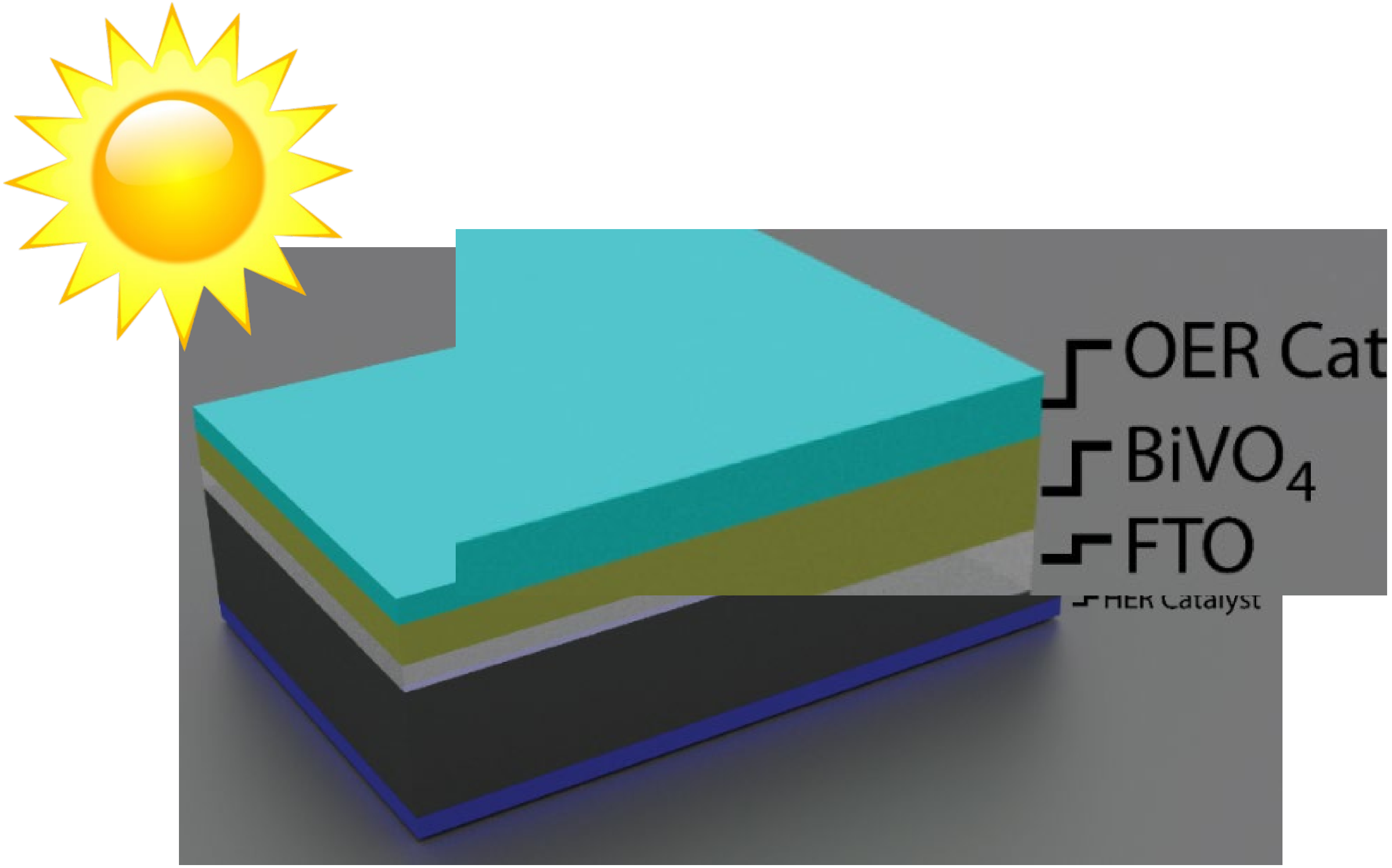
$$O_2 + 4H^+ + 4e^- \rightleftharpoons 2H_2O$$

$$4H^+ + 4e^- \rightleftharpoons 2H_2$$

$$2H_2O \longrightarrow 2H_2 + O_2$$

Thermodynamic requirements E = 1.23 V
with kinetics E = 1.7 V

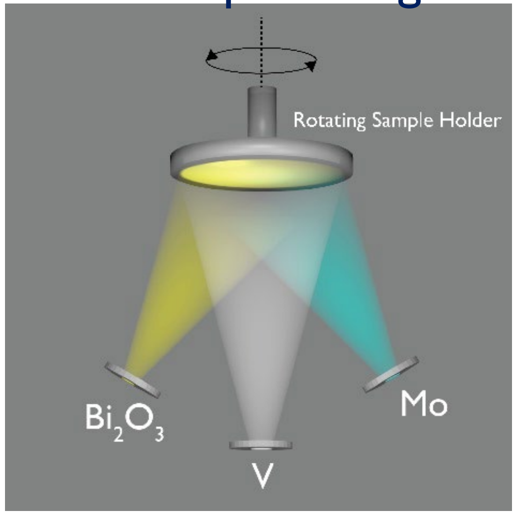
Artificial Photosynthesis: Why $BiVO_4$?

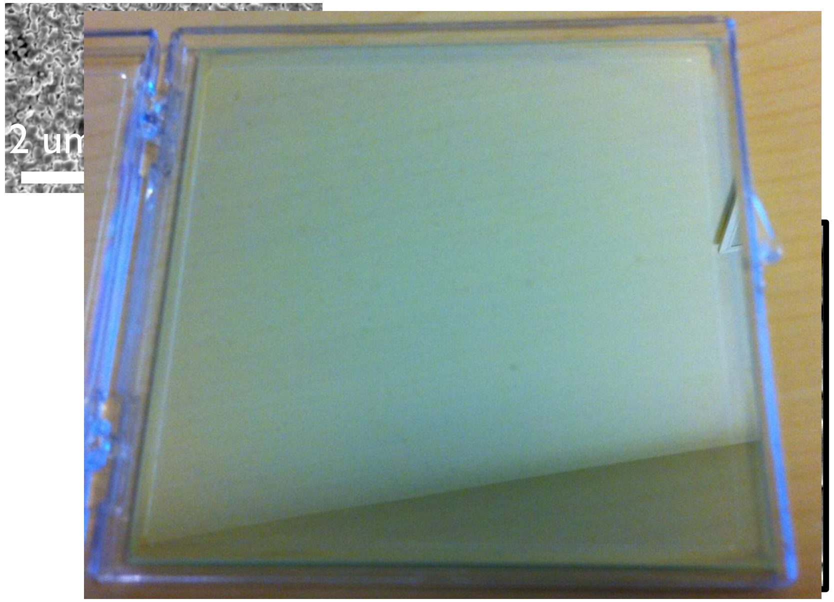


- Band gap of ~2.4-2.5 eV
- Photovoltage > 1 V
- Suitable valence band for water oxidation
- (Nominally) stable

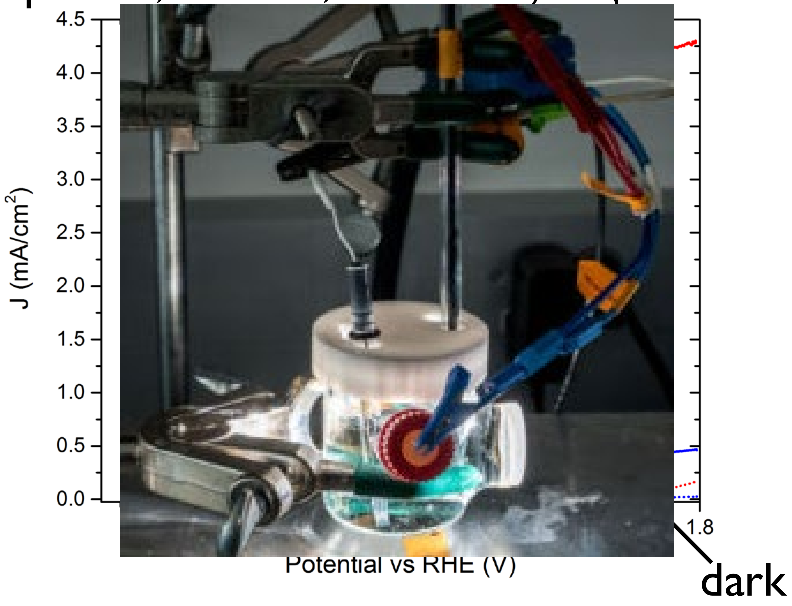
Synthesis of Homogeneous and Reproducible $BiVO_4$ Substrates

Reactive Sputtering





pH 6.8, 1M KPi, 0.1 M Na_2SO_3



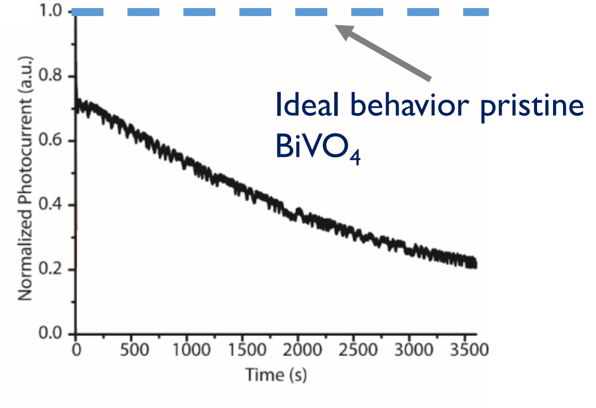
- Scalable and reproducible synthesis
- Improved performance

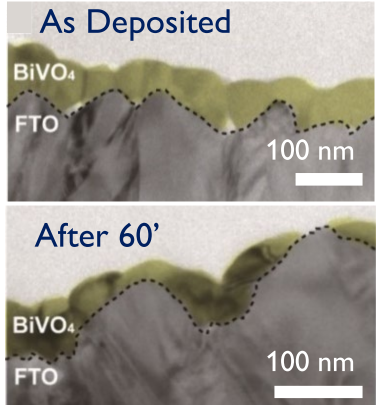
Demonstrate stability over a prolonged (100 h) amount of time

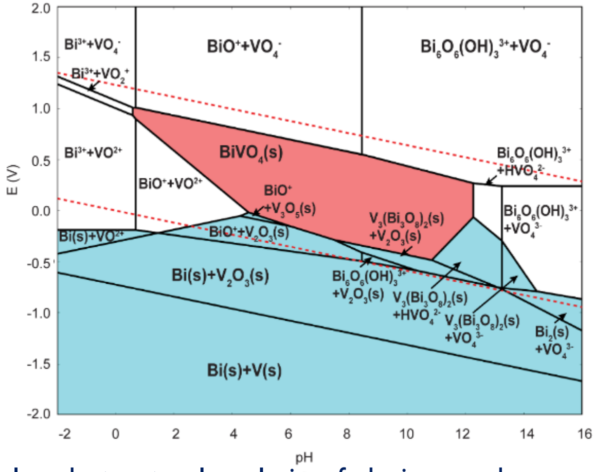
L. Chen, F. M. Toma, J. K. Cooper, A. Lyon, Y. Lin, I. D. Sharp, J. W. Ager, ChemSusChem 2015, 8, 1066-1071

Understanding evolutions of (P)EC materials

Redefining description of materials stability



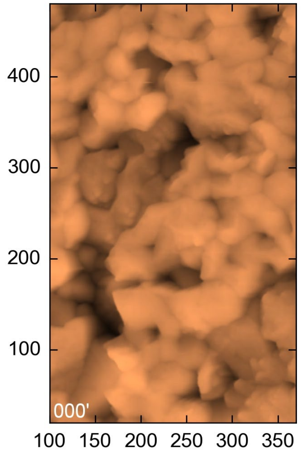




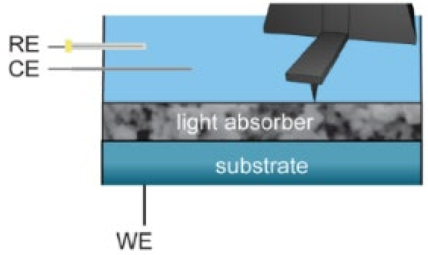
Through chemical and structural analysis of devices under operating conditions, I informed computational methods

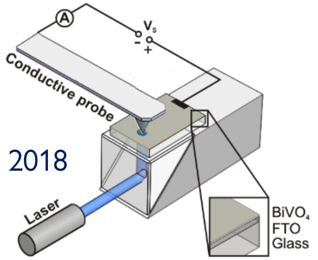
*Nat. Comm 2016

Revealing real-time transformations and charge transport at the nanoscale

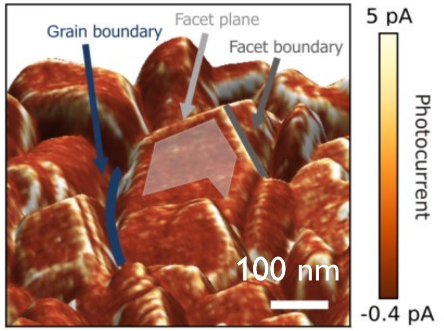


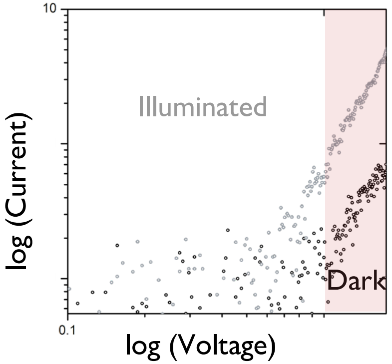
*Nat. Comm 2016





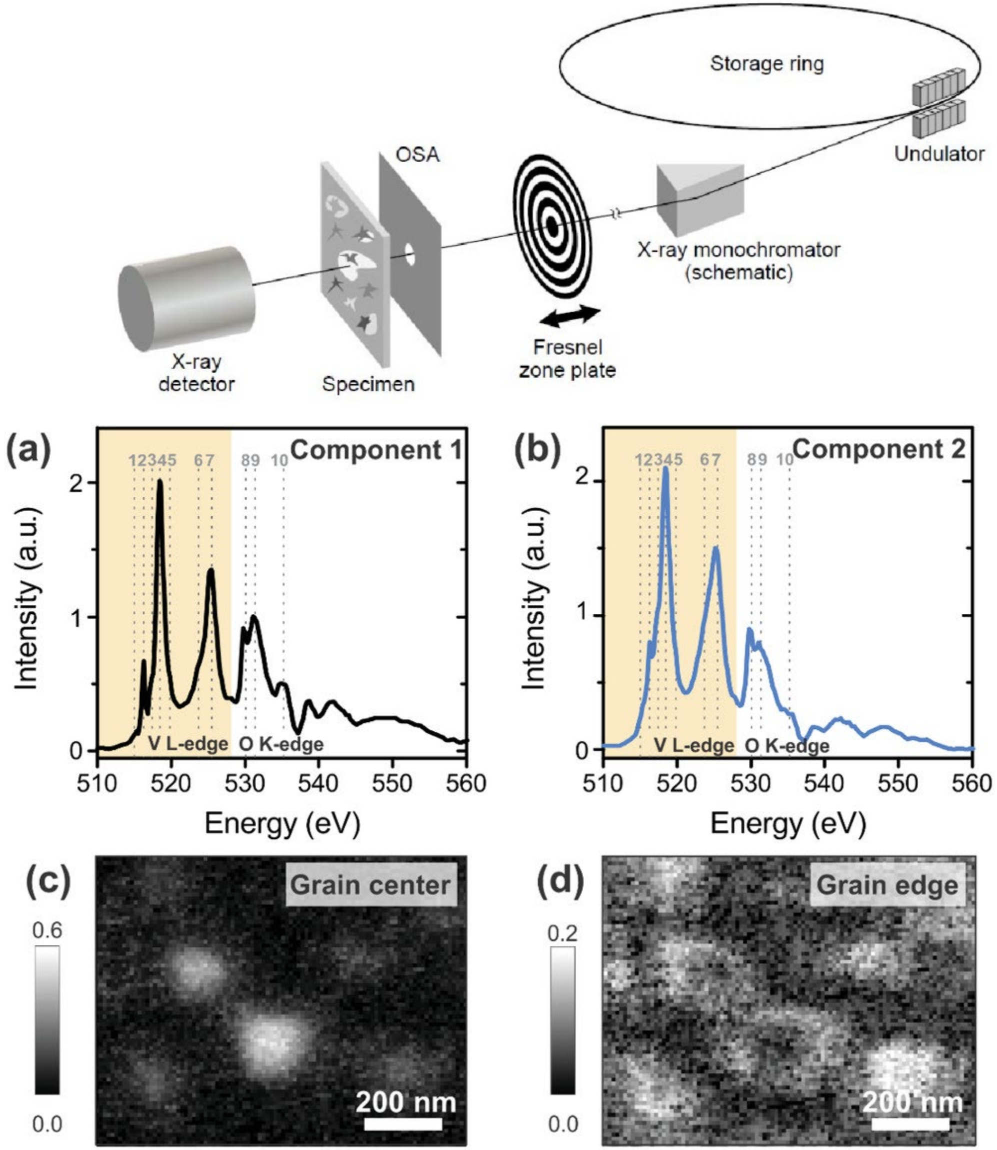
*Nat. Comm 2018, *ACS AMI 2018





Through development of novel nanoscale methods, I revealed materials transformation and effects of interfacial chemical interactions

Elucidating chemical heterogeneity *via* STXM



- STXM is a powerful technique to locally resolve variations in the electronic and chemical structure of materials with a lateral resolution of ~20 nm

- Principal component analysis can help infer the main spectral components

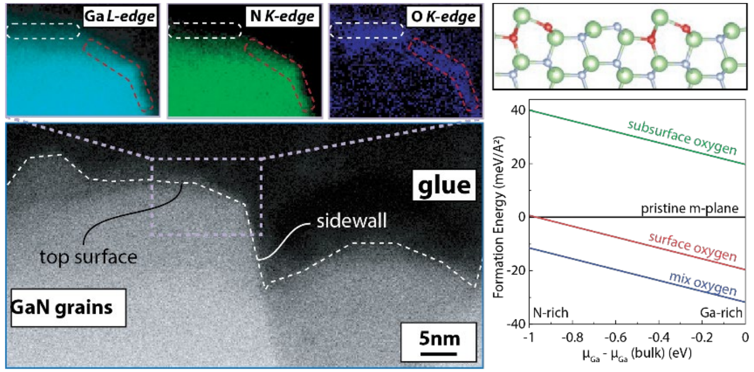
- Grain centers and grain boundaries/voids correspond to different spectral components

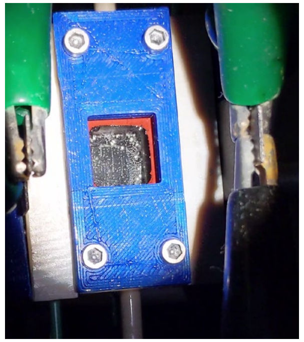
- These changes are compatible with the presence of V_2O_5 at grain boundaries

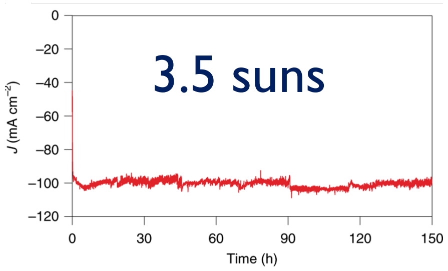
Some of my most recent work


Sehun Seo   Hojoong Choi

Oxynitride on GaN sidewalls improves stability and increases catalytic sites

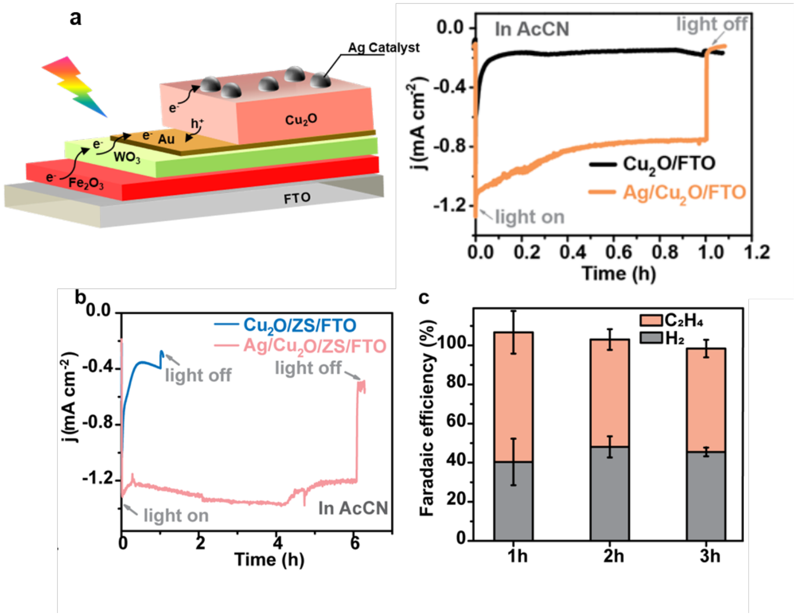






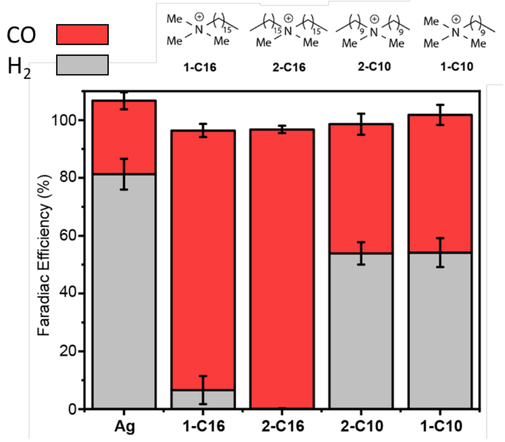
G. Zeng, […], F. M. Toma* et al, Nat. Mater. 2021,

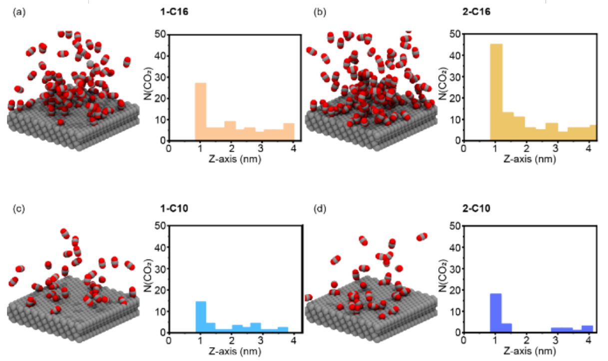
The interaction with the electrolyte determines degradation rate of Cu_2O



G. Liu, […], F. M. Toma* et al, Nat. Energy. 2021,
G. Liu, […], F. M. Toma* et al, PNAS 2021,

Controlling and understanding the local reaction environment



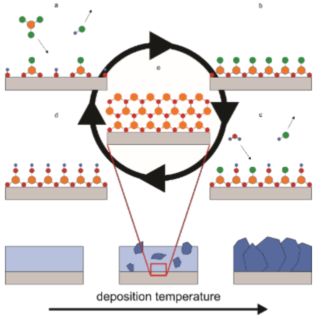


A. Buckley, […], F. M. Toma* et al, JACS. 2019,
A. Buckley, […], F. M. Toma* et al, ACS Catalysis 2021,

A few of the ongoing projects (I)


Mauricio Schieda Thomas Klassen

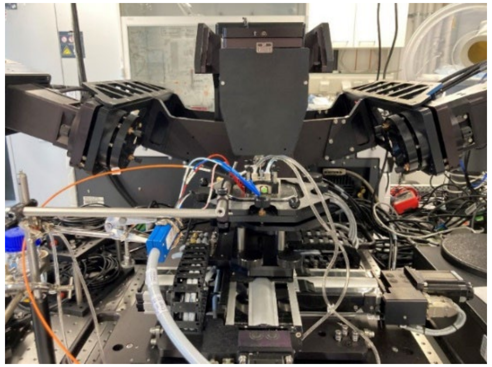
Redefining description of materials stability

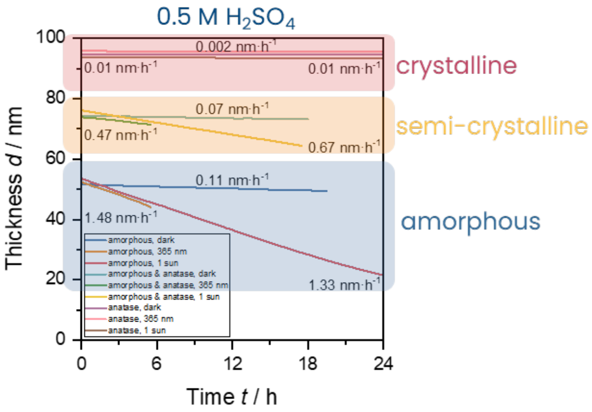


Atomic Layer Deposition (ALD). Tuning of process parameters enables control of coating microstructure.

Jiri Kollmann

Photoelectrochemical *operando* spectroscopic ellipsometry.

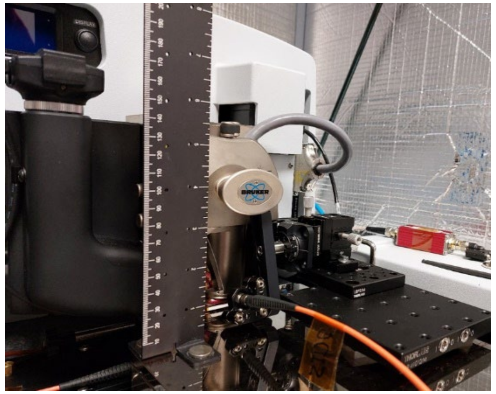




Direct characterization of degradation rates of ALD deposited protective layers by *operando* ellipsometry .

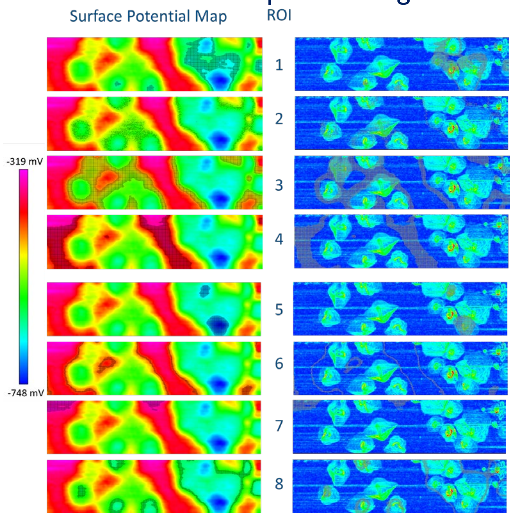
Kollmann et al. in preparation

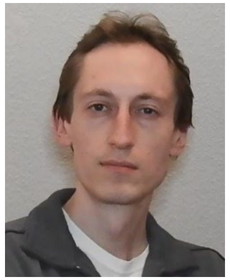
Advanced atomic force microscopy (AFM) characterization



- AFM and related conductive characterization methods for spatially resolved, functional characterization of photoelectrodes
- Understanding photoelectrochemical stability through in-situ and operando studies
- Data analysis to extract time-dependent information on transient photovoltage

Surface potential (KPFM) on a mixed-phase TiO_2 coating. *Photovoltage response of matrix and crystalline inclusions.*





Steffen Fengler

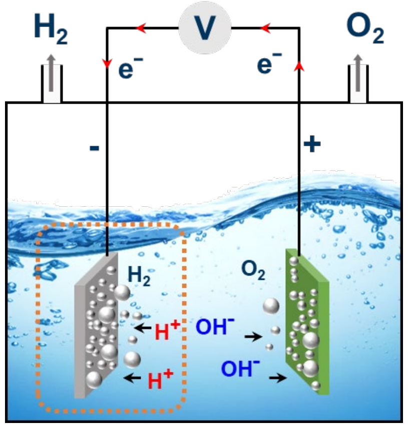
Maryam Pourmahdavi

Pourmahdavi et al. in preparation

A few of the ongoing projects (II)

Bubble management on photoelectrodes

Bubble adsorptions hinders mass transfer and scatters light.




Makafui Folikumah


Axel Neffe


Mauricio Schieda

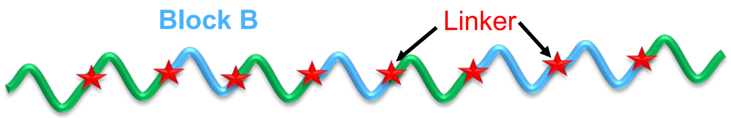
Superhydro**philic** gels are superaero**phobic**. We will study structure-activity properties to control bubble formation and time of residency at the electrode.

Development of angiogenetic blockcopolymers

- Chemistry: robot-assisted parallel synthesis
- Analytics: Sequence structure, branching, degradation, ...
- Biology: angiogenesis assays, mechanistic studies
- Processing and analytics: chemical structure vs. physics


Kirchhecker


Balk




Ma

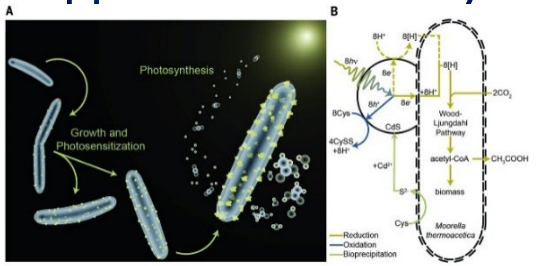

Eselem Bungu


Neffe

This project brings together the existing experience in polymers and is based on preliminary results of angiogenic effects (heart).

Biotechnological approaches to catalysis

- Polymer upcycling
- Degradation of materials
- Transformation of renewable carbon sources
- Biohybrid catalytic approaches




Tarrazona


Pasch

Additional presentations

- Developing printed electronics
- Characterizing stereocomplexes for bio-applications
- Emitters for thermophotovoltaic applications (previous WG work)


Wang


Mandlule


Krishnamurthy

KIT Karlsruher Institut für Technologie

HELMHOLTZ MDMC

Correlative Characterization
Analytical Method Development


Pasch


Eselem Bungu


Lützow


Emmler

Mechanical Properties and Rheology

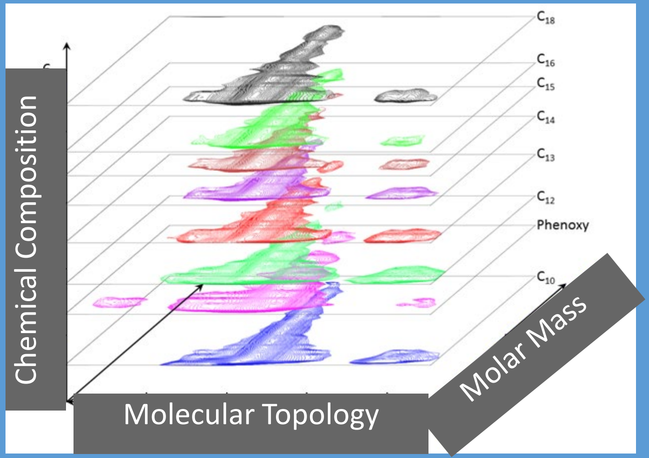
Surface Analysis

Thermal Properties

Electron Microscopy

X-Ray techniques

Multidimensional Molecular Structure Characterization



Fractionation

- Multidetector GPC
- HPLC
- 2D-HPLC
- Prep GPC/HPLC

Mass Spectrometry

- MALDI-ToF
- ESI-MS
- LC-MS
- GC-MS

Spectroscopy

- NMR
- FTIR/Raman
- UV
- Fluorescence
- IR/Raman Imaging

Acknowledgments

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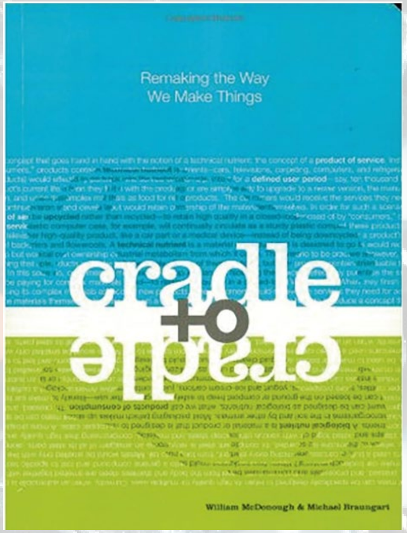

Zetian Mi
Bill Goddard
Yi Liu
Anh Pham
Tadashi Ogitsu
Junko Yano
Ethan Crumlin
Todd Deutsch
Myles Steiner
James Young
Ian Sharp
Jason Cooper
Dean Toste
Joel Ager
Aditya Mohite
Alex Bell
Adam Weber
Kristin Persson
Martin Head-Gordon
David Prendergast
Jeff Reimer
Sebastian Reyes Lillo

Johanna Eichhorn
Guosong Zeng
Aya Buckley
Olivia Alley
Guiji Liu
Michelle Lee
Tao Cheng
Alex King
Srinivas Vanka
Keenan Wyatt
David Larson

U.S. DEPARTMENT OF ENERGY
Office of Science

HydroGEN
Advanced Water Splitting Materials

DOE-EERE

BERKELEY LAB

LDRD Program

JCAP
JOINT CENTER FOR ARTIFICIAL PHOTOSYNTHESIS

DOE-BES

ALS
ADVANCED LIGHT SOURCE

LiSA
LIQUID SUNLIGHT ALLIANCE

MOLECULAR FOUNDRY

The WG team with the extended PL family ☺
…Towards remaking the way we make things…