

Materials and Chemical Research





Materials and Chemical Research

UCI Samueli School of Engineering

Manufacturing Science





Diran Apelian



Julie Schoenung



Lorenzo Valdevit



Tim Rupert



Ramin Bostanabad



D. R. Mumm



Institute for Design and Manufacturing Innovation (IDMI) UCI Samueli School of Engineering





IDMI – Advanced Casting Research Center







Irvine Materials Research Institute (IMRI)

UCI Samueli School of Engineering

Laboratory for Electron & Xray Instrumentation (LEXI)



Magellan 400 SEM GAIA-3 GMH FIB-SEM

Surface Science Facility (SSF)



AXIS Supra by Kratos Analytical

Center for Transmission Electron Microscopy (CTEM)



NION HERMES Grand ARM CryoTEM 2100F

TEMPR Facility for Soft Materials Characterization



A cross-disciplinary institute offering world-class facilities to researchers engaged in the discovery, development and commercialization of all types of materials.



- Direct imaging of single atoms, 3D atomic structure, chemical bonds, and local electronic properties
- *In situ* observation of the phase transition and dynamic behaviors of materials under different conditions and environments with the atomic resolution.
- The unique Nion UltraSTEM HERMES200 is an ideal microscopy for the study of 2D materials.
- The world record energy resolution (4.2 meV) allows one to measure the molecular vibration and phonons in crystal.





Why Additive / Metal Manufacturing

Metal Additive Manufacturing Genome





UCI expertise in:

- Metal processing
- \circ Machine learning
- Big data

CI

Sensors and control





- Architected materials
- Scalable nano-manufacturing
- o Metal AM
- Optimal design for AM

Scalable Nanomanufacturing







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Laser Powder Bed Fusion: Shell-based PH steel metamaterials L. Valdevit, D. Apelian (UCI), M. Begley (UCSB), A. Asadpoure, M. Tootkaboni (UMass Dartmouth)







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Direct Energy Deposition - Processing Science of Functionally graded materials J. Schoenung, L. Valdevit, P. Cao



Image courtesy of Optomec













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Oxide

Cold Spray for Large Area Additive Manufacturing D. Apelian, L. Valdevit, D. R. Mumm







Powder characterization

- Microstructural
- Mechanical



Spraying





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ACRC Consortium



Thixotropic Casting













Materials and Chemical Research





Diran Apelian



Julie Schoenung



Penghui Cao



Tim Rupert



Xiaoqing Pan



D. R. Mumm



ICME – Structural Materials Design

UCI Samueli School of Engineering



Center for Complex and Active Materials UCI MRSEC

Funded by National Science Foundation \$18 million over 6 years Premier Center Program in MSE Total MRSECs Nationwide: 19

Director: Professor Xiaoqing Pan

Participants: 19 Faculty 25 Junior Research Fellows





Xiaoqing Pan, Pl

IRG 1 – Complex Concentrated Materials



IRG 2 – Bioinspired Active Materials



Materials Research Science and Engineering Centers (MRSECs) support interdisciplinary and multidisciplinary materials research and education of the highest quality while addressing fundamental problems in science and engineering that are important to society.

https://ccam.uci.edu/ https://www.mrsec.org/mrsec-program-overview



ICME – Structural Materials Design

UCI Samueli School of Engineering

Conventional Alloy: Dilute Solid Solution



High Entropy Alloys: Disordered Solid Solution



Specifically investigate the role of interfaces





Conventional Alloy

- Equiatomic HEA
- Non-equiatomic HEA









Tim Rupert

Diran Apelian

Julie Schoenung

Penghui Cao



ICME – Structural Materials Design





Design Philosophy for Advanced Materials Refractory MPEAs for Extreme Environments





Design Philosophy for Advanced Materials Refractory MPEAs for Extreme Environments





Biomimetic and Nanostructured Materials



• Synthesis – Structure - Function (mechanical, optical, thermal) analysis of biological materials













• Biomimetic Synthesis of Impact, Abrasion, Thermal Resistant Multifunctional Materials



•











Low temperature, Bio-mediated / inspired syntheses of nanomaterials for energy and environmental applications



Enzyme driven synthesis

Self-cleaning, adaptive membranes



Fast charging 3D batteries



Impact & abrasion resistant coatings



Multifunctional nanofibers: Gas sensing, catalysis











Lorenzo Valdevit



P. Cao



UCI Samueli

School of Engineering

R. Bostanabad



A 0.9

18.0 ℃

enght ratio, lenght ratio, len

Rigid section le

0.01

0.11

0.21

Hinge aspect ratio, $t/\ell = 2t/(L(1-R))$

Architected Materials for Impact Mitigation L. Valdevit

UCI Samueli School of Engineering



non-technical

109

1010

ceramics

108

metamaterials [19]

106

Compressive strength (Pa)

107

ultralight

104

metallic microlattices [28]

10²

10

0.41

0.31

energytrapping

metmaterials [3]

10³



Architected Materials as Mesoscale Materials (Pending) UC-NL Collaborative Research and Training Award







Materials and Chemical Research





Maxim Shcherbakov



Filippo Capolino



UCI Samueli

School of Engineering

Odzal Boyraz



Howard Lee



Daryl Preece



Controlled Light-Matter Interactions



photonics

light sources



Maxim Shcherbakov



Howard Lee



Daryl Preece



Filippo Capolino



Odzal Boyraz



Dmitry Fishman

And others!

Nanophotonic devices: Shcherbakov lab Dynamic designer nanomaterials wavelength CMOS-compatible / integrated Platform Large-scale Externally controlled $\mathbf{P}(\mathbf{r},t) = \varepsilon_0 \int \chi(\mathbf{r},t,t') \mathbf{E}(\mathbf{r},t') dt'$ 🗲 🕒 🕒 Concepts S S S 666 Deep-subwavelegth nanolithography Time-variant materials Search and optimization algorithms $PD \qquad I(V_g; s_1, s_2, s_3)$ and Polarize Devices a-Si:H $V = \lambda^3 / 100$ absorption modulated probe Polarization synthesizer Perfect Liquid crystal lens Photonic switch Optoelectronic analyzers gratings Use scenarios Ultralight Beam steering/LiDAR AR/VR/ On-chip Extreme

head-up displays

imagers



Photonic Metasurfaces and Metamaterials Lee Nano Optics Lab

UCI Samueli School of Engineering

Extreme light-matter interaction, optical metasurfaces and metamaterials, tunable optical materials, quantum/bio-photonics, and photonic applications at nanometer scale



Active optical metasurfaces



Novel optical materials







Howard Lee

Member of Beckman Laser Institute



Nanomaterials for Quantum Science



UCI Eddleman Quantum Institute

UCI Samueli

School of Engineering



Quantum Materials Eddleman Quantum Institute

UCI Samueli School of Engineering

UCI Eddleman Quantum Institute



Spintronics Jauregui, Krivorotov, Wu **cules** Furche, , Wu

> Quantum Materials Burke, Ho, Pan, Xin, Wu, Yu

Quantum Design

Superconductivity Fisk, White, Chernyshev, Yu, Krivorotov, Wu **2D Quantum Materials** Xia, Chernyshev, White, Jauregui, Sanchez-Yamagishi

Quantum Magnetism Chernyshev, White, Wu, Romhányi, Sanchez-Yamagishi



Concentrated efforts in:

- Quantum materials and rare-earth metals
- Theory of quantum systems, especially for correlated systems and rare earth-containing materials



Quantum Materials Eddleman Quantum Institute

UCI Samueli School of Engineering

Eddleman Quantum Institute Faculty

Faculty from both School of Engineering and School of Physical Sciences





Quantum Materials Research Jauregui, Sanchez-Yamagishi

UCI Samueli School of Engineering



Luis A. Jauregui

Electrical and optical properties of van der Waals quantum materials and devices.

Growth of high-quality topological quantum materials:







Quantum optoelectronic devices

Acoustic control of excitons:



Funded by NSF

Thin topological field effect devices:



Javier Sanchez-Yamagishi

New measurement and fabrication techniques for quantum materials



In-situ nanomanipulation of van der Waals heterostructures





Squeeze-grown 2D topological materials



ultrathin and atomically flat bismuth

In collaboration with: Michael Pettes from LANL

Huolin Xin

Stacy Copp

Zuzanna Siwy

Regina Ragan

UCI Samueli

School of Engineering

Allon Hochbaum

Accelerating Materials Science with Informatics UCI Samueli School of Engineering Xin Group, Copp Group

"Artificially Intelligent" Transmission Electron Microscopy (TEM)

Huolin Xin

Overcoming the limitations of conventional TEM and electron tomography through deep learning

ADF-STEM micrograph of Co₃O₄

Inpainting De-artifacts WBP SART TVM Au nanorod image Au nanorod FFT

R. Lin, et al., Sci Rep. 2021; G. Ding, et al., Sci Rep. 2019

Chemistry-informed machine learning (ML)

DNA-stabilized silver nanoclusters as sequence-encoded materials for quantum plasmonics, sensing, and bioimaging

S. Copp, et al., Chem. Mater. 2020; P. Mastracco, et al., In prep.

Stacy Copp

Deep Learning-Enabled Nanomaterials Devices UCI Samueli Siwy; Ragan and Hochbaum

Deep learning enabled mechanotyping

Harnessing supervised and unsupervised machine learning to identify cell types by mechanical property differences

Combs, et al. Bioarxiv 2021

Fingerprinting vibrational spectra of bacterial metabolites

Rapid Antimicrobial Susceptibility Tests Latent space representations provide mechanistic insights

Thrift*, et al. ACS Nano* 2017 Thrift*, et al. ACS Nano* 2020 Surface enhanced Raman scattering sensors with controlled nanogap chemistry produce rapid, sensitive, and reproducible data for ML analysis.

Regina Ragan

Allon Hochbaum

Bio- and bio-inspired materials

(A)

2 Flow

Materials and Chemical Research

UCI Samueli School of Engineering

Herdeline Ardoña

Seunghyun Sim

Ken Shea

Bioinspired Active Materials UCI MRSEC

Life exists far from equilibrium – why not synthetic materials?

Out of equilibrium materials in biology

Essential Cell Biology, 4th Ed.

1. Reaction networks for

actively assembling conductive materials Energy-dissipating tubulin assembly

Vision: Develop *supramolecular materials* that mimic biological function and interface with biological systems.

models for emergent

properties

2. In situ TEM and spectroscopy and molecular modeling

Center for Complex and Active Materials

UCI MRSEC

MRSEC Interdisciplinary Research Group 2: **Bioinspired Active Materials**

Guan, Ragan, Patterson, Hochbaum, et. al. in review; Ing, et al., ACS Nano 2018

Understanding Dissipative Assembly Ragan, Wickramasinghe, Patterson, Tobias

UCI Samueli School of Engineering

Surface enhanced Raman spectroscopy and photo-induced force microscopy (PiFM)

Characterizing complex, out-of-equilibrium soft matter systems

Multi-scale molecular dynamics modeling of supramolecular assembly

Patterson Si2NA chip TEM holder Si₃N₄ cell Coated Window RE WE pH

Electrochemical nanoreactor

Thirft, Hochbaum, Ragan et al, ACS Nano, 2017, 11, 11317; Rajaei, Wickramasinghe et al, Opt Expr, 2018, 26, 26365; Wong, Tobias et al, Biochemistry, 2019, 58, 3691; Ianiro, Patterson et al, Nature Chem, 2019, 11, 320.

Charge Transport in Biomolecular Materials Sharifzadeh, Wu, Hochbaum, Copp

UCI Samueli School of Engineering

Electronic structure of supramolecula CDFT informs state-coupling in peptide assemblies through all atom **MD-DFT** calculations

hopping charge transport conduction model

0.9 1.0 1.1 Variation of Hopping

1.4

1.6

0.6 0.8 1.0 1.2

Machine learning-enabled study and design

Self-assembling conductive peptide fibers

Metal-enhanced **DNA** nanowires

Materials for the Biological Interface

UCI Samueli School of Engineering

Molecular design of functional soft materials for biointerfacing

Probing Biological Processes

Herdeline Ardoña

Polymer-Assisted Patterning of Optoelectronic Peptides (*with A. Yee*)

Seunghyun Sim

Programmable living functionality within soft materials

Synthetic Antibodies Ken Shea

Synthetic hydrogel copolymers engineered with antibody-like affinity and selectivity for biological

Ken Shea

Materials and Chemical Research

Energy Conversion and Storage

WHAT

HOW

WHY

UCI Samueli School of Engineering

Vojislav Stamenkovic

Plamen Atanassov

Iryna Zenyuk

Jack Brouwer

Shane Ardo

Jenny Yang

Matt Law

Reg Penner

Electrochemical Technologies Readiness Level

TRL: Batteries >> Fuel Cells >> Electrolyzers

CHARGE **Electrochemical Technologies** Fuel Cells | Electrolyzers | Batteries electrons flow through a circuit generating direct electric current Current (AI) Li⁺ Ior urrent (Cu) Graphite H₂ Fuel Cell **Electrolyzer** Li Battery Charging electrons electrons current O₂/Air DC current -Electrolyte 6 64 Θ Discharging current Hydrogen protons H₂O Θ Current collector Cathode Cathode Current H_2 Electrolyte/Membrane Separator Anode collector Anode

Electrochemical Technologies: Common Denominator ELECTROCHEMICAL INTERFACES

Solid-Aqueous

Solid-Organic

Solid-Solid

Challenges

- Performance (reaction rate, capacity)
- Efficiency
- Durability
- Cost

an in the start

Topics

- Structure-function properties
- Modification of electrochemical interfaces
- Guided synthesis of functional materials
- Formation of interfaces and role of impurities

ELECTROCHEMICAL INTERFACES:

H₂

M+

reactants

H₂

Η,

hydratic

M+

RESEARCH TOPICS

- 1. ACTIVITY GAIN FROM SOLID PHASE
- 2. TUNING OF THE DOUBLE LAYER
- 3. STABILITY OF INTERFACES

ELECTROCHEMICAL INTERFACES BY DESIGN

1. Ultra High Vacuum & Surface Science Approach

Single Crystals

Thin Films N

Nanomaterials

Electrochemical Interfaces @ Play

STM: Pt[10 9 9] - CO_{ad}

→Larger terraces lead to higher reaction rate for ORR: improvement factor 100

Design @ Atomic Scale: nature of active sites

FeN₄/Graphene Structure

Durability @ Atomic Scale

NATURE of active sites:

Dynamic stability for OER

alkaline electrolytes

 Resolved the nature of active sites and mechanism for OER through the balanced Fe dissolution and redeposition over TM-oxide

• The strong interaction between Fe and TMO_xH_y is the key to control the average number of Fe active sites present at the interface

• The Fe-M adsorption energy is a reaction descriptor that unifies OER on 3d TM hydr(oxy)oxides, and extends the design rules for active and stable electrochemical interfaces

REFERENCE

a) Isotope exchange between the electrode (⁵⁶Fe) and electrolyte (⁵⁷Fe) by ICP-MS
b) Schematic of the dynamic stable Fe active site during OER in alkaline electrolyte

Nature Energy 5 (2020) 222

Electrochemical Technologies are <u>Complementary</u>

Batteries -- Fuel Cells -- Electrolyzers

Electrification in Transportation: Batteries and Hydrogen Fuel Cells The Electric-Truck Battle to Come: Batteries vs. Hydrogen Fuel Cells

Levels of Autonomous Driving Network

	Level Definition	LO: Manual Operation & Maintenance	L1: Assisted Operation & Maintenance	L2: Partial Autonomous Network	L3: Conditional Autonomous Network	L4: Highly Autonomous Network	L5: Full Autonomous Network
Ę	Execution (Hands)	(P)	() C	ê	ê	ie.	ê
0	Awareness (Eyes)	(F)	(B)	() C	ê	ê	ê
Ð	Decision (Minds)	(P)		(P)	B	ê	ŵ
Ð	Service Experience	(P)		(P	(P)	(P)	ê
¢	System Complexity	Not Applicable	Sub-Task Mode-Specific	Unit Level Mode-Specific	Domain Level Mode-Specific	Service Level Mode-Specific	All Modes

0001

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