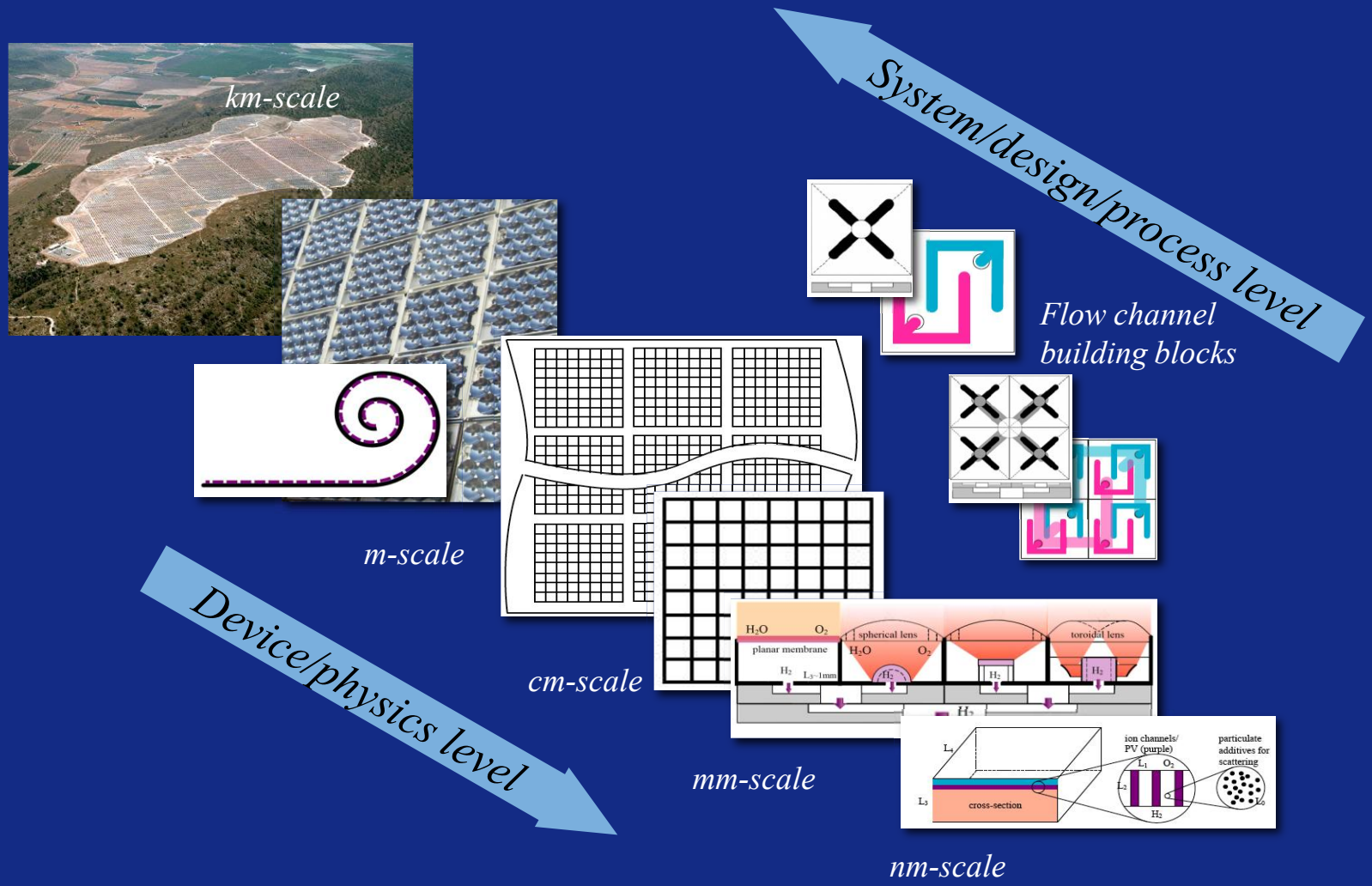
JCAP: DOE's Solar Fuels Energy Innovation Hub



The Solar Fuels Challenge

A Bold Challenge:

"The proposed Energy Innovation Hubs will take a very different approach: they will be multi-disciplinary, highly collaborative teams ideally working under one roof to solve priority technology challenges, such as artificial photosynthesis (creating fuels from sunlight)."

Secretary of Energy Steve Chu
Congressional testimony, May 19, 2009

Our Bold Response:

JCAP: The Joint Center for Artificial Photosynthesis

JCAP at a Glance

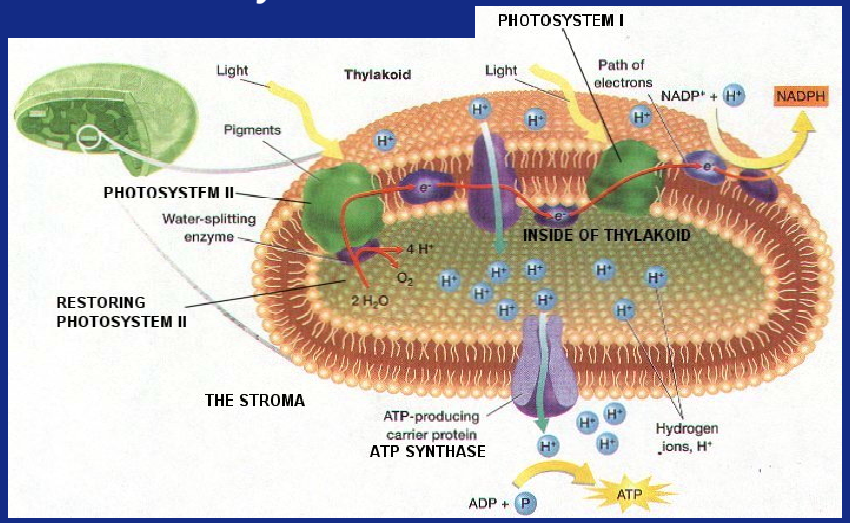
- Start-up company approach
- Highly focused research agenda
- Single, safe operation and unified facilities ("under one roof")
- Two Science and Technology Divisions
  - Accelerated Discovery
  - Science-Based Scale Up
- Eight Partners
  - Two DOE National Laboratories (LBL, SLAC)
  - Six Research Universities (Caltech, UCB, Stanford, UCSB, UCI, UCSB)

- Translational Research:
  - Parallel R&D
  - From science to prototypes
  - From nanoscale to macroscale
- Scalable and sustainable manufacturing considered throughout
- Impacts
  - "Bell-lablet"
  - Perform functions only a Hub can do
  - Agile, dynamic structure
  - Serve as integrative focal point for Solar Fuels R&D community

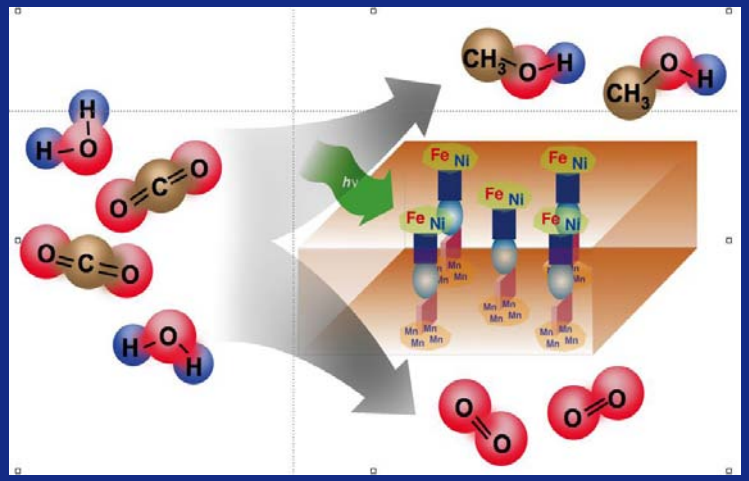
Mission of JCAP

- **Melvin Calvin, 1982**: It is time to build an actual artificial photosynthetic system, to learn what works and what doesn't work, and thereby set the stage for making it work better
- **10-year JCAP Goal, 2010**: To demonstrate a manufacturably scalable solar fuel generator, using earth-abundant elements, that, with no wires, robustly produces fuel from the sun, 10 times more efficiently than (current) crops

Photosynthesis



Artificial Photosynthesis



Fuel from Sunlight

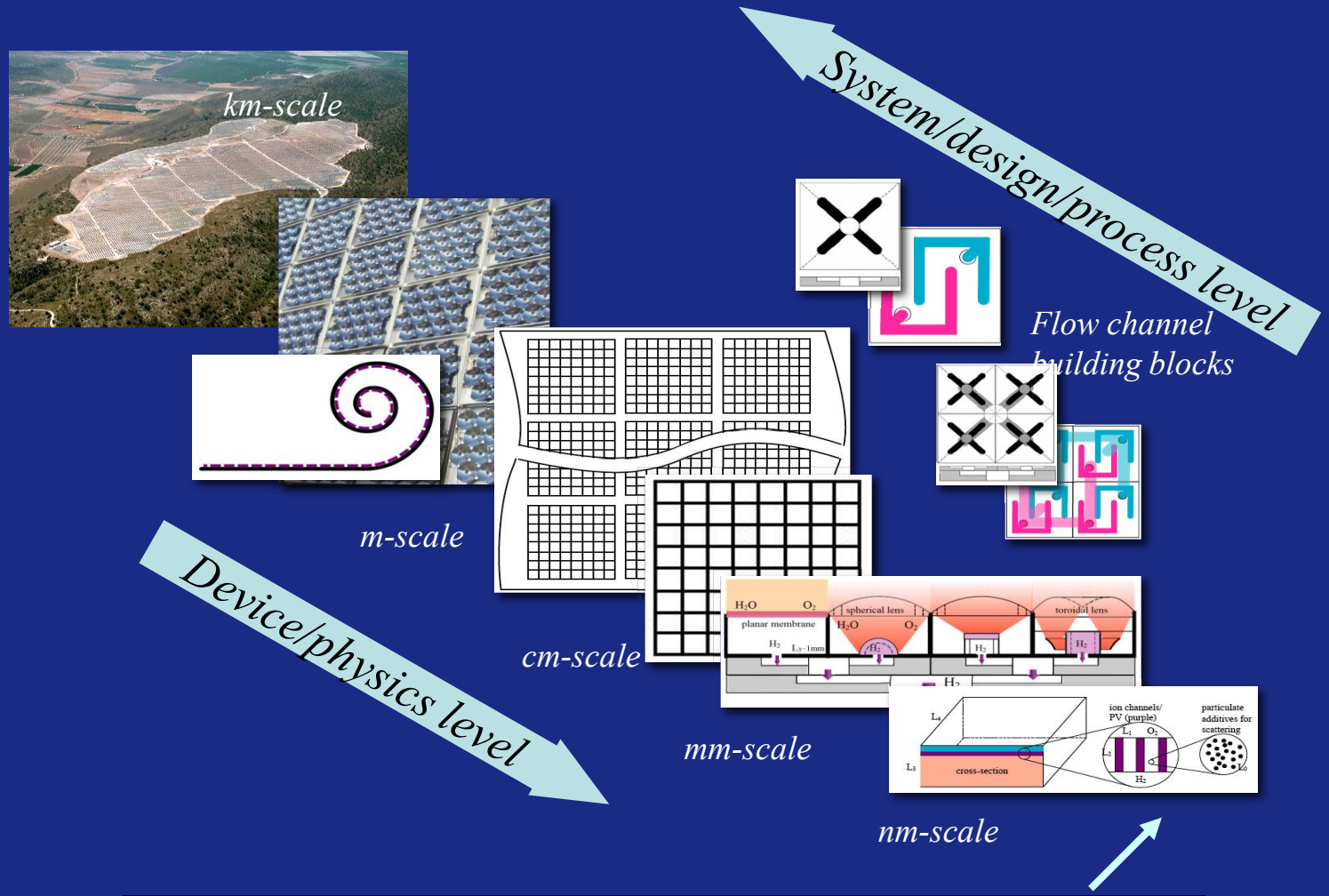
JCAP Parallel Research Goals

- **Short-term research** (five-year time frame): discovery of robust, Earth-abundant light absorbers, catalysts, linkers, membranes, and scale-up science that are required components for a complete system that produces fuels from sunlight.

- **Intermediate-term research** (five- to 10-year time frame): synergistic operation and assembly of these components and scale-up methods into a fully operational, scalably manufacturable system for the production of fuels from sunlight.

- **Long-term research** (10- to 15- year time frame): approaches to achieve very high efficiency as well as to provide optionality in the types of fuels (H_2, CH_3OH, C_4H_9OH, liquid hydrocarbons) that can be produced from sunlight by scalable, robust artificial photosynthesis.

Science and Technology Gaps

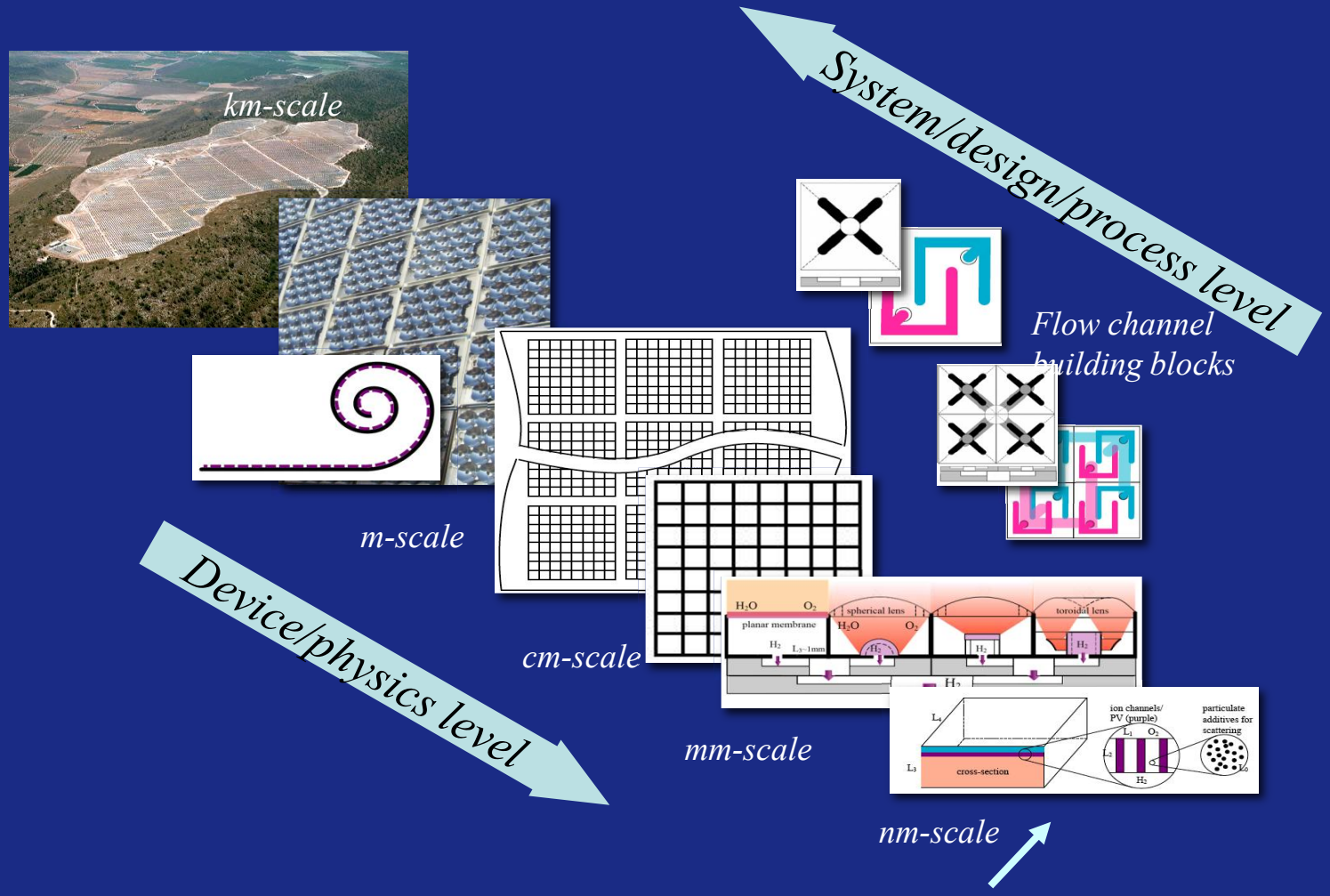


Earth-abundant Light Absorbers & Photocatalysts

JCAP JOINT CENTER FOR ARTIFICIAL PHOTOSYNTHESIS

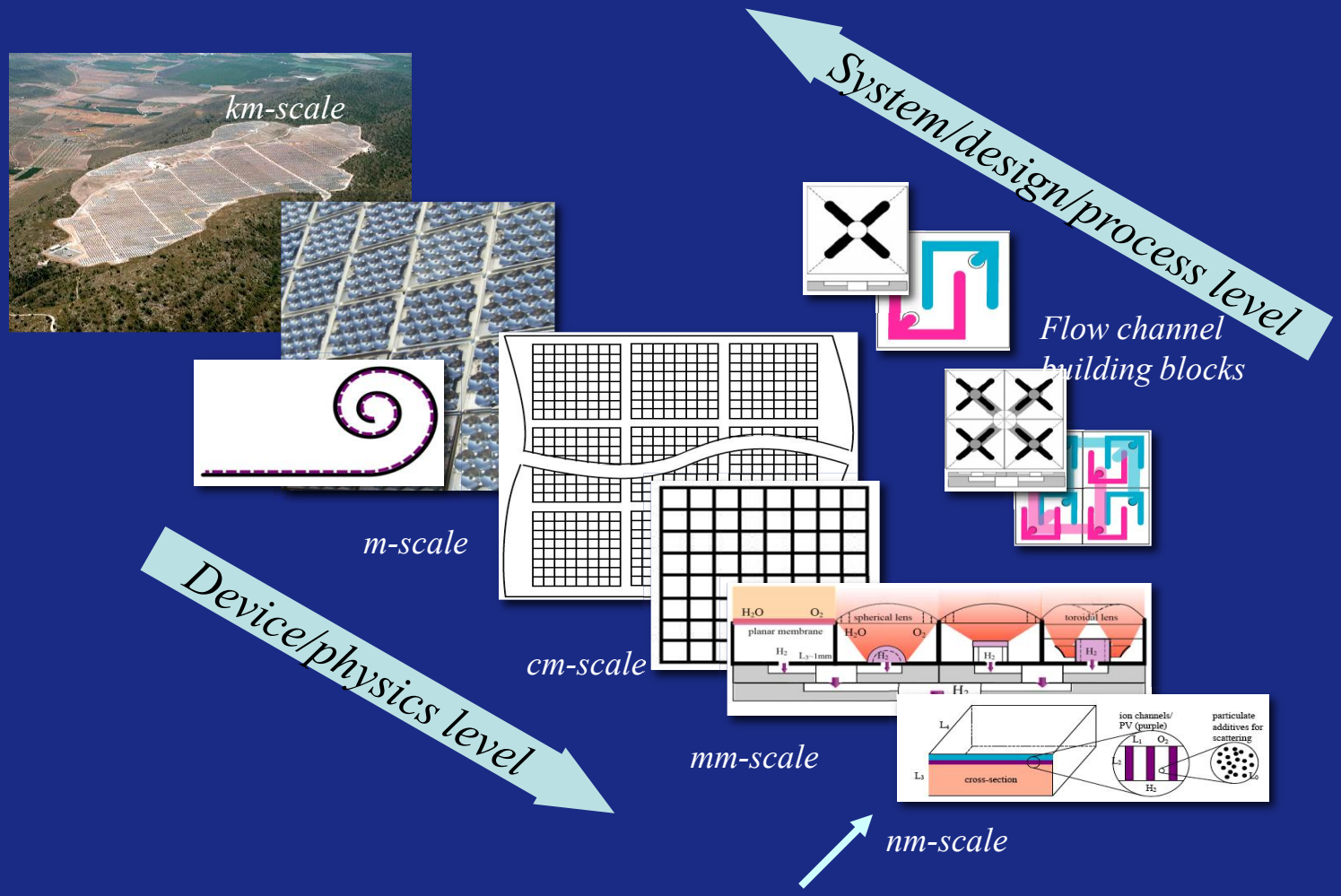
BERKELEY LAB

Science and Technology Gaps



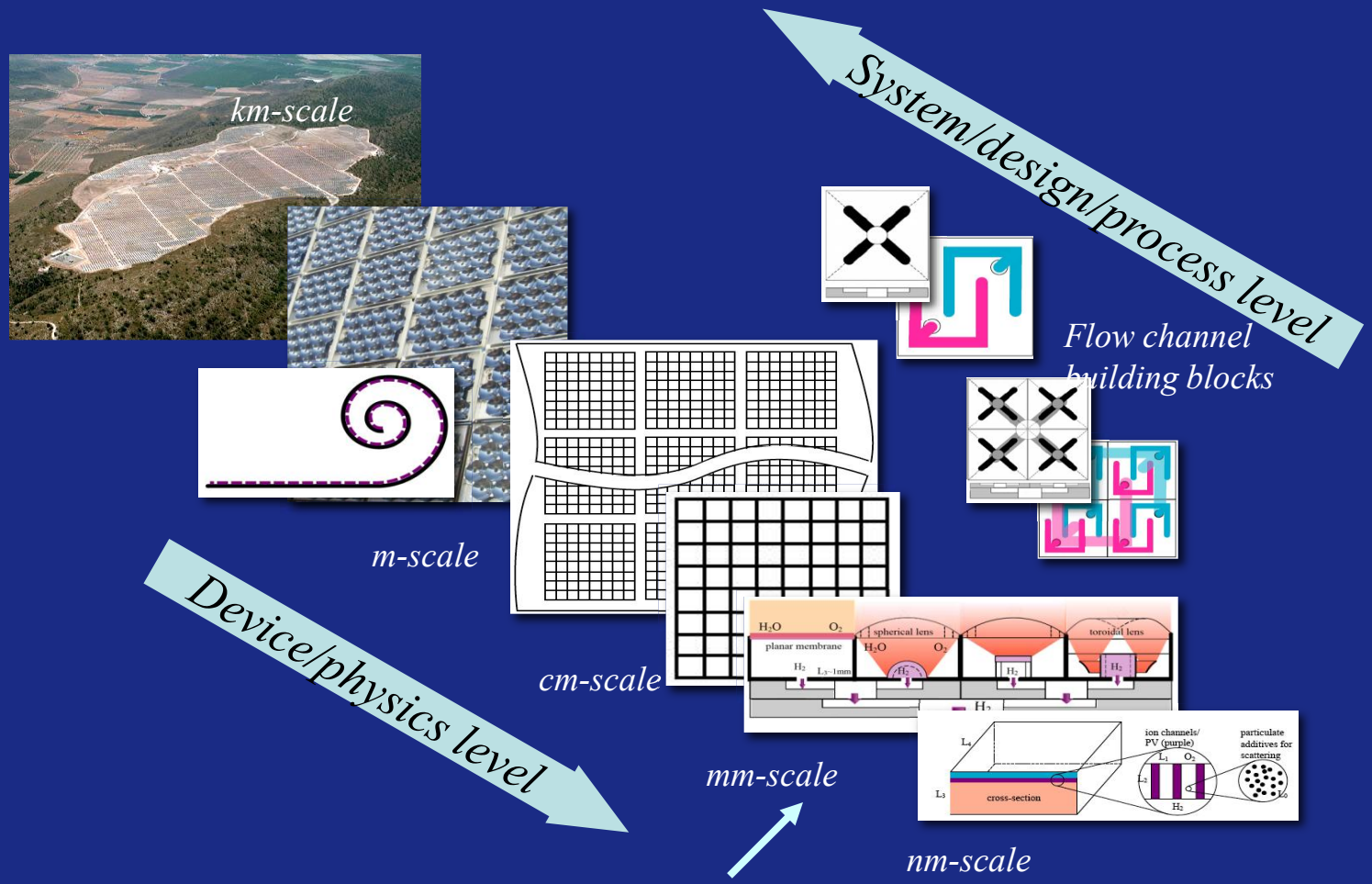
Earth-abundant, Low-overpotential, Catalysts
(Homogeneous; Heterogeneous; "Hybrid")

Science and Technology Gaps



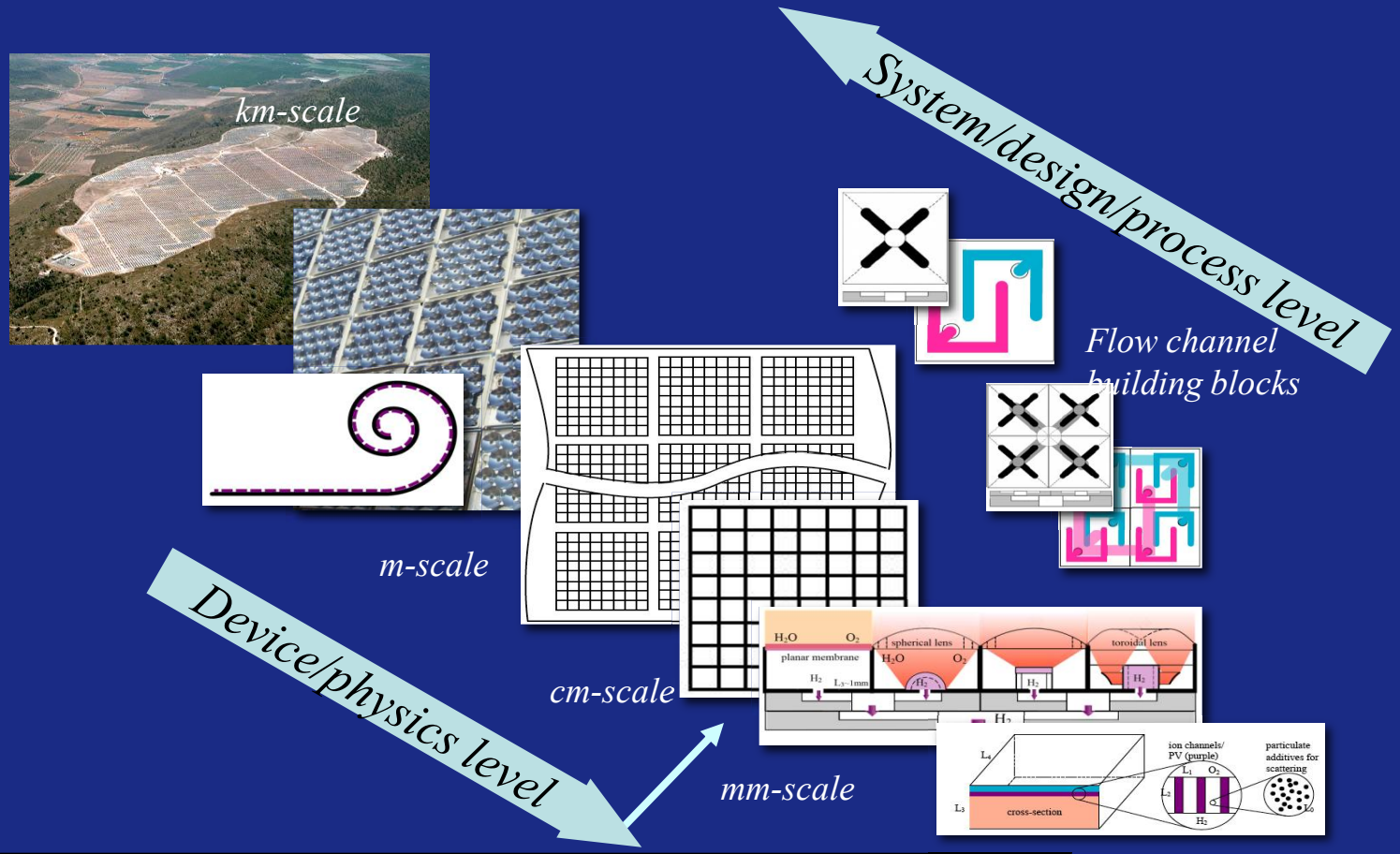
Photoelectrochemical Membranes

Science and Technology Gaps



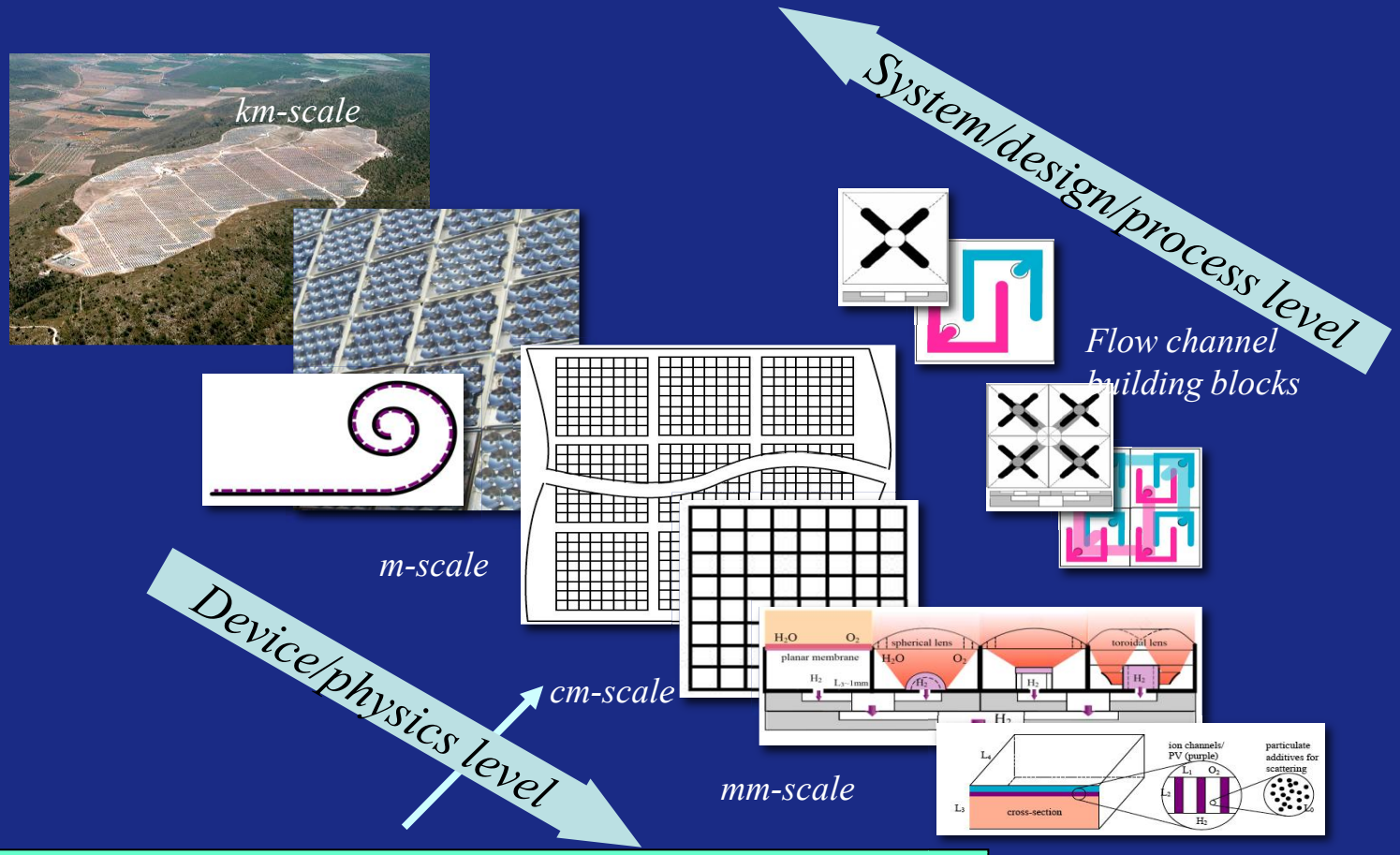
Integration of Components

Science and Technology Gaps



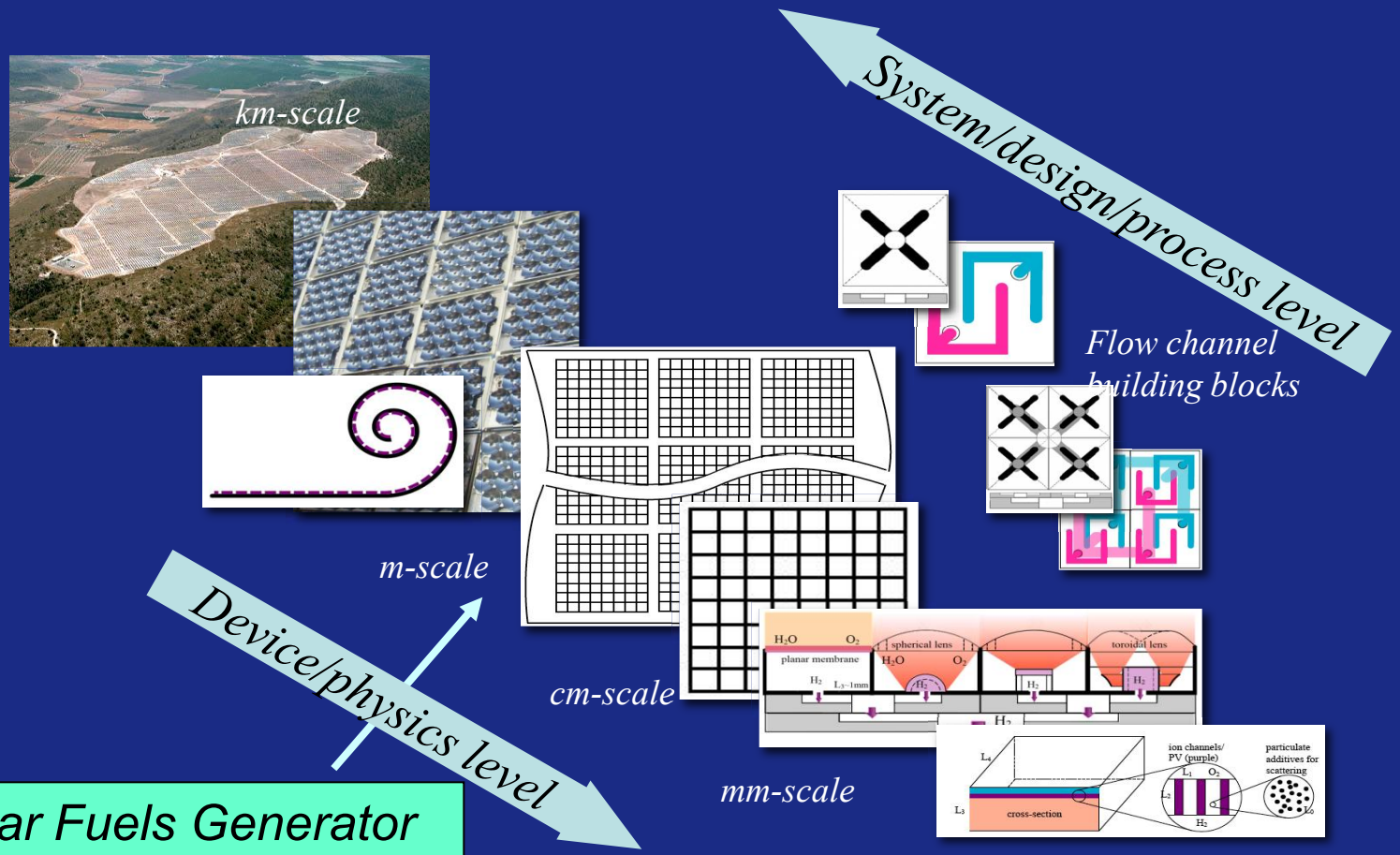
Emergent Phenomena on Mesoscale

Science and Technology Gaps



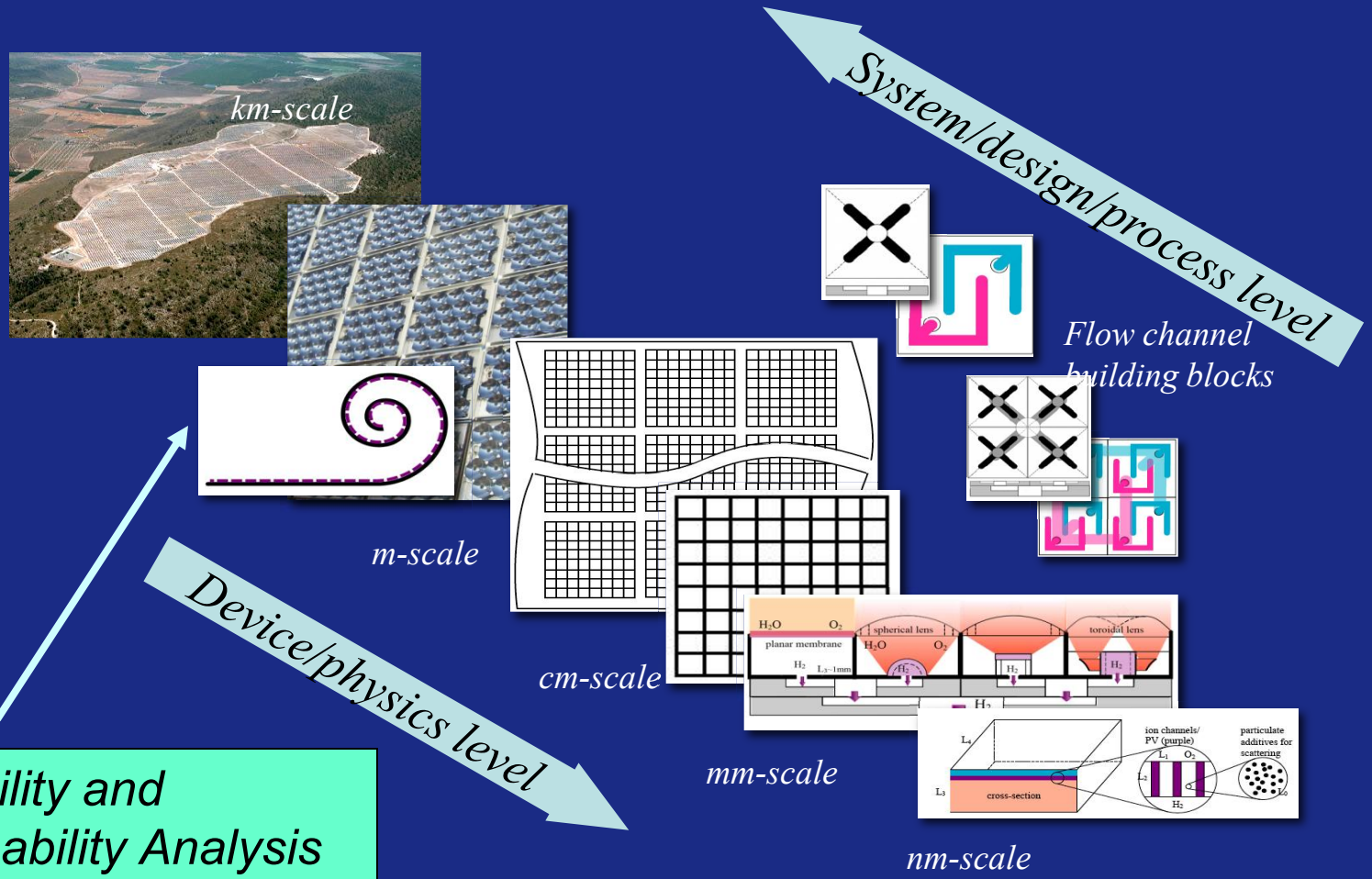
Scale-Up from Mesoscale to Macroscale

Science and Technology Gaps



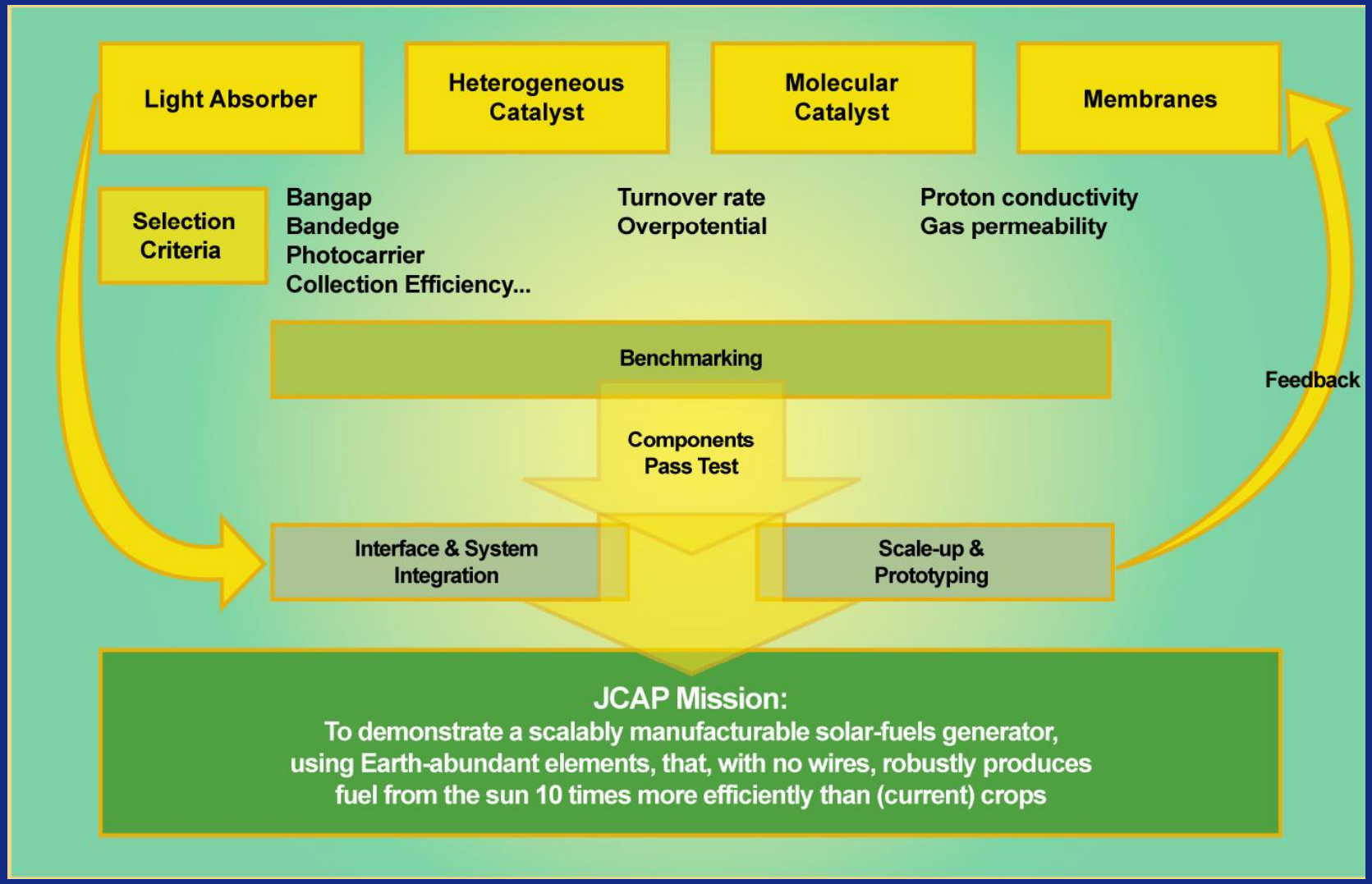
Solar Fuels Generator Prototypes

Science and Technology Gaps

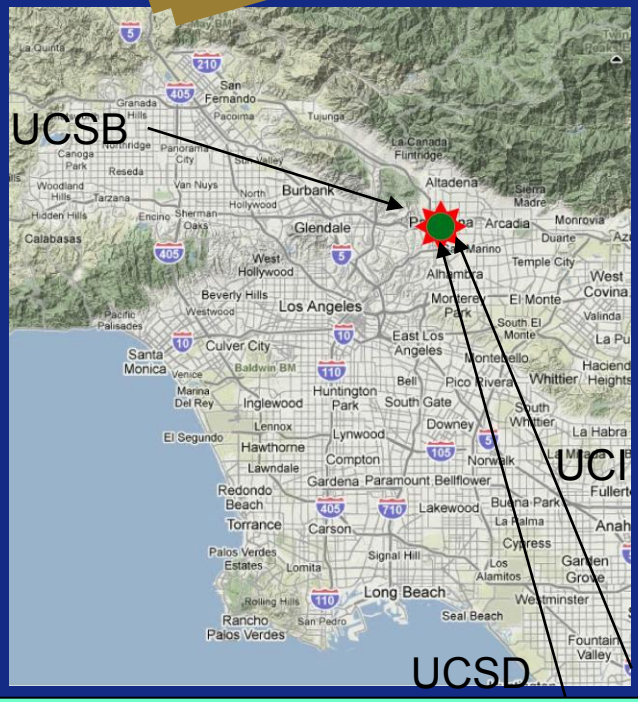


Scalablility and Sustainability Analysis

JCAP as an Integrative Hub

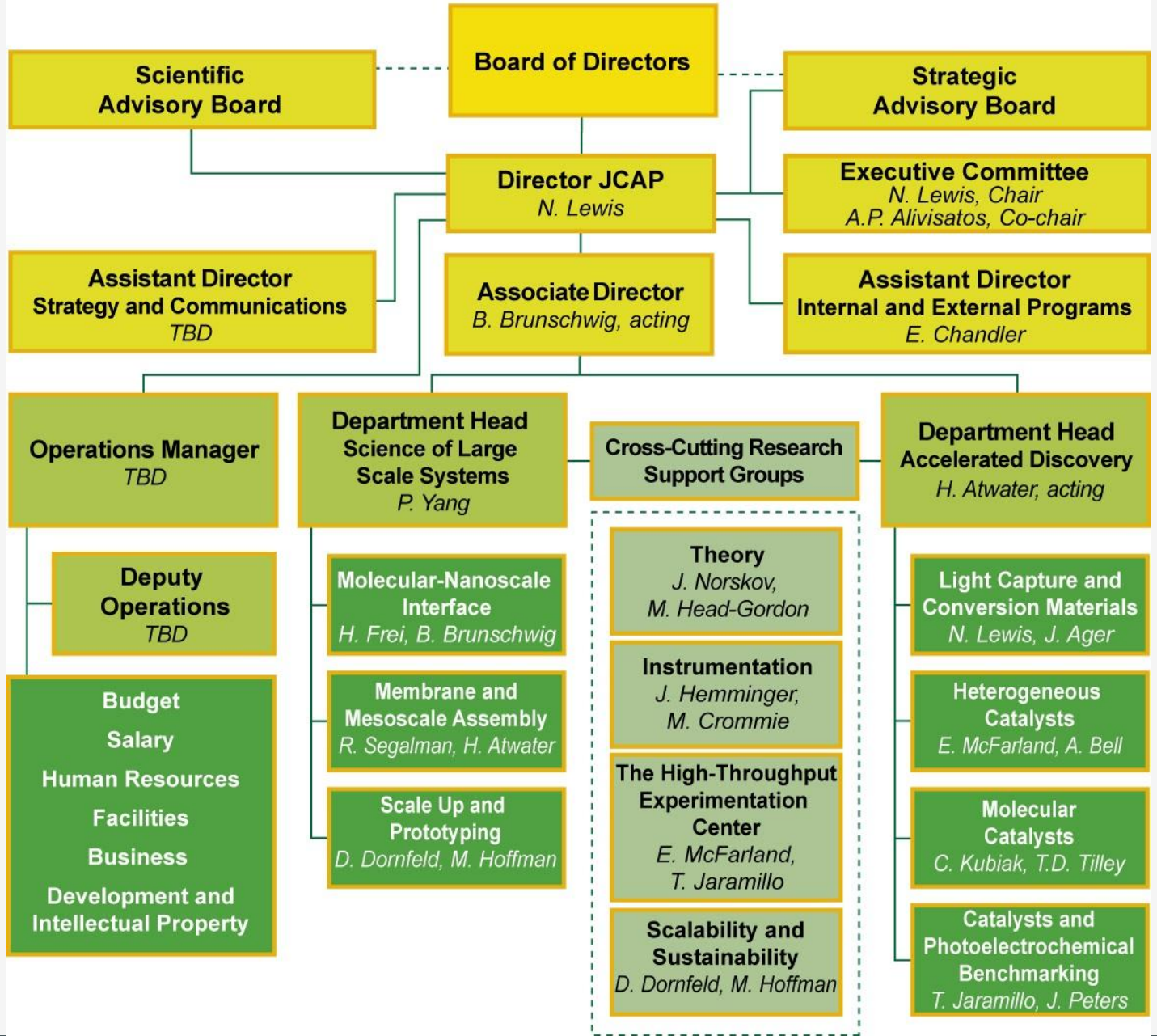


JCAP Structure: “Under One Roof”



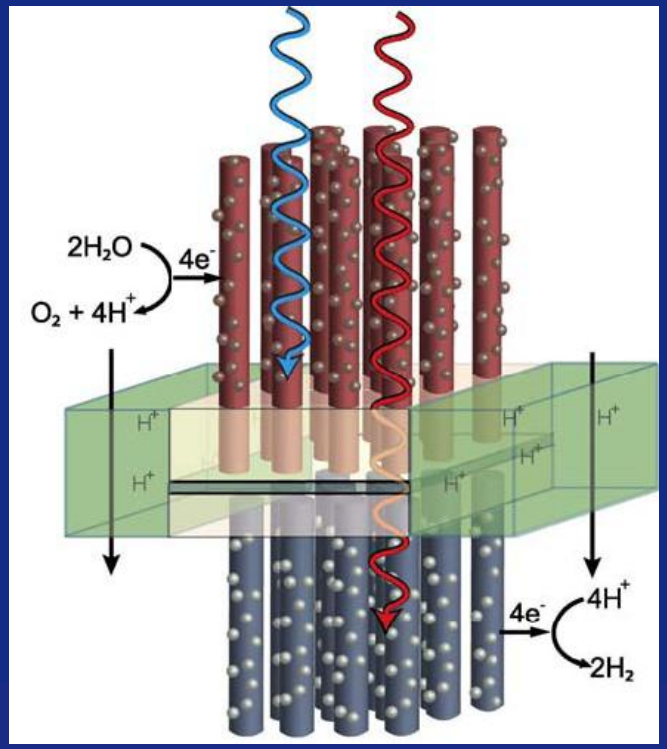
No JCAP-funded work performed outside of the JCAP buildings (except for DOE Facilities: SLAC/SSRL and ALS)

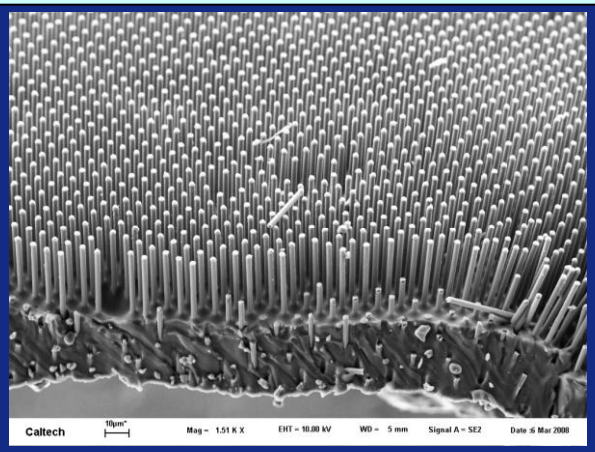
JOINT CENTER FOR ARTIFICIAL PHOTOSYNTHESIS

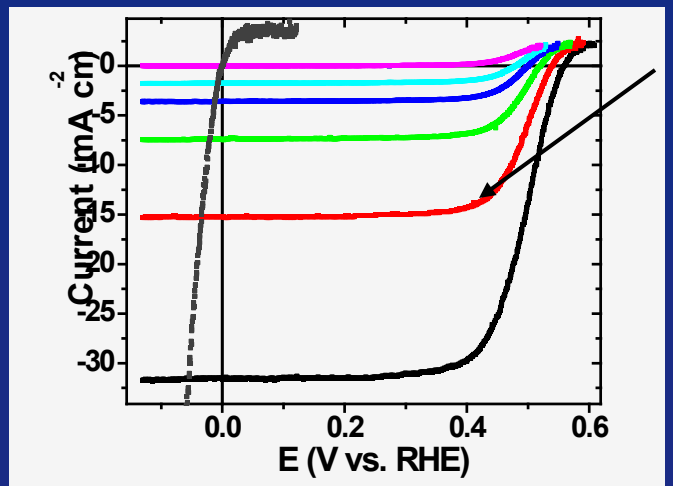


Fundamental Design Principles and Progress

- Require >1.23 V of photovoltage
- Require membrane to neutralize pH gradient and separate products
- Require catalytic sites to transform individual e^--h^+ pairs into multi-electron transfer reactions







7% to H_2

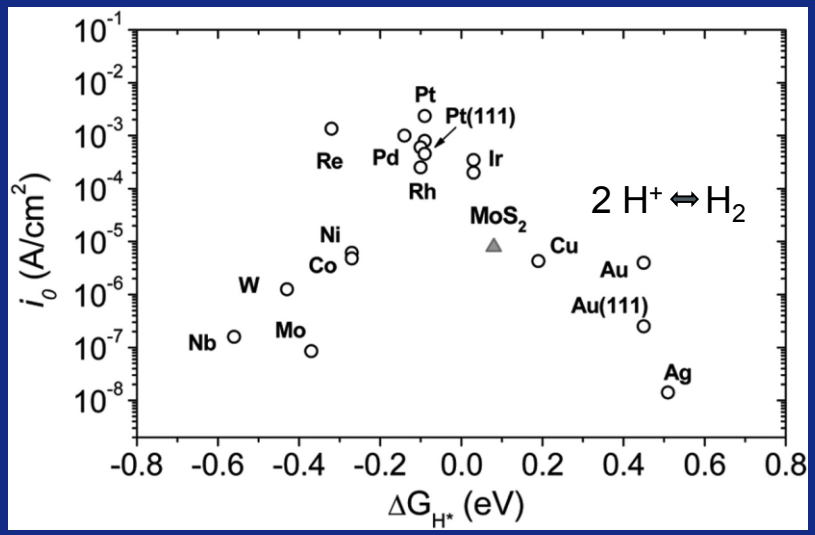
(w only 60% absorption)

Scope and Focus of JCAP

- Robustness of Components:
  - >98% of commercial catalysts are heterogeneous
  - Significant JCAP effort into heterogeneous catalyst development
  - Also active development of homogeneous, inorganic surface attached catalysts
- Historical rate of catalyst discovery for solar fuels reactions is too low
  - Pt; RuO_2, IrO_2, Co_3O_4; Ru_2"blue dimer"
  - Must dramatically accelerate rate of catalyst discovery
- Need earth-abundant, robust, inorganic light absorbers with optimal band gaps
- Need science base to incorporate components into functioning devices and systems, as well as scale-up and prototyping
- Need to address in parallel the many scale lengths involved, from nanoscale to macroscale

Heterogeneous Catalyst Discovery

Gaps: Need active, earth-abundant catalysts for H_2, O_2, and for $e^- + CO_2$

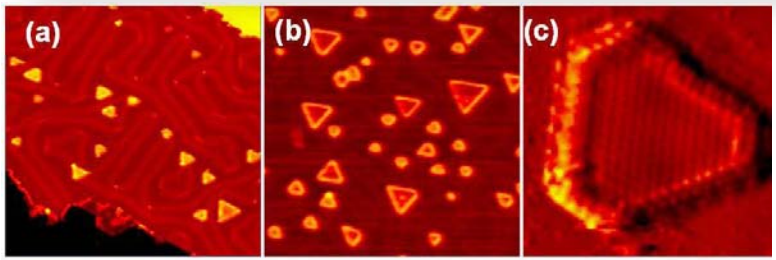


Starting Points:

H_2: Ni-Mo, MoS_2 CO_2: Cu, Ag, GaP

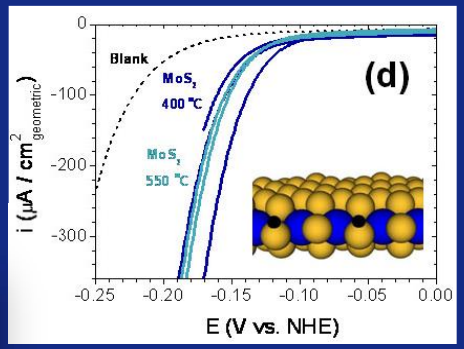
O_2: RuO_2, NiO_x

Approach: Develop structure-function relationships for "best systems"

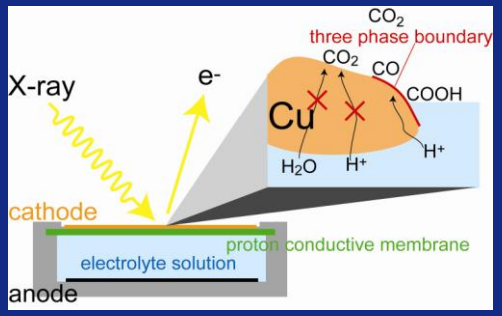


STM images of MoS_2 nanoparticles on Au(111)

Electrochemistry

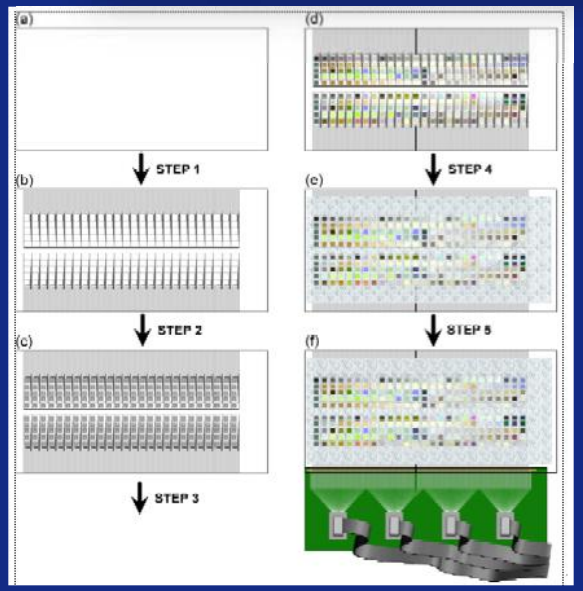


In-situ XPS (SSRL)

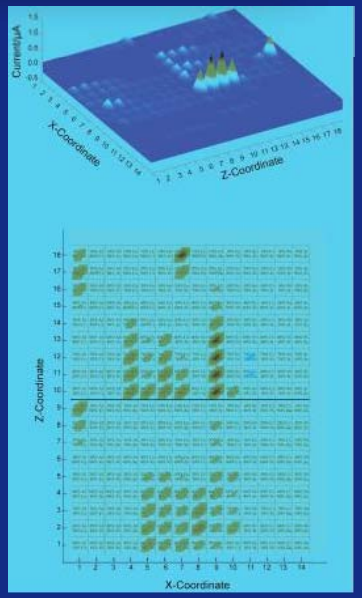


Heterogeneous Catalyst Discovery

Gaps: Complement with Ultra-high Throughput Experimentation



Schematic of the process of preparing the substrate and making electrical contact to 130 individual materials on a single piece of FTO-coated glass.

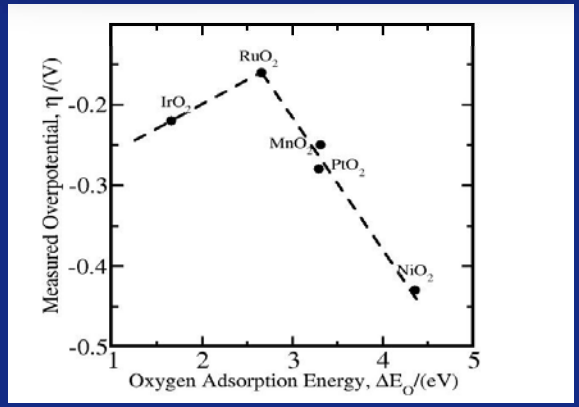


False color images of the photocurrent of a slide that contained spots of binary mixed-metal oxides (top). Three-dimensional plot (bottom). Top-down view.

Starting Points:

H_2/CO_2: MS_x; O_2: MO_x, MO_xN_y

Outputs: Tie together theory, surface science, electro-chemistry, X-ray spectroscopy, high-throughput experimentation



Measured OER overpotential vs calculated adsorption energy

Activity Metrics/Goals:

~x 10^2 for H_2; ~x 10^4 for O_2

>x 10^5 for CO_2

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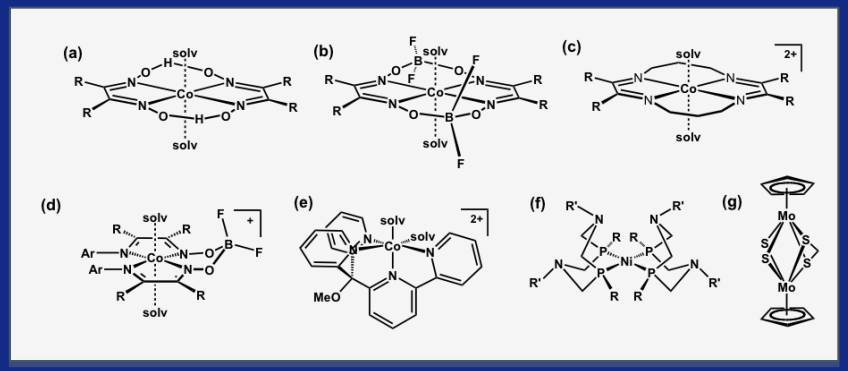
CALIFORNIA INSTITUTE OF TECHNOLOGY

BERKELEY LAB

Molecular Catalyst Discovery

Gaps: No robust, active homogeneous catalysts for H_2, O_2, or CO_2 reduction

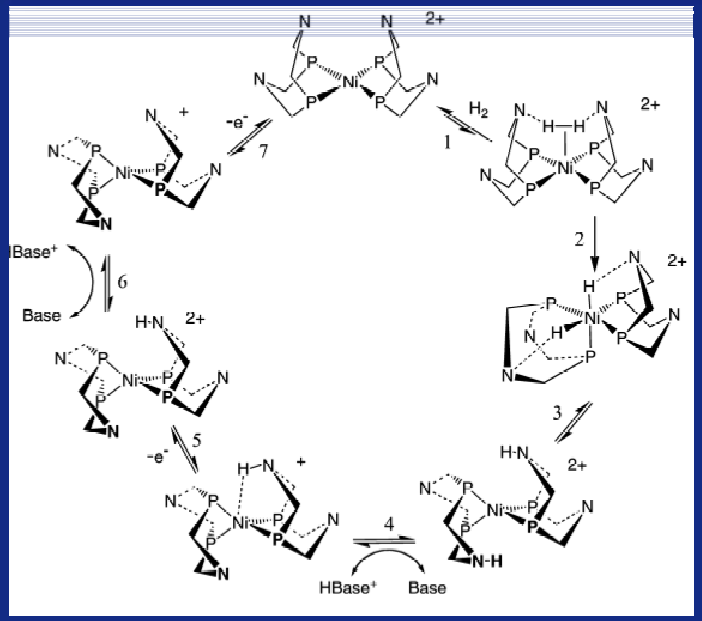


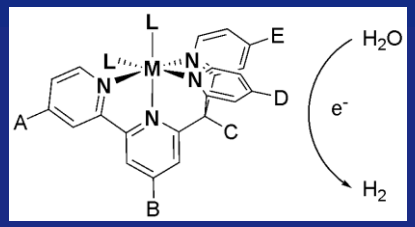
Starting Points:

H_2/CO_2: Co/Ni/Fe (II,I,0) species

O_2: Mo, W, Co (IV, V, VI) species

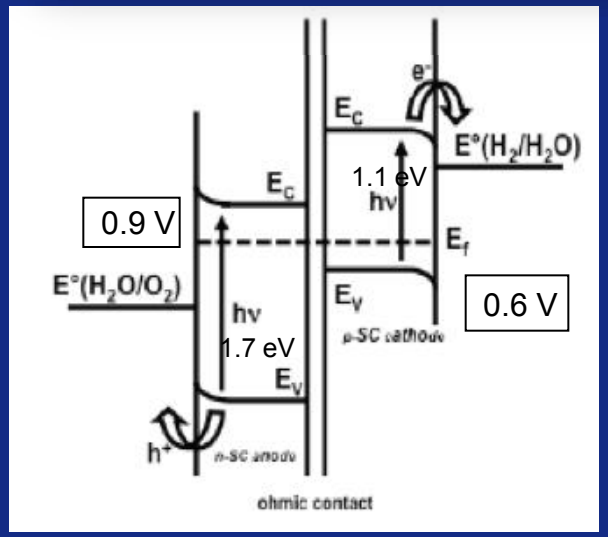
Approach: Understand mechanistically which classes of catalyst work (better) on surfaces





Light Absorbers

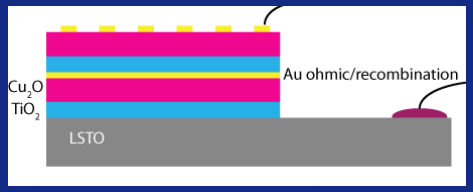
Gaps: Earth-abundant, 1.7 eV light absorbers

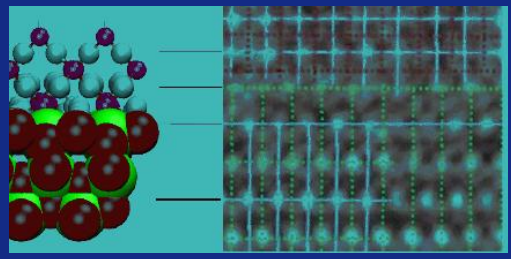


p/n-type photoanode/photocathode cell

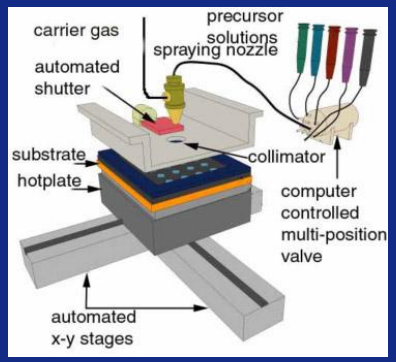
Starting Points:
Cathodes: Si, FeS_2
Anodes: MO_x

Approach: Develop systems with earth-abundant elements

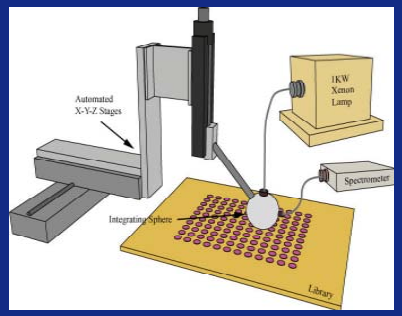




Directed: p-Cu_2O, p-type minerals, N-doped WO_3



spray pyrolysis

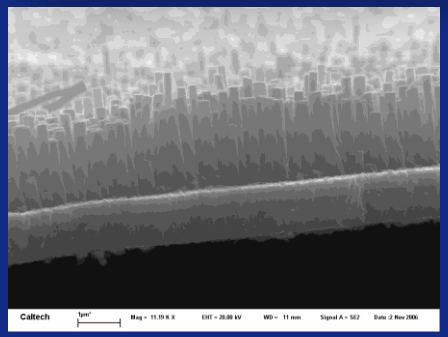


absorbance

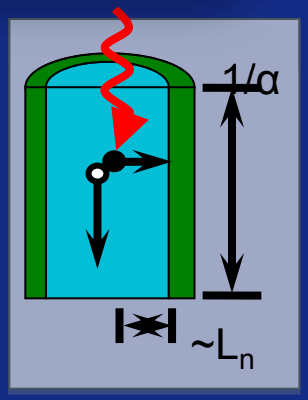
HTE: Metal oxides, oxy-nitrides, sulfides

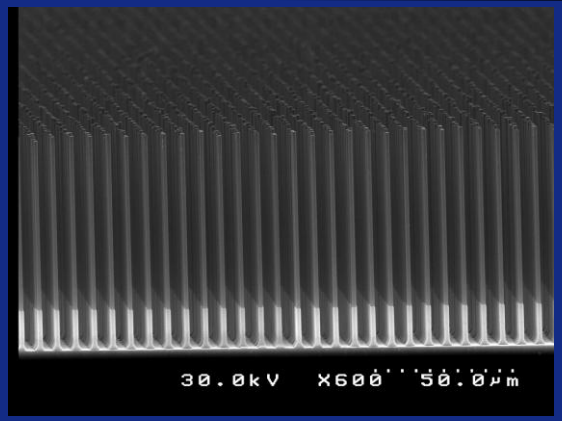
Light Absorbers

Gaps: Accelerate development to obtain required photocurrent and photovoltage

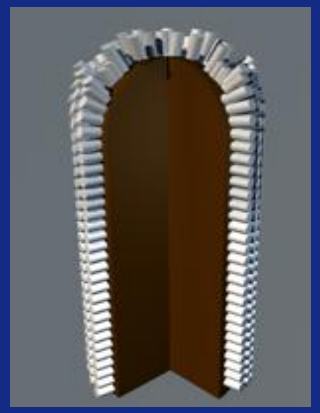


CdSeTe from AAO



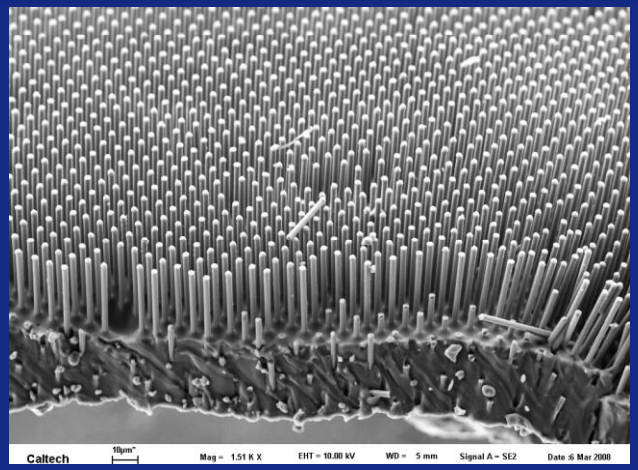


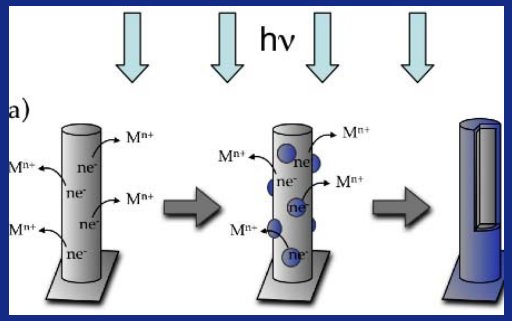
N^+-p radial Si junctions



InGaN/Si core shell nanowire

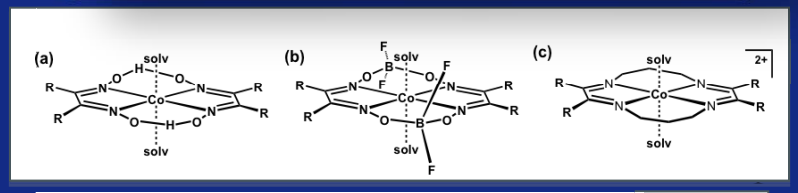
Approach: Use nanostructures to accelerate rate of discovery and to enhance catalytic surface area

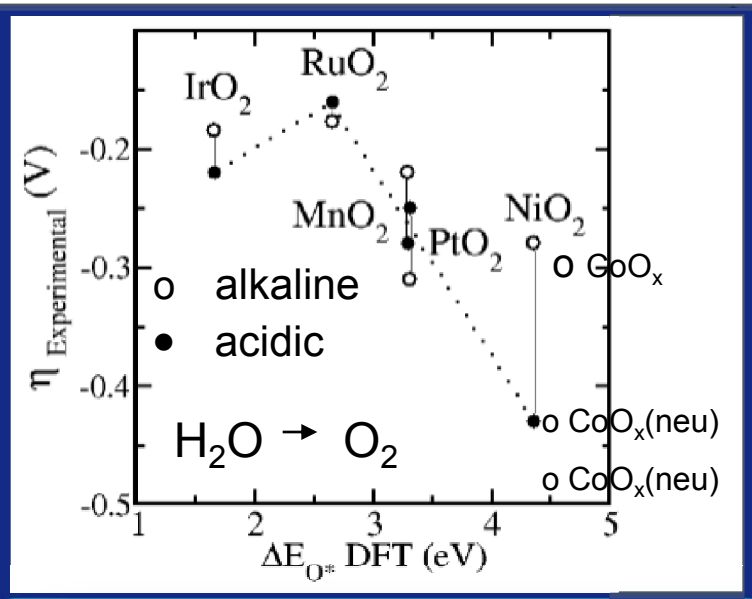




Catalyst Benchmarking

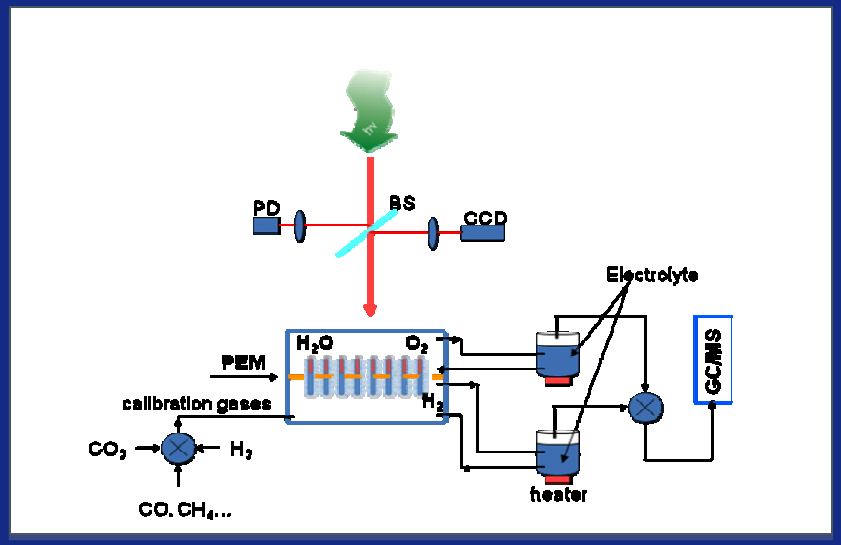
Gaps: Lack of consistent reporting of catalytic activity





Starting Points: Co, Ni complexes vs Co, Ni alloys/oxides

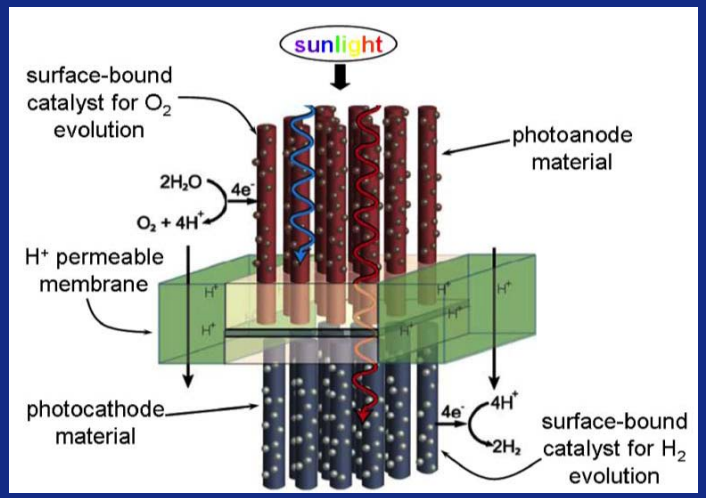
Approach: Develop standard protocols for assessing and comparing activity of homogeneous and heterogeneous catalysts and photocatalysts



Output: comparative activity reporting and database on catalytic and photocatalytic activity

Molecular-Nanoscale Interface

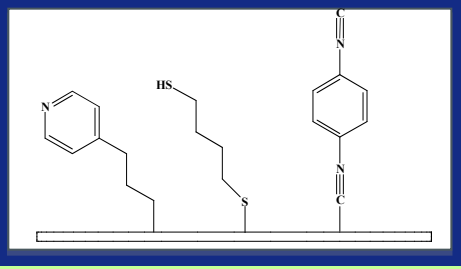
Gaps: How to combine components into working system; functionality of components individually vs collectively



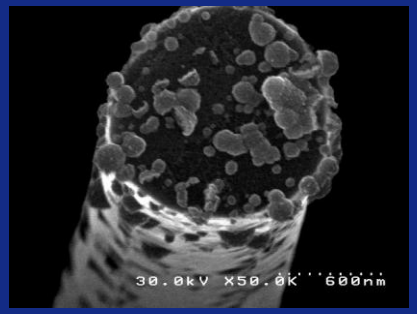
Starting Points:
Si-H; M(OH) surfaces
M^o or M_{coll}; ligand+A

Approach: Develop library of linkers; understand what controls functionality of integrated components

Methods of linking pieces together with minimal charge carrier losses



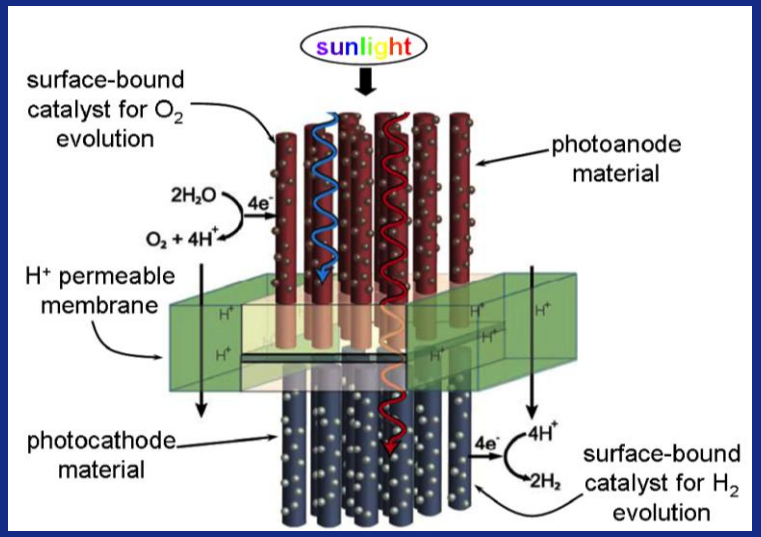
Preserve (or exploit new) functionality of assembly vs individual components



Pt/Si vs Pt/CH_3-Si

Molecular-Nanoscale Interface

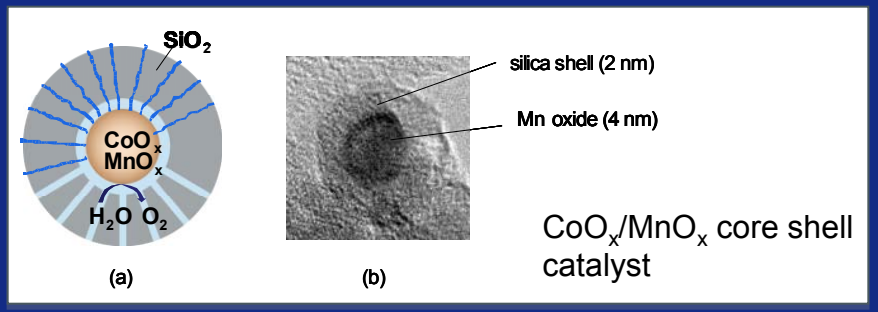
Gaps: How to combine components into working system; functionality of components individually vs collectively



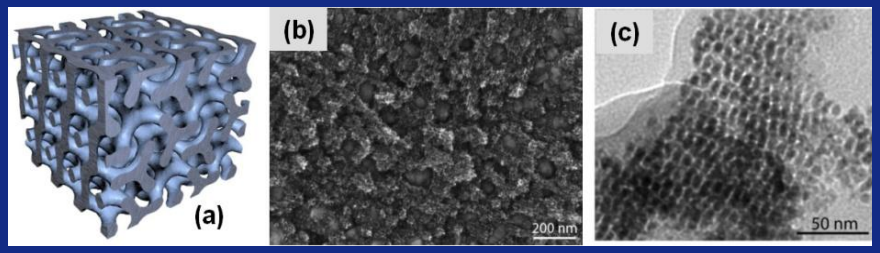
Starting Points:
MnO_x; CoO_x
Ni-Mo

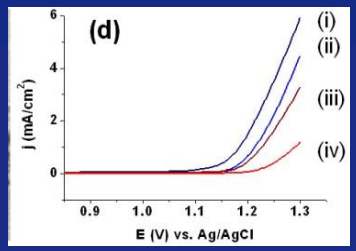
Approach: Control functionality of integrated components

Exploit 3-D to achieve desired activity and/or functionality



CoO_x/MnO_x core shell catalyst



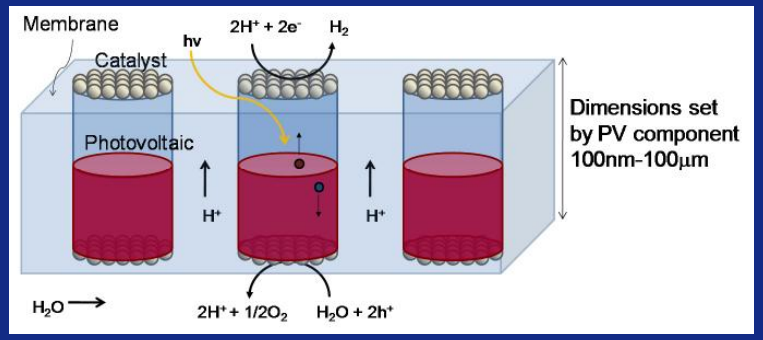


Synthesis and catalytic activity of Ru double gyroid vs planar Ru for O_2 evolution

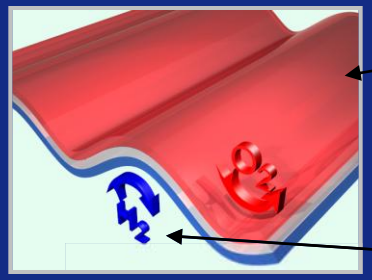
Membrane and Mesoscale Assembly

Gaps: Controlling mesoscale properties

Require directed assembly



Requires multi-functionality



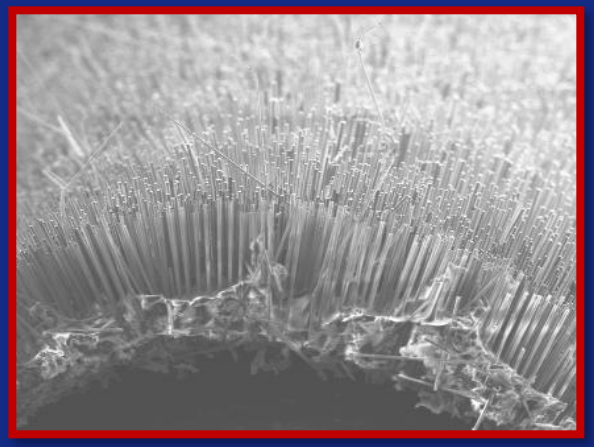
Multi-functional components

mechanical properties and fluidics

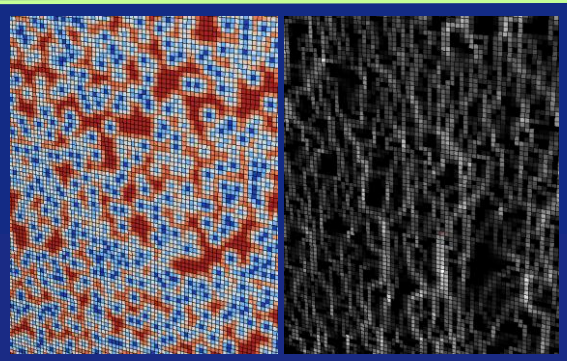
Starting Points:
Si, CdSe rods;
Nafion & OH^- permeable PEDOT composites

Approach: Develop directed, integrated components with multi-functionality

Directed assembly



Si/PDMS Microwire composites

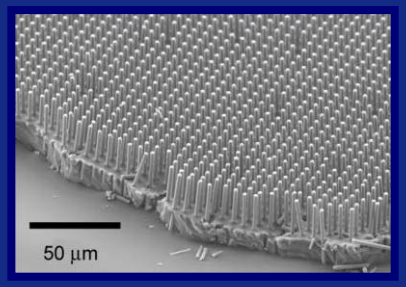


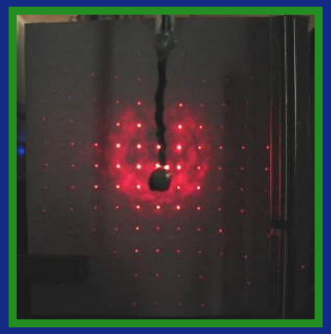
H^+/e^- conductive block co-polymers

Membrane and Mesoscale Assembly

Gaps: Emergent Optical and Transport Phenomena on Mesoscale

Si/polymer composites



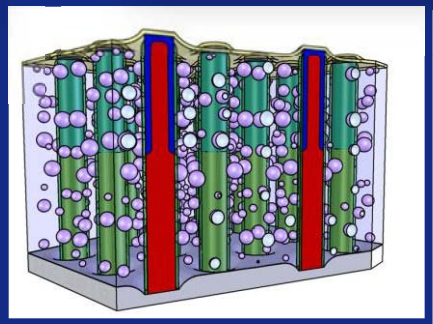


Optical diffraction from microrod arrays

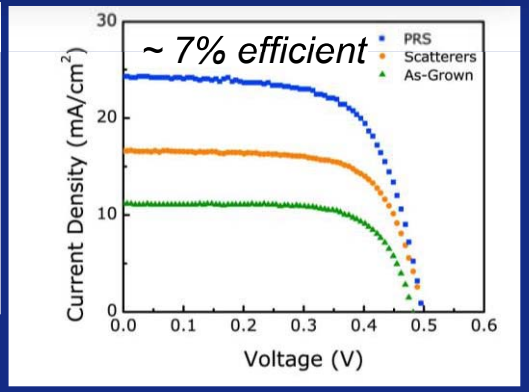
Gas Bubbles Diffract Light

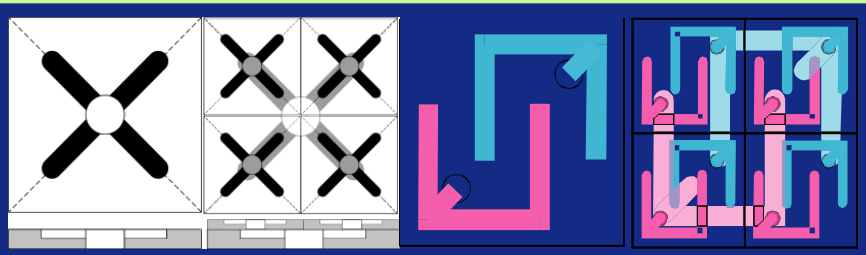
Starting Points:
Pt/$SrTiO_3$ rods
"photo-MEA"

Approach: Exploit Emergent Phenomena



Optical scatters to achieve light management



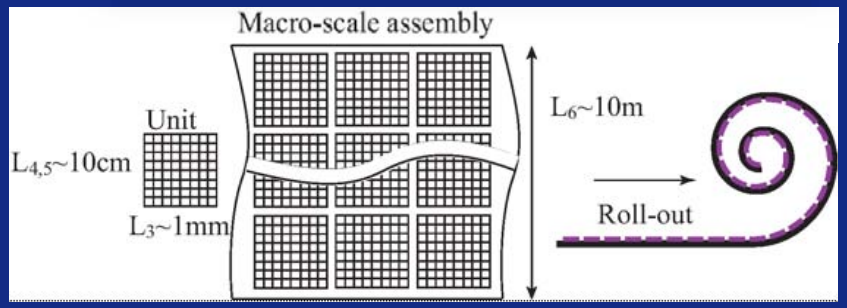


Fluid flow channels in building block

Supply liquid water or water vapor?

Hardware Prototyping

Gaps: Form Factor of Prototypes



Deployment of a flexible product using self-similar asssembly for a 16-cell unit.

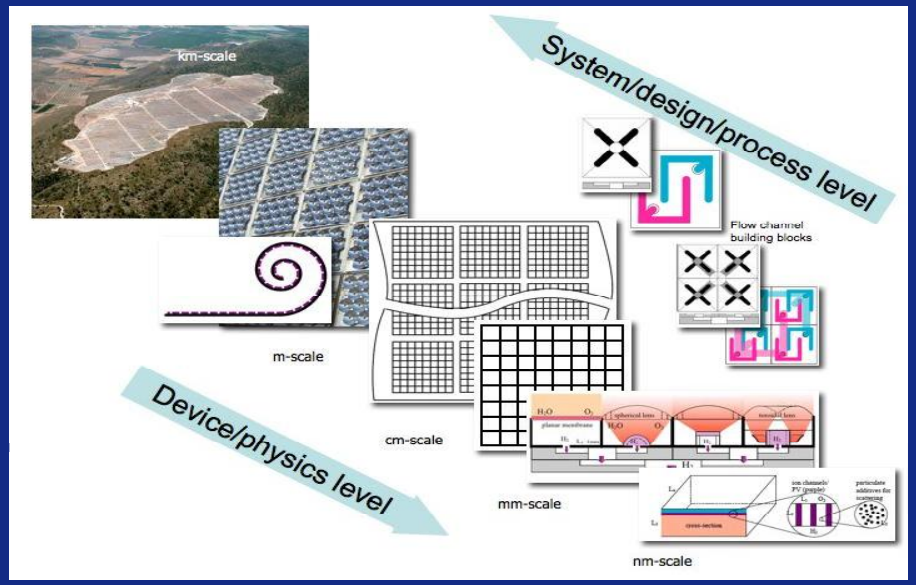
Starting Points:

$SrTiO_3$/Pt

Pt/GaAs-Si p-n dual assembly

Nafion as membrane

Approach: Build, and evolve, 4-5 different designs"



Will build full system simulator model of prototypes; from nanoscale to macroscale (Spice; Aspen; model of the cell)

Cross-Cutting Capabilities

Theory: *Catalysts, photocatalysts, membranes, mesoscale, fluidics*

Instrumentation: *end stations, high-throughput support, component characterization, system characterization*

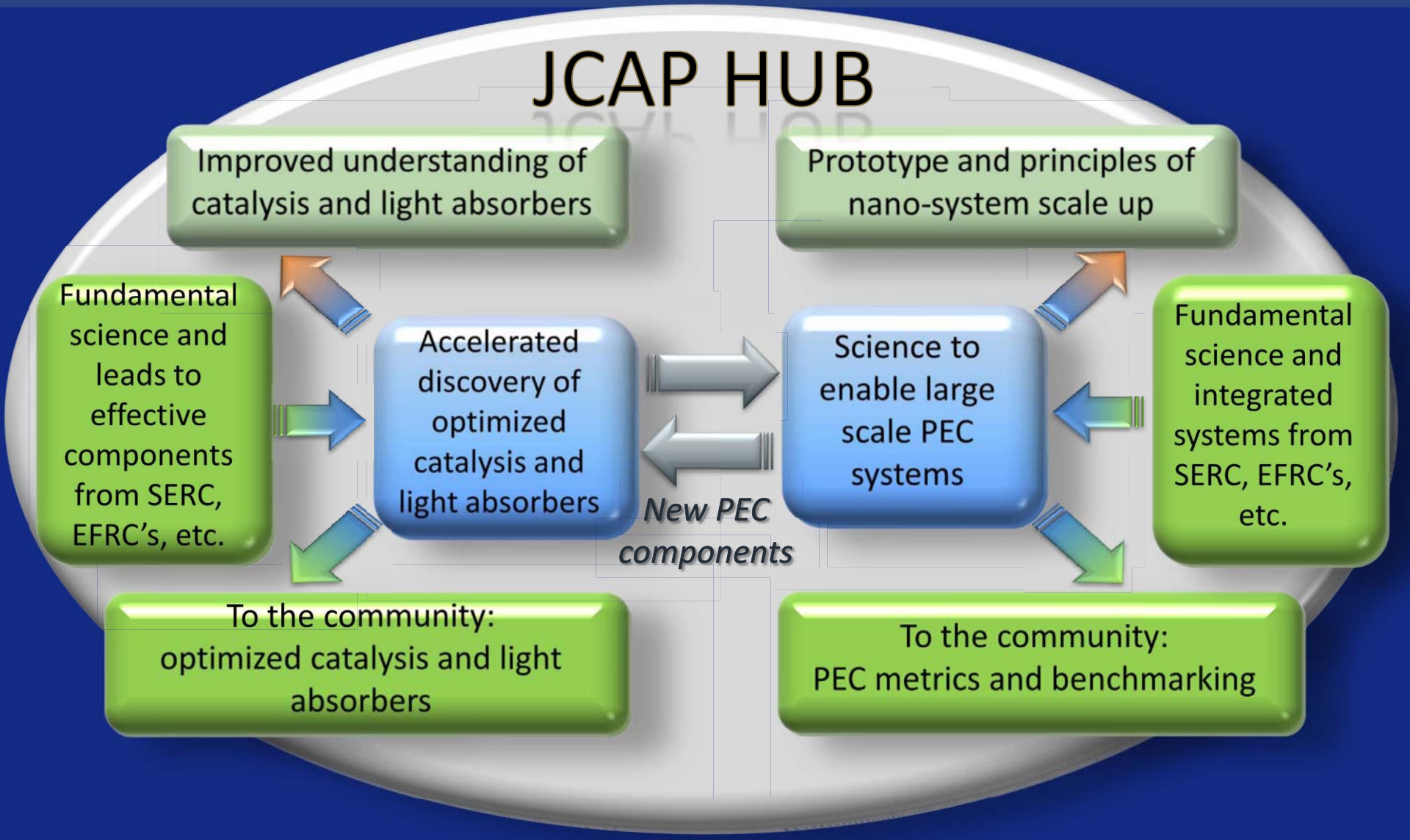
High-Throughput Resource Center: *Catalysts, light absorbers, membranes*

Benchmarking: *components level, system level*

Databases: *HTE data, benchmarking data*

Scalability and Sustainability: *materials, methods, processes*

JCAP's Role as a Solar Fuels Hub



Flexible, Adaptive Internal Decision Making

- Organization modeled after start-up company
- Project goals and budgets reside with JCAP Line Management
  - Responsible for implementation and success of program
  - Commission work by staff, grad students, post-docs to meet goals and tasks sanctioned by JCAP Executive Management Team/JCAP Director
- Weekly JCAP Management team meetings
- Internal progress evaluation monthly
- Internal progress roll-ups quarterly to JCAP Executive Management Team
- Presentation to SAB semi-annually
- In consultation with the JCAP Executive Management Team, the JCAP Director will dynamically evaluate progress, redefine tasks, and re-assign budgets

So. Cal. JCAP Scientific Leadership

- N. Lewis (PI; Caltech; Interfaces, electrochemistry, overall oversight)
- H. Gray (Caltech; inorganic chemistry, reaction mechanisms)
- B. Brunschwig (Caltech; multi-electron transfers)
- H. Atwater (Caltech; earth-abundant light absorbers, devices)
- J. Peters (Caltech; homogeneous catalyst development)
- M. Hoffmann (Caltech; full system design and prototyping)
- J. Hemminger (UC Irvine; directed catalyst development)
- E. McFarland (UCSB; ultra-high throughput instrumentation and heterogeneous catalyst discovery)
- C. Kubiak (UCSD; homogeneous catalyst discovery)

No. Cal. JCAP Scientific Leadership

- P. Yang (LBL/UCB lead: science-based scale up; nanostructures for light absorption and collection)
- H. Frei (LBL: inorganic reaction chemistry)
- P. Alivisatos (LBL/UCB, science-based scale-up from nano to macro systems)
- M. Crommie (LBL: instrumentation)
- R. Ramesh (LBL: APS beam line facilities)
- Alex Bell (UCB: heterogeneous catalysis)
- J. Newman (UCB: electrochemical systems engineering)
- C. Chang (UCB: Inorganic reaction mechanisms)
- D. Tilley (UCB: Heterogeneous inorganic catalysts)
- E. Chandler (LBL: Program development/oversight)
- R. Segalman (UCB/LBL: membranes)
- P. Marcus (UCB/LBL; fluid mechanics)
- D. Dornfeld (UCB: scalable manufacturing)
- T. Martinez (Stanford, SLAC: theory)
- T. Jaramillo (Stanford, SLAC; heterogeneous catalysis and photocatalysis)
- J. Norskov (Stanford/SLAC; theory)
- A. Nilsson (Stanford/SLAC; in situ X-ray spectroscopy)

Advantages of JCAP as a Hub

- Streamlined access to world's brightest soft X-ray source (ALS) and hard x-ray source (SSRL/SLAC)
  - unique beam line instrumental capabilities constructed and operated by JCAP personnel
- ALS access through an "approved program"

  10.3.2 *μ-XANES and EXAFS from 2-10 keV*; **3 weeks/year**

  7.0.1 *Soft X-ray spectroscopy, L-edges of transition metals and K-edges of low Z atoms*; **3 weeks/year**

  6.0.1, 6.0.2 *Ultrafast X-ray spectroscopy*; **2 weeks/year**
- SLAC (SSRL, LCLS) access: JCAP "single proposal"

  9-3/7-3: *Hard X-ray spectroscopy, K-edges and EXAFS of transition metals*; **4 weeks/year**

  6-2 *Advanced in-situ X-ray spectroscopy*; **4 weeks/year**

  4-3 *Intermediate energy (Ru and Pd L-edges), Intermediate Energy (Cl, S, Ti, Ca etc) XANES and EXAFS*; **3 weeks/year**

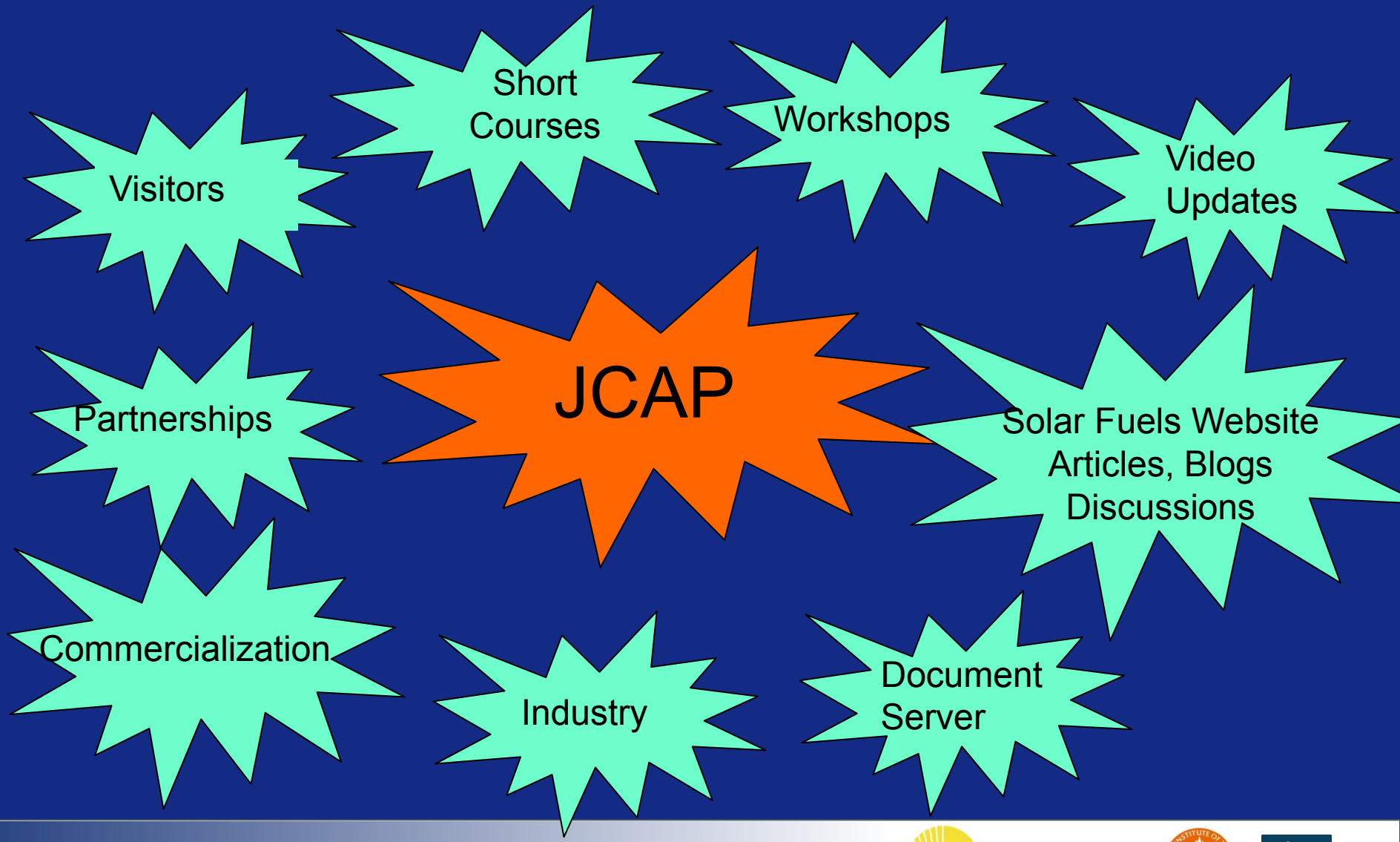
  13-2 *XPS for UHV surface science, Hard and Soft x-ray Ambient pressure XPS*; **5 weeks/year**

  11-2 *EXAFS and XANES of K and L edges in grazing incidence*; **2 weeks/year**

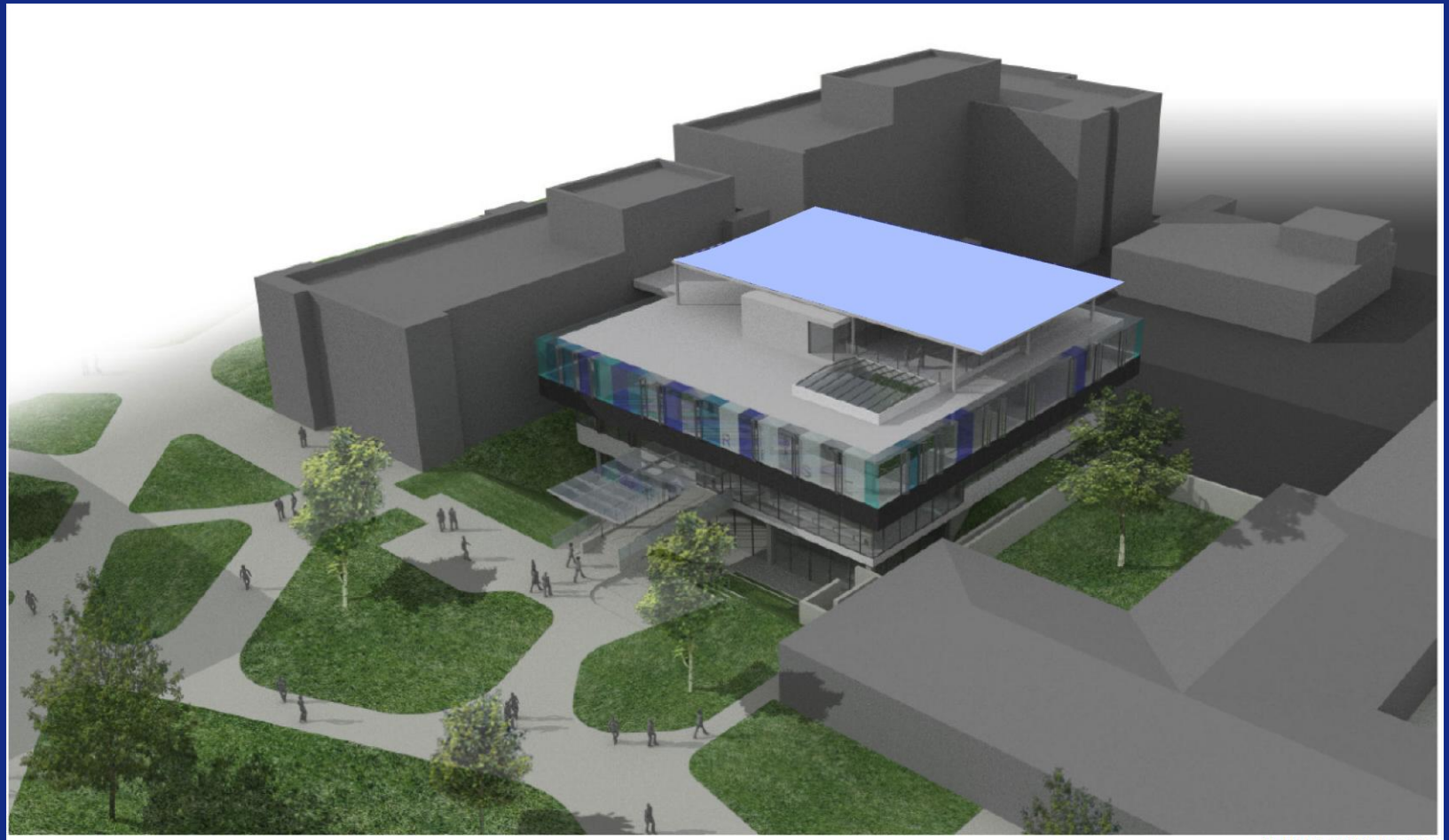
  Also, ALS 8.0.1 or 10.0.1, and SSRL: 13.1, 13.2 13.3 for *XPS*

  SSRL 1.4, ALS 7.3.3 for *small angle X-ray scattering*
- DOE's high performance computation facility: NERSC
- Nanoscience synthesis and characterization capabilities: Molecular Foundry
- National Center for Electron Microscopy: LBL

JCAP Scientific Outreach/Partnerships



JCAP Facilities (South)



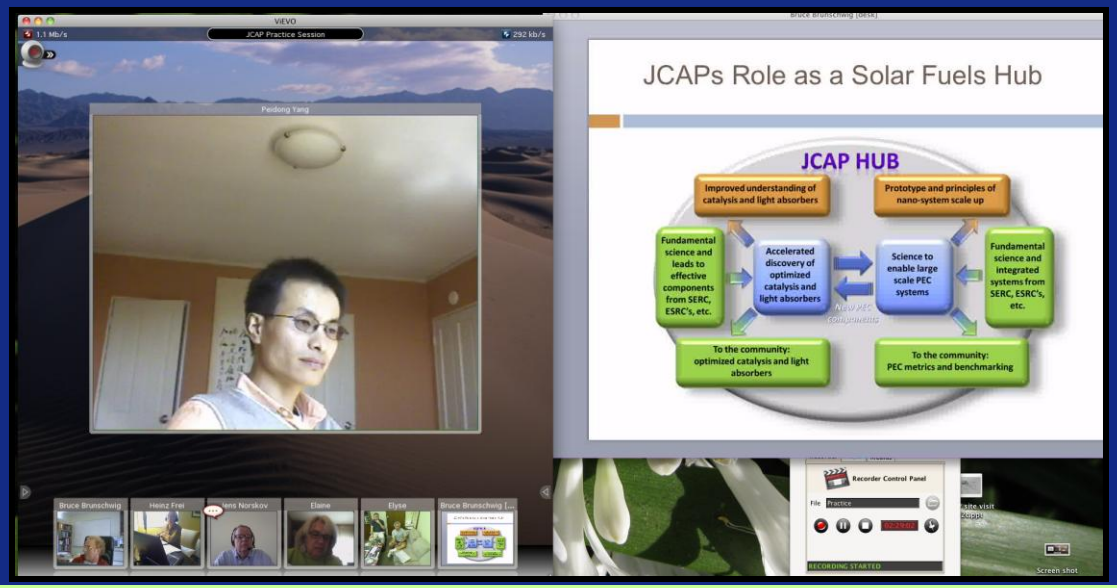
AERIAL RENDERING

JCAP (North) on LBL campus

New $54.4 M facility: $14.4M gift, $10M Cal Public Utilities Commission grant, $30M State Lease Revenue Bonds

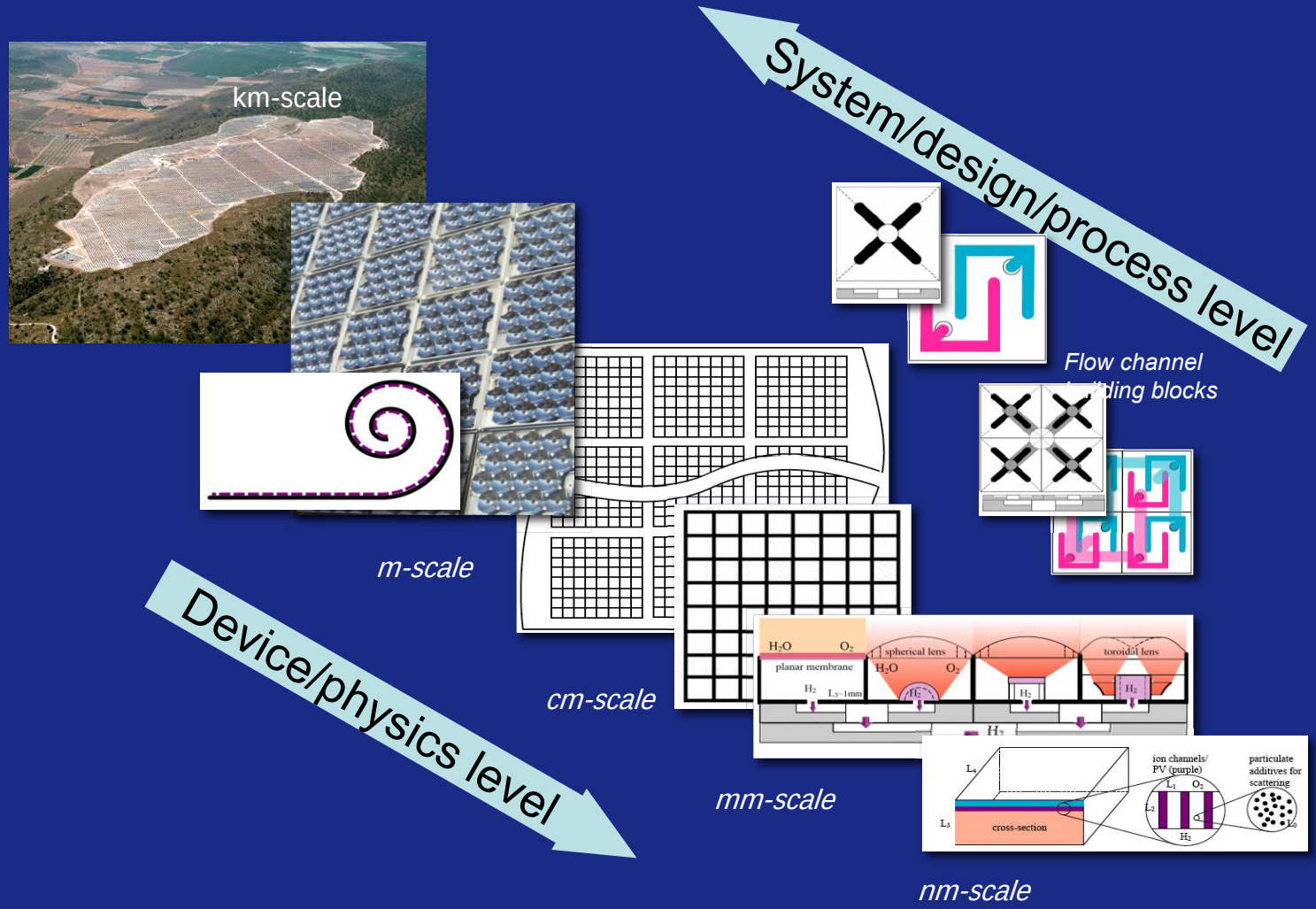
JCAP Cyber-connectivity

EVO (DOE) video/audio links in all seminar rooms, office, alcoves, and labs



Lifesize telepresence in selected meeting rooms:
Secretary Chu's "virtual lunchroom"

Commercializing JCAPs Products



Impacts of JCAP

Development of a commercially viable artificial photosynthesis technology

JCAP will performs functions that only a Hub can perform:

- Ultra-high throughput synthesis facilities and databases
- Unique instrumentation and capabilities
- Streamlined access to light sources and nanoscience facilities
- Catalyst and photosystem benchmarking
- Scale-up from components to full systems
- System integration
- Device design
- Hardware prototyping

Deliver an artificial photosynthesis research center with a critical mass of researchers: a true "Bell-lablet"

Accelerate the rate of discovery in semiconductors and OER and HER catalysts

Provide an integrative center for translational research

Serve as a unique focal point for the solar fuels R&D community, bringing together EFRC's, SISGR's, individual PI's both as inputs and outputs

An agile dynamic research center of world-recognized scientific leaders

Key Attributes of JCAP

- Builds upon successful solar fuels research programs
  - DOE Helios SERC program at LBL
  - NSF CCI led by Caltech
  - LMI EFRC with LBL/Caltech
- Caltech and UC have long track records for managing projects at scale (JPL, LIGO, SIRTF, Owens Valley, Keck, TMT, LBL)
- World famous academic and research institutions
  - Student inspiration, training and support
  - Internationally renowned scientists provide research directions
- JCAP PI's are some of the most preeminent communicators advocating for increased clean energy R&D
- Diverse, distinguished advisory boards

JCAP Science Advisory Board

- **Hector Abruna**
  Emile M. Chamot Professor of Chemistry Cornell University
  Electrochemistry, in-Situ synchrotron methods for electrode characterization, photoelectrochemisry ; Director EFRC
- **Michael L. Klein**
  Laura H. Carnell Professor of Science Temple University
  Theory, National Academy of Sciences, Royal Society
- **Karl Wieghart**
  Director, Max Plank Institute for Bioinorganic Chemistry
  Inorganic chemistry of transition metal catalysts
- **Charles Lieber**
  Mark Hyman Jr. Professor of Chemistry Harvard University
  Nanoscience and nanotechnology, Science-based scale up
  National Academy of Sciences
- **Gerhard Ertl**
  Former director, Fritz-Haber Institut der Max-Planck Gesellschaft
  Surface chemistry and electrochemistry, Nobel Laureate

JCAP Strategic Advisory Board

- **Bill Banholzer**

  VP of R&D, Dow; Scale-up, Electrochemistry, Membranes, Catalysts
- **Ellen Williams**

  Chief Scientist, BP; Fuels, Catalysts, Materials
- **Om Nalamasu**

  VP and CTO, Applied Materials; Manufacturing Scale-up
- **Amol Deshpande**

  Kleiner, Perkins Venture Capital; Commercial Feasibility and Value Proposition
- **Rob Socolow**

  Princeton Carbon Mitigation Initiative; Portfolio of Low-carbon technologies for mitigation of climate change
- **Maxine Savitz**

  Pres. Council on Science and Technology, fmr DOE, V.P. NAE; Program directions
- **Dave Whelan**

  VP, Strategic Innovation, Boeing Phantom Works
  Innovation, Fuels, systems integration

Technology Transfer from JCAP

- Master JCAP IP agreement
  - Letter of intent in place
  - Caltech, as lead, controls all licensing of JCAP IP
  - Royalties flow pro rata to inventing institutions and to inventors
- In the U.S., UC is #1 in patent filings and issued patents; Caltech is #2
- Strategic Advisory Board to provide guidance on IP strategy and IP portfolio
- Early commercialization opportunities:
  - new PV materials
  - catalysts for better electrolyzers to firm up solar, wind electricity and for fuel cells;
  - HTE systems for batteries and other catalysts

Clean Energy Technology in California

- Extensive capital available (60% of all clean-tech investment in U.S. in CA; 500% greater than next highest state)
- Talent
- Intellectual environment
- Public support

Favorable Regulatory Framework in California for Clean-Technology

- Assembly Bill 32: Global Warming Solutions Act:
  Cut emissions by 20% by 2020 relative to 1990 levels
- Gov's Executive Order: Cut Emissions by 2050 by 80% from 1990
- Pavley: Tailpipe emissions regulations: 22% by 2012; 30% by 2016; federal standard followed Pavley/CA bill
- SB1: Million Solar Roofs, $50 MM RD&D Program
- Low-Carbon Fuel Standard; 10% reduction by 2020
- California Air Resources Board (Mary Nichols, chair)
  - strongest clean air regulatory framework in the U.S.

will drive and facilitate early and widespread adoption of alternative fuel technology in home state market, largest in the U.S.

California State Support for JCAP

- Sales tax exemption on JCAP equipment (9% of $12 MM = $1 MM)
- Worker training as support for JCAP graduate students and post-docs (est $2-3 MM)
- AB112 Funding for general JCAP support (est. $3 MM)

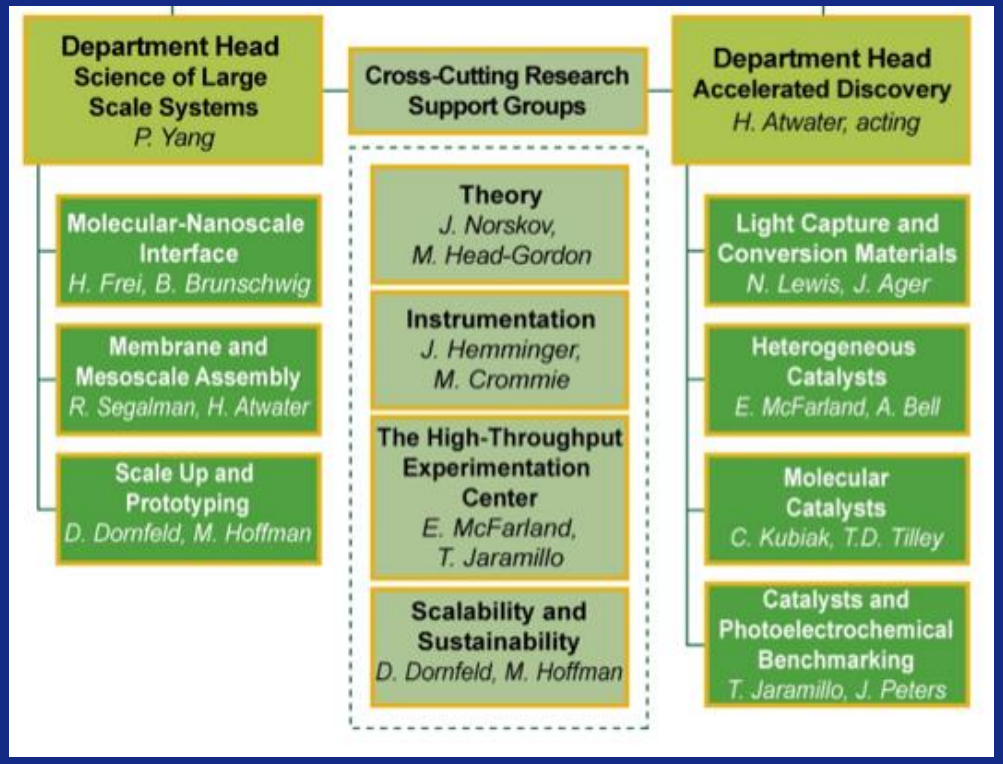
  CA can not definitively commit funds to a Hub that does not yet exist

- JCAP Hub would be visible at many levels:
  - Local: Pasadena, Berkeley
  - County: San Gabriel Valley, Alameda County
  - Region: Los Angeles County, S.F. Bay Area
  - CA: Sacramento, CEC, CARB
  - Federal Level: Reps Schiff (House Appropriations), Drier (fmr House Rules Chairman); Pelosi (House Speaker); Feinstein (Senate Energy and Water Appropriations), Boxer (Senate Global Warming Committee)
  - NGOs and Business groups: Environment Now, E2, Apollo Alliance

Strategy and Organization

Strategy for operating the Hub and organization structure:

- Researchers under one integrated roof, in two fully cyber-connected buildings, to focus solely on artificial photosynthesis: a true "Bell-lablet"
- A start-up company organizational structure enables strong, agile, decision making
- Two Scientific Divisions and 4 Cross-cutting units
- Support teams devoted to
  - ✓ Operations, Safety,
  - ✓ IP, Tech Transfer
  - ✓ Program Management
- Program features
  - ✓ Communications
  - ✓ Scientific partnerships
  - ✓ Educational outreach



Staff and Oversight

Exceptional quality and flexibility of staff

- World class scientists intimately involved in all key JCAP strategic and tactical decisions
- Mix of internal staff, graduate students and post-docs, to enable JCAP to rapidly reconfigure to pursue new opportunities
- Senior leadership team consists of personnel with demonstrated scientific leadership, program and project management, educational expertise, and technology transfer to industry

Careful oversight and evaluation

- Constant evaluation and/or benchmarking of component performance, identifying and using the best available systems regardless of where they are developed
- Monthly internal progress updates for each Director-level task
- Quarterly internal and external status reports to Executive Committee and Director
- Semi-annual status reports, with internal action items, reported to outstanding SAB and StAB

Research Infrastructure

Modern research infrastructure built specifically for this Project

- One new and one newly-renovated building devoted to housing JCAP operations

  On the campus of a leading DOE BES laboratory: LBL
  On the campus of a preeminent research and educational institution: Caltech

- Both buildings centrally located where they can take advantage of the educational and complementary research environments of Caltech and LBL including

  - ✓ nanoscience facilities
  - ✓ specialized instrumentation
  - ✓ chemical synthesis laboratories
  - ✓ other solar energy projects and programs

$10 MM in first-year renovation/rehab funds supplemented by extensive state, private, and other matching funds to allow for rehabilitation of a combined >50,000 gsf of space for JCAP

Appropriateness of Budget

Appropriateness of proposed budget

Two sites: JCAP South (Caltech, UCSB, UCSD, UC Irvine) and JCAP North (LBL, SLAC, Stanford)

Complementary, but cross-matrixed tasks involving members of both sites

Mix of professional staff, faculty joint appointments, and graduate student/post-doc personnel on all tasks; different ratios for each task and as a function of time, as warranted

Personnel ramp-up to ~3/4 full strength by end of year 3, ~ 90% by end of year 4

Balanced, but dynamically adjustable, funding for each of the JCAP tasks

Responsibility for executing each task resides with the JCAP line management, who will justify their budget requests semi-annually. All requests must be prioritized and resolved within the constraint of the total available JCAP funding

Overcoming Challenges

Ability of investigators to overcome scientific challenges

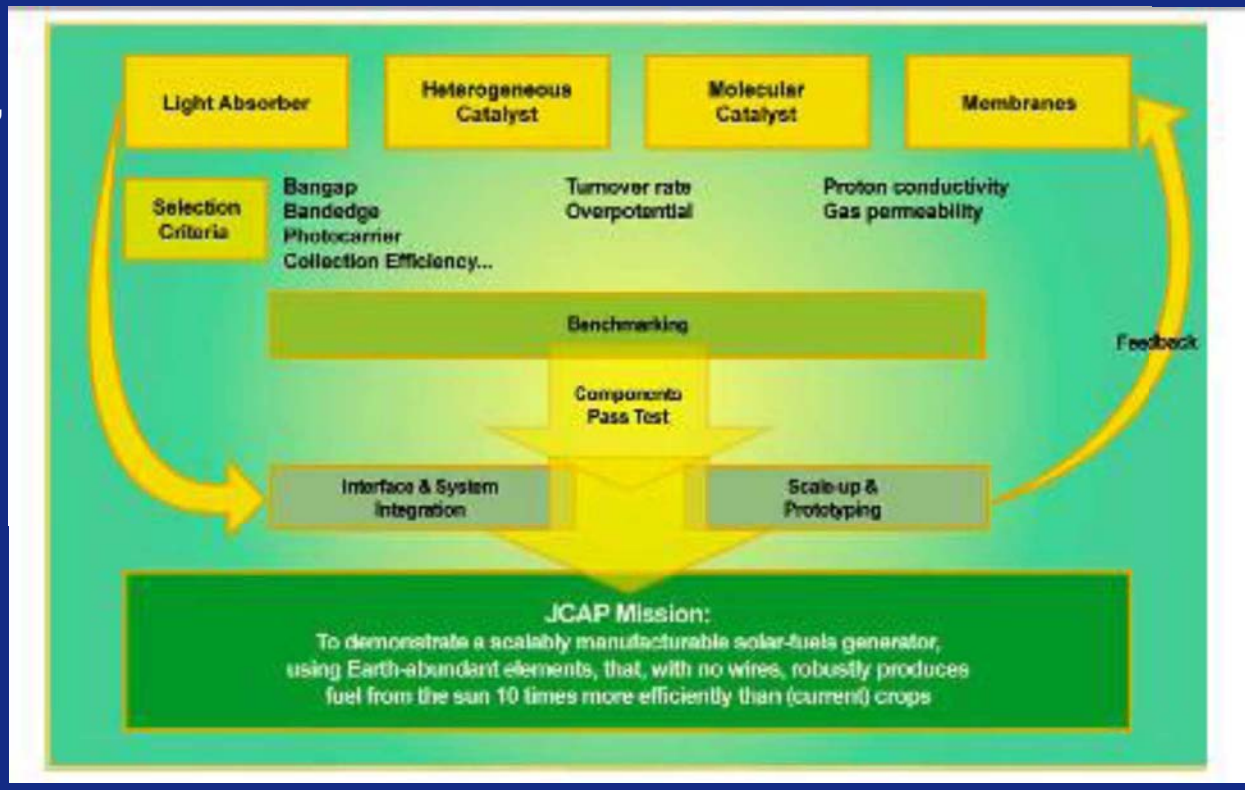
- Have recruited committed, world-class scientific leaders as JCAP Director, Department Heads, and PI's on all tasks
- Clear goals and metrics for success
- Skills of PI's well-matched to goals of JCAP
- Parallel approaches to success; risk mitigation and optionality at all stages

Integration of Basic and Applied R&D

Integration of basic and applied research and development in the Hub

Fully integrated from inception

- Pursue in parallel all needed levels of complexity, from discovery of components at the nanoscale to assembly of prototypes at the macroscale
- All efforts iteratively linked at the systems level
- Quantitative measure of progress at all stages
- Benchmarking and evaluation of competitive landscape to insure that most promising systems are being pursued



Engagement of Extramural Entities & DOE User Facilities

Suitability of plans to engage entities extramural to the Hub, including the utilization of DOE user facilities

Partnerships; developing with over a dozen EFRC's already; more to come

Attractive for partnerships for external PI's and SISGR's developing components

- JCAP will characterize, benchmark, and optimize components for anybody as a service to the community
- JCAP will integrate highest performers into the JCAP hardware prototypes

Streamlined access to the world's brightest soft X-ray light source (ALS), the world's brightest hard X-ray light source (SSRL) and the world's fastest time-resolved X-ray source (SLAC) to provide facile access for JCAP R&D and, in partnership with SSRL, to develop unique instrumental capabilities (atmospheric pressure XPS) that will benefit the scientific community at large

Presence at 2 National Labs and 6 Research universities

Extensive outreach programs including short courses, hands-on workshops, academic and industrial visitors to the Hub, "state of the science and technology" authoritative, updated reviews available both in journals and on-line for wide dissemination

Likelihood of Success

Increased likelihood of success of due to pathway that

- Starts with robust components with state-of-the-art performance
- Systems level view from inception of JCAP
- Constructs hardware prototypes and links nanoscale to macroscale performance and operational characteristics at all time and scale lengths
- Embraces compelling advantages of a fully integrated artificial photosynthesis system (water vapor feed, system synergies, etc.) for high scalability and low ultimate cost
- Pursues parallel paths with risk mitigation and optionality at all stages

Related opportunities include

Better catalysts for electrolyzers for firming up wind and solar electricity; better catalysts for fuel cells

New materials for PV systems

New, widely applicable ultra-high throughput materials synthesis and characterization techniques

New membranes for fuel cells and batteries

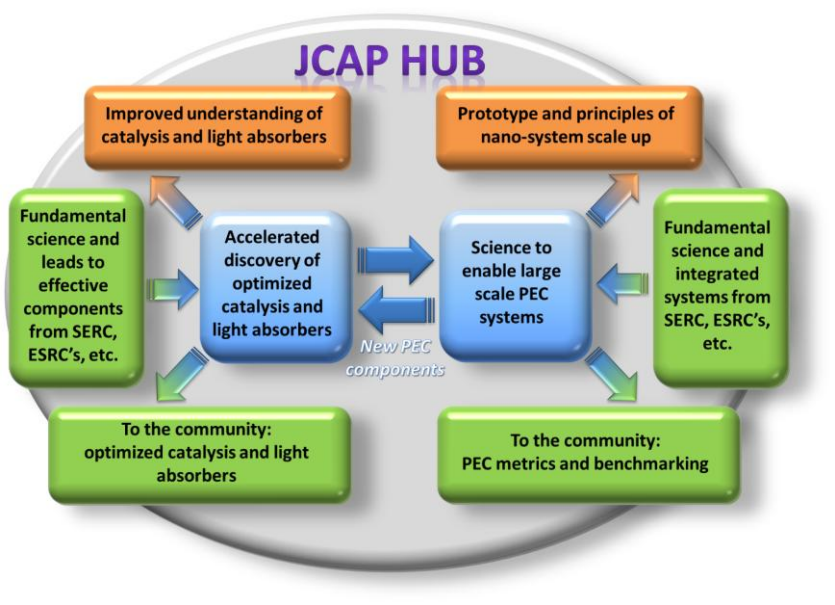
JCAP is bold, incredibly exciting, and an opportunity not to be missed!

Holds unprecedented opportunities for the next generation of science R&D workforce in renewable energy systems

Impact of JCAP

International efforts at single PI and center level

BES core program: single PI & SISGR projects



NSF artificial PS centers

BES EFRCs, Helios SERC

- JCAP will fulfill a critical accelerating role in the national and international effort of making artificial photosynthesis a technological option for society, by providing the missing pieces of accelerated discovery and the development of large scale systems science.
- By adapting, optimizing and integrating the most promising components available from anywhere into viable solar fuel generators, JCAP will augment the combined BES effort in the fields of solar photochemistry, solar and energy materials.