Welcome to

Stanford Sierra Conference Center

The following information will help you during your stay at our lakeside retreat and enjoy your visit to the fullest!

The best way to keep in touch with the office and home is to bring a laptop with wireless capability. Our wireless network is available throughout the camp, including lodge rooms, meeting rooms, and common areas in the main lodge, as well as in the cabins.

Cell service is spotty and inconsistent at Fallen Leaf Lake so plan to be without cell reception during your stay.

You can receive phone messages at 530-541-1244. You can receive faxes at 530-541-2212.

Registration, registration payment, and registration concerns can be emailed to aacg@comcast.net. Visit www.crystalgrowth.org to register and/or pay online.

We post phone messages and faxes on the guest message board across from the office. Check out time on departure day is 10:00 a.m.

Our website is www.stanfordsierra.com.

Morgan Marshall
Sales & Marketing Director
(530) 541-1244 ext.125
mdmarshall@stanford.edu
Conference Contacts

Conference Chair:
Peter Vekilov
University of Houston
vekilov@uh.edu

Fundamentals of crystal growth
Organizer: Kristen Fichthorn, Penn State
kaf2@nyu.edu

Local Arrangements:
Luis A. Zepeda-Ruiz, AACG Treasurer
Lawrence Livermore National Laboratory
zepedaruiz1@llnl.gov

Molecular crystals in process: Growth, ripening, phase transformations
Co-organizers:
Bart Kahr, NYU
bk66@nyu.edu
Alex Shtukenberg, NYU
shtukenberg@mail.ru

Program Committee:
Non-classical mechanisms of crystallization and self-assembly
Organizer: Steven Whitelam, LBNL
swhitelam@lbl.gov

Stanford Sierra Camp Contact:
Morgan Marshall
Sales & Marketing Director
(530) 541-1244 ext.125
mdmarshall@stanford.edu

Biological crystallization
Organizer: Jinhui Tao, PNNL
Jinhui.Tao@pnnl.gov

Registration Support:
Shoshana Nash
303-539-6907
aacg@comcast.net

Functional materials
Organizer: Moneesh Upmanyu, NEU
mupmanyu@neu.edu

Moneesh Upmanyu, NEU
mupmanyu@neu.edu

Fundamentals of crystal growth
Organizer: Kristen Fichthorn, Penn State
kaf2@nyu.edu

Molecular crystals in process: Growth, ripening, phase transformations
Co-organizers:
Bart Kahr, NYU
bk66@nyu.edu
Alex Shtukenberg, NYU
shtukenberg@mail.ru

Biological crystallization
Organizer: Jinhui Tao, PNNL
Jinhui.Tao@pnnl.gov

Registration Support:
Shoshana Nash
303-539-6907
aacg@comcast.net
Conference Sponsors & Supporters

AACG

COHERENT®

Heraeus

IPG Photonics

Lawrence Livermore National Laboratory
Main Lodge Facilities

Cell Phone reception at Fallen Leaf Lake is inconsistent. High-Speed Internet available in all rooms and on main lodge decks.
# Program Guide

## Sunday, June 10

<table>
<thead>
<tr>
<th>Location</th>
<th>Time</th>
<th>Event</th>
</tr>
</thead>
<tbody>
<tr>
<td>Old Lodge Deck</td>
<td>3:00 P.M. – 6:00 P.M.</td>
<td>Check-In &amp; Registration</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(Before checking in, please register and pay online: <a href="http://www.crystalgrowth.org">www.crystalgrowth.org</a>)</td>
</tr>
<tr>
<td>Old Lodge Deck</td>
<td>4:30 P.M. – 6:00 P.M.</td>
<td>Welcome Reception</td>
</tr>
<tr>
<td>Dining Room</td>
<td>6:00 P.M. – 7:30 P.M.</td>
<td>Dinner</td>
</tr>
<tr>
<td>Cathedral Room</td>
<td>7:30 P.M. – 9:10 P.M.</td>
<td>Biological Crystallization</td>
</tr>
</tbody>
</table>

## Monday, June 13

<table>
<thead>
<tr>
<th>Location</th>
<th>Time</th>
<th>Event</th>
</tr>
</thead>
<tbody>
<tr>
<td>Dining Room</td>
<td>7:30 A.M. – 9:00 A.M.</td>
<td>Breakfast</td>
</tr>
<tr>
<td>Cathedral Room</td>
<td>9:00 A.M. – 10:30 A.M.</td>
<td>Molecular Crystals</td>
</tr>
<tr>
<td></td>
<td>10:30 A.M. – 11:00 A.M.</td>
<td>BREAK</td>
</tr>
<tr>
<td>Cathedral Room</td>
<td>11:00 A.M. – 12:00 P.M.</td>
<td>Molecular Crystals</td>
</tr>
<tr>
<td>Dining Room</td>
<td>12:00 P.M. – 1:30 P.M.</td>
<td>Lunch</td>
</tr>
<tr>
<td></td>
<td>1:30 P.M. – 4:00 P.M.</td>
<td>Camp Activities</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Unscheduled Time</td>
</tr>
<tr>
<td>Angora Room</td>
<td>4:00 P.M. – 6:00 P.M.</td>
<td>Poster Session (1 of 2)</td>
</tr>
<tr>
<td>Dining Room</td>
<td>6:00 P.M – 7:30 P.M.</td>
<td>Dinner</td>
</tr>
<tr>
<td>Cathedral Room</td>
<td>7:30 P.M. – 9:10 P.M.</td>
<td>Fundamentals of Crystal Growth</td>
</tr>
</tbody>
</table>
**Tuesday, June 14**

<table>
<thead>
<tr>
<th>Location</th>
<th>Time</th>
<th>Activity</th>
</tr>
</thead>
<tbody>
<tr>
<td>Dining Room</td>
<td>7:30 A.M. – 9:00 A.M.</td>
<td>Breakfast</td>
</tr>
<tr>
<td>Cathedral Room</td>
<td>9:00 A.M. – 10:40 A.M.</td>
<td>Functional Materials</td>
</tr>
<tr>
<td></td>
<td>10:40 A.M. – 11:00 A.M.</td>
<td>BREAK</td>
</tr>
<tr>
<td>Cathedral Room</td>
<td>11:00 A.M. – 12:00 P.M.</td>
<td>Functional Materials</td>
</tr>
<tr>
<td>Dining Room</td>
<td>12:00 P.M. – 1:30 P.M.</td>
<td>Lunch</td>
</tr>
<tr>
<td></td>
<td>1:30 P.M. – 4:30 P.M.</td>
<td>Camp Activities</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Unscheduled Time</td>
</tr>
<tr>
<td>Angora Room</td>
<td>4:00 P.M. – 6:00 P.M.</td>
<td>Poster Session (2 of 2)</td>
</tr>
<tr>
<td>Dining Room</td>
<td>6:00 P.M. – 7:30 P.M.</td>
<td>Dinner</td>
</tr>
<tr>
<td>Cathedral Room</td>
<td>7:30 P.M. – 8:50 P.M.</td>
<td>Non-Classical Mechanisms</td>
</tr>
</tbody>
</table>

**Wednesday, June 15**

<table>
<thead>
<tr>
<th>Location</th>
<th>Time</th>
<th>Activity</th>
</tr>
</thead>
<tbody>
<tr>
<td>Dining Room</td>
<td>7:30 A.M. – 9:00 A.M.</td>
<td>Breakfast</td>
</tr>
<tr>
<td>Cathedral Room</td>
<td>9:00 A.M. – 10:30 A.M.</td>
<td>Biological Crystallization</td>
</tr>
<tr>
<td></td>
<td>10:30 A.M. – 11:00 A.M.</td>
<td>BREAK</td>
</tr>
<tr>
<td>Cathedral Room</td>
<td>11:00 A.M. – 12:00 P.M.</td>
<td>Fundamentals of Crystal Growth</td>
</tr>
<tr>
<td>Dining Room</td>
<td>12:00 P.M.</td>
<td>Snack Lunch</td>
</tr>
<tr>
<td></td>
<td>1:30 P.M.</td>
<td>Departure</td>
</tr>
</tbody>
</table>
Sunday, June 10, 2018

19:30 - 21:10 Biological Crystallization
Cathedral Room
Chair: Jinhui Tao

19:30-20:00 CRystallization by Particle Attachment in Biominerals
Pupa Gilbert, UW-Madison, Physics, USA

20:00-20:30 Biological Crystallization of UltraHard Teeth and Translation to Multi-Functional Materials
David Kisailus, Department of Chemical and Environmental Engineering, University of California, Riverside, CA/USA

20:30-20:50 Barrier-Free Nucleation of 2D Phage-Selected Peptide Films on Mos2 Surfaces
Jiajun Chen1, Enbo Zhu2, Juan Liu3, Hendrik Heinz3, Yu Huang2, James De Yoreo4; 1University of Washington, WA/Us, 2University of California, Los Angeles, CA/USA, 3University of Colorado-Boulder, CO/USA, 4Pacific Northwest National Laboratory, WA/USA

20:50-21:10 Role of Amyloid-Like Amelogenn Nanoribbons in Enamel Mineralization
Susrut Akkineni1, Sarah Engelberth2, Jinhui Tao3, Johan Bonde4, Stefan Habelitz2, James De Yoreo5; 1University of Washington, USA, 2University of California, CA/USA, 3 USA, 4Lund University, SE, 5Pacific Northwest National Laboratory, WA/USA

Monday, June 11, 2018

09:00 - 10:30 Molecular Crystals
Cathedral Room
Chair: Alex Shtukenberg

09:00-09:30 Crystallization of Molecular Glasses: A Central Role for Surface Diffusion
Lian Yu, University of Wisconsin-Madison, WI/USA

09:30-10:00 Expanding the Scope of Viedyma Ripening
Louis Cuccia, Concordia University, QC/CA
10:00-10:30 POLYMORPHIC PHASE TRANSFORMATIONS OF ACTIVE PHARMACEUTICAL INGREDIENTS DURING EXTRUSION INTO CRYSTALLINE SOLID DISPERSIONS
Vilmali Lopez-Mejias¹; Torsten Stelzer²; Jose Hernandez Espinell¹; ¹University of Puerto Rico, Rio Piedras Campus, Pr, ²University of Puerto Rico, Medical Sciences Campus, Pr

11:00 - 12:00 Molecular Crystals
Cathedral Room
Chair: David Kisailus

11:00-11:30 EARLY ONSET OF KINETIC ROUGHENING DUE TO FINITE STEP WIDTH IN HEMATIN CRYSTALLIZATION
Peter Vekilov¹; Katy Olafson²; Jeffrey Rimer¹; ¹University of Houston, TX/USA, ²MIT, USA

11:30-12:00 L-CYSTINE CRYSTAL GROWTH INHIBITION BY TAILOR-MADE ADDITIVES
Alexander Shtukenberg¹; Laura Poloni¹; James Lee-Thorp²; Robert Kohn³; Michael Ward¹; ¹New York University, Department of Chemistry, NY/USA, ²New York University, Courant Institute of Mathematical Sciences, USA, ³New York University, Courant Institute of Mathematical Sciences, NY/USA

16:00 - 18:00 Poster Session (1 of 2)
Angora Room
Chair: Peter Vekilov

P1-1 CHARACTERIZATION OF BIOMINERALS IN THE FULLY MINERALIZED RADULAR TEETH OF THE CHITON, CHITON ARTICULATUSA
Ruoheng Zhao¹; Steven Herrera¹; Wangxiang Li¹; Misha Itkis¹; Laura Alvarez-Cerrillo²; Omar Avila-Poveda²; David Kisailus³; ¹Department of Chemical and Environmental Engineering, University of California, Riverside, CA/USA, ²Facultad de Ciencias del Mar, Universidad Autonoma de Sinaloa, Mx, ³University of California, Riverside, CA/USA

P1-2 THE ROLE OF ORGANIC ADDITIVES IN DIRECTING THE CRYSTALLIZATION PATHWAY OF SOL-GEL DERIVED HYDROXYAPATITE
Reum Scott¹; Lara Estroff²; ¹Cornell University, USA, ²Cornell University, NY/USA
P1-3  ANTAGONISTIC COOPERATIVITY BETWEEN ANTIMALARIALS CONTROLLING HEMATIN CRYSTALLIZATION BY ATTENUATION OF STEP PINNING
Peter Vekilov1; Wenchuan Ma2; James Lutsko3; Jeffrey Rimer2; 1, TX/Us, 2University of Houston, TX/USA, 3Université Libre de Bruxelles, Be

P1-4  OLanzapine Crystals Grow by Association of Preformed Solute Dimers
Peter Vekilov1; Monika Warzecha2; Alastair Florence2; 1, TX/USA, 2University of Strathclyde, Gb

P1-5  A New Look on the Formation of Electrical Centers in Silicon Single Crystals
Vitalyi Igorevich Talanin1; Igor Evgenievich Talanin2; Vladyslav Vladimirovich Kondratiev3; 1Zaporozhye Institute of Economics & Information Technologies, Ua, 2Zaporozhye Institute of Economics & Technologies, Ua

P1-6  TiO2 Crystal Nucleation and Competitive Growth Along [001] on Template Stripped Gold
Brandon Gunn1; Joachim Schuder2; Michael Sanchez3; Andrew Ichimura4; Chris Tassone5; 1Department of Chemistry & Biochemistry, San Francisco State University, CA/USA, 2San Francisco State University, USA, USA, 4San Francisco State University, CA/USA, 5Stanford Synchrotron Radiation Lightsource, CA/USA

P1-7  X-Ray Topography Study of Yttrium Aluminum Garnet Single Crystal Fibers
Subhabrata Bera1; Craig Nie2; James Harrington3; Balaji Raghothamachar4; Jianqiu Guo4; Ailihumaer Tuerxun4; Michael Dudley4; 1National Energy Technology Laboratory, USA, 2Corning Inc., NY/USA, 3Rutgers University, NJ/USA, 4Stony Brook University, NY/USA

P1-8  Synchrotron 2D-Diffraction Study of Anatase Film Growth
Brandon Gunn1; Kyle Kulinski2; Andrew Ichimura2; Chris Tassone3; 1Department of Chemistry & Biochemistry, San Francisco State University, CA/USA, 2San Francisco State University, CA/USA, 3Stanford Synchrotron Radiation Lightsource, USA

P1-9  Thermo-Physical Properties of La2Ce2O7 Nanoparticles Synthesized by Co-Precipitation Method
HOZEFa Tinwala1; Dimple Shah2; Ranjan Pati1; Jyoti Menghani1; 1SARDAR Vallabhbhai National Institute of Technology, In, 2Sardar Vallabhbhai National Institute of Technology, In
P1-10  GROWTH AND CHARACTERIZATION OF HIGHLY PROPORTIONAL INTRINSIC SCINTILLATOR CS$_2$HFCL$_6$
Rastgo Hawrami$^1$; Elsa Ariesanti$^1$; Liviu Matei$^1$; Vlad Buliga$^1$; Arnold Burger$^1$; Stephanie Lam$^2$; Shariar Motakef$^2$; $^1$Fisk University, TN/USA, $^2$CapeSym, Inc., MA/USA

P1-11  EX-SITU AFM STUDY OF HETEROEPITAXIAL ANATASE TiO$_2$ GROWTH ON SAPPHIRE
Joachim Schuder$^1$; Brandon Gunn$^2$; Michael Sanchez$^1$; Andrew Ichimura$^3$; $^1$San Francisco State University, USA, $^2$Department of Chemistry & Biochemistry, San Francisco State University, CA/USA, $^3$San Francisco State University, CA/USA

P1-12  HIGH POWER IMPULSE MAGNETRON SPUTTERING OF W THIN FILMS
Alison Engwall; Yinmin Wang; Lawrence Livermore National Laboratory, CA/USA

19:30 - 21:10  Fundamentals of Crystal Growth
Cathedral Room
Chair: Kristen Fichthorn

19:30-20:00  THEORETICAL AND COMPUTATIONAL ADVANCES IN SOLUTE PRECIPITATE NUCLEATION
Baron Peters, UC Santa Barbara, CA/USA

20:00-20:30  PREDICTING THE FORMATION OF INCLUSION-TYPE SILICON PHASES: INSPIRED BY THE ANALOGY BETWEEN SILICON AND WATER
Tianshu Li$^1$; Yuanfei Bi$^1$; Enshi Xu$^1$; Timothy Strobel$^2$; $^1$George Washington University, DC/USA, $^2$Geophysical Laboratory, Carnegie Institution of Washington, DC/USA

20:30-20:50  STRUCTURE AND COLLECTIVE DYNAMICS OF BOEHMITE ORIENTED AGGREGATION
Elias Nakouzi$^1$; Jennifer Soltis$^2$; Benjamin Legg$^2$; Gregory Schenter$^2$; Xin Zhang$^2$; Trent Graham$^2$; Kevin Rosso$^2$; Lawrence Anovitz$^3$; James De Yoreo$^4$; Jaehun Chun$^2$; $^1$Pacific Northwest National Laboratory, $^2$Pacific Northwest National Laboratory, USA, $^3$Oak Ridge National Laboratory, USA, $^4$Pacific Northwest National Laboratory, WA/USA

20:50-21:10  TRYING A DIFFERENT APPROACH TO THE FREEZING OF LIQUID WATER
Charles Knight, National Center for Atmospheric Research, CO/USA
Tuesday, June 12, 2018

09:00 - 10:40 Functional Materials
Cathedral Room
Chair: Moneesh Upmanyu

09:00-09:30 EPITAXIAL GROWTH OF HBN ATOMIC LAYERS ON COPPER VIA HETEROGENEOUS A PYROLYSIS: ATOMIC-SCALE GROWTH MECHANISMS
Badri Narayanan\textsuperscript{1}; Cristian Ciobanu\textsuperscript{2}; Gene Siegel\textsuperscript{3}; Michael Snure\textsuperscript{3}; Stefan Badescu\textsuperscript{3};
\textsuperscript{1}Argonne National Laboratory, IL/USA, \textsuperscript{2}Colorado School of Mines, CO/USA, \textsuperscript{3}Air Force Research Laboratory, OH/USA

09:30-10:00 TBD
Hanchen Huang

10:00-10:20 CONGRUENTLY MELTING PEROVSKITE SOLID SOLUTIONS
Vincent Fratello\textsuperscript{1}; Lynn Boatner\textsuperscript{2}; Hanna Dabkowska\textsuperscript{3}; Antoni Dabkowski\textsuperscript{3}; \textsuperscript{1}Quest Integrated, LLC, USA, \textsuperscript{2}Oak Ridge National Laboratory (retired), TN/USA, \textsuperscript{3}McMaster University, CA

10:20-10:40 TITANIA NANOPARTICLE CRYSTAL GROWTH WITHIN POLYMER-CARBON NANOFIBER MATRICES
Luz Cruz\textsuperscript{1}; David Kisailus\textsuperscript{2}; \textsuperscript{1}University of California Riverside, CA/USA, \textsuperscript{2}University of California, Riverside, USA

11:00 - 12:00 Functional Materials
Cathedral Room
Chair: Luis Zepeda-Ruiz

11:00-11:20 IN SITU SCANNING TUNNELING MICROSCOPY STUDIES OF GROWTH AND STRUCTURE OF HEXAGONAL BORON NITRIDE MONOLAYERS ON PD(111)
Pedro Arias\textsuperscript{1}; Abdulfattah Abdulsalam\textsuperscript{2}; Abbas Ebnonasir\textsuperscript{1}; Cristian Ciobanu\textsuperscript{2}; Suneel Kodambaka\textsuperscript{1}; \textsuperscript{1}University of California Los Angeles, CA/USA, \textsuperscript{2}Colorado School of Mines, CO/USA

11:20-11:40 GROWTH MECHANISM OF FIVEFOLD-TWINNED AG NANOWIRES IN SOLUTION
Kristen Fichthorn; Xin Qi; Penn State University, PA/USA
THE ROLE OF SOLUTION COMPLEXATION IN THE HYBRID ORGANIC-INORGANIC PEROVSKITE CRYSTALLIZATION PATHWAY

Amnon Ortoll-Bloch; Henry Herbol; Blaire Sorenson; Paulette Clancy; Lara Estroff; Cornell University, NY/USA

16:00 - 18:00 Poster Session (2 of 2)
Angora Room
Chair: Peter Vekilov

P2-1 ALTERED SELF-ASSEMBLY OF PROTEIN 2D CRYSTAL AT SOLID-LIQUID INTERFACE
Shuai Zhang\textsuperscript{1}; Robert Alberstein\textsuperscript{2}; F Akif Tezcan\textsuperscript{2}; Jim Deyo\textsuperscript{1}; \textsuperscript{1}Pacific Northwest National Laboratory, USA, \textsuperscript{2}University of California, San Diego, USA

P2-2 EFFECT OF TRANSITION METAL (FE, CO) ION DOPING ON TIO2 NANO PARTICLES.
Kiritkumar Siddhapara; Patij Shah; Dimple Shah; Svnit, In

P2-3 HIERARCHICALLY ASSEMBLED PLANT STRUCTURES AS BIO-INSPIRATION FOR WATER PURIFICATION
Morgan Dundon; David Kisailus; University of California, Riverside, USA

P2-4 TRANSPORT, NUCLEATION, AND PHASE TRANSFORMATION OF IRON-BASED MINERAL IN THE ULTRAHARD TEETH OF CRYPTOCHITON STELLERI
Steven Herrera\textsuperscript{1}; Omar Avila-Poveda\textsuperscript{2}; Julia McCoey\textsuperscript{3}; David Simpson\textsuperscript{3}; Jeremy Shaw\textsuperscript{4}; Michiko Nemoto\textsuperscript{1}; David Kisailus\textsuperscript{1}; \textsuperscript{1}University of California Riverside, CA/USA, \textsuperscript{2}Universidad Autónoma de Sinaloa, Mx, \textsuperscript{3}University of Melbourne, Au, \textsuperscript{4}University of Western Australia, Au, \textsuperscript{5}Okayama University, Jp

P2-5 SOLID STATE DIFFUSION AND CATALYSIS IN METAL NANOPARTICLE-DOPED CARBON FIBER
Thomas Dugger\textsuperscript{1}; Hongjie Tang\textsuperscript{1}; Luz Cruz\textsuperscript{2}; Jessica Devine\textsuperscript{3}; David Kisailus\textsuperscript{4}; \textsuperscript{1}University of Delaware, DE/USA, \textsuperscript{2}University of California Riverside, CA/USA, \textsuperscript{3}California Baptist University, CA/USA, \textsuperscript{4}University of California, Riverside, USA

P2-6 INVESTIGATION ON THE GROWTH AND CHARACTERIZATION OF BISTHIOUREA DOPED DISODIUM HYDROGEN PHOSPHATE SINGLE CRYSTALS
Manickam R; SRINIVASAN G; Government Arts College for Men (Autonomous), In
INVESTIGATION ON THE GROWTH AND CHARACTERIZATION OF BISTHIOUREA DOPED DISODIUM HYDROGEN PHOSPHATE SINGLE CRYSTALS
Manickam R; SRINIVASAN G; Government Arts College for Men (Autonomous), In

TRANSITION METAL (COBALT) DOPED ZNO MICRO/NANORODS SYNTHESIZED BY SOL GEL SPIN COATING METHOD
SRINIVASAN G; Nadhiya D; Trixy Priscilla; Government Arts College for Men (Autonomous), In

INVESTIGATION ON LITHIUM NITRIDE ZNO THIN FILMS GROWN ON SAPPHIRE USING SOL-GEL SPIN COATING PROCESS
SRINIVASAN G; Priya S; Jayabharathi P; Government Arts College for Men (Autonomous), In

ENERGY ABSORPTIVE BIO-MINERALIZED SEED COATINGS: THE FINAL DEFENSE AGAINST FOREST FIRES
Ramya Mohan1; Sarah McElligott2; David Kisailus3; 2University of California, Riverside, USA, 3Department of Chemical and Environmental Engineering, University of California, Riverside, CA/USA

SYNTHESIS OF Ta3N5 HOLLOW NANOSPHERES, NANORODS AND THEIR PHOTOCATALYTIC BEHAVIOR
Taifeng Wang1; David Kisailus2; 1University of California, Riverside, CA/USA, 2Department of Chemical and Environmental Engineering, University of California, Riverside, CA/USA

GROWTH DIFFICULTIES OF EUROPIUM DOPED STRONTIUM IODIDE (SrI2:Eu2+) SCINTILLATOR SINGLE CRYSTAL FOR RADIATION DETECTION APPLICATIONS
Raja Arumugam; Ramasamy P; SSN College of Engineering, In

HIERARCHICAL ASSEMBLY OF LIGHT WEIGHT BEETLE EXOSKELETONS
JesUSARivera1; David Arango2; Satoshi Murata3; Pablo Zavattieri2; Atsushi Arakaki3; David Kisailus4; 1University of California, Riverside, USA, 2Purdue university, IN/USA, 3Tokyo University of Agriculture and Technology, Jp, 4Department of Chemical and Environmental Engineering, University of California, Riverside, CA/USA
19:30 - 20:50 Non-Classical Mechanisms
Cathedral Room
Chair: Steven Whitelam

19:30-20:00  MULTI-STEP PATHWAYS IN DNA SELF-ASSEMBLY
William Jacobs, Harvard University, USA

20:00-20:30  ENGINEERING AND IN SITU CHARACTERIZATION OF DNA CRYSTAL
JOINING, HEALING AND SELECTIVE MELTING
Rebecca Schulman, Johns Hopkins University, USA

20:30-20:50  STRUCTURAL DEVELOPMENT AND BIOMINERALIZATION OF THE
MANTIS SHRIMP DACTYL CLUB
Nicholas Yaraghi\(^1\); Julian Kosacki\(^1\); Albert Fernandez\(^1\); Mikhail Zhernenkov\(^2\); Richard Wuhrer\(^3\); Pablo Zavattieri\(^4\); David Kisailus\(^5\); \(^1\)University of California, Riverside, CA/USA, \(^2\)Brookhaven National Laboratory, NY/USA, \(^3\)Western Sydney University, NSW/Au, \(^4\)Purdue university, IN/USA, \(^5\)University of California, Riverside, USA

Wednesday, June 13, 2018

09:00 - 10:30 Biological Crystallization
Cathedral Room
Chair: Jim DeYoreo

09:00-09:30  UNIVERSAL BACKBONE CONFORMATION IN PEPTOID POLYMER
CRYSTALS
Sunting Xuan; Doug Greer; Nitash Balsara; Ronald Zuckermann; Lawrence Berkeley
National Laboratory, USA

09:30-10:00  CONTROLLING SILICA BINDING AND TITANIA PRECIPITATION WITH
SOLID-BINDING PROTEINS
François Baneyx, University of Washington, USA

10:00-10:30  CONTROLLED SYNTHESIS OF HIGHLY-BRANCHED PLASMONIC GOLD
PARTICLES THROUGH PEPTOID ENGINEERING
Chun-Long Chen, WA/USA
11:00-11:20  IN SITU STUDIES OF THE NUCLEATION AND GROWTH OF NANOCRYSTAL SUPERLATTICES  
Yixuan Yu; Chris Orme; LLNL, USA

11:20-11:40  DIRECT OBSERVATION OF NUCLEATION FLUCTUATIONS WITH IN SITU AFM  
Benjamin Legg¹; Marcel Baer¹; Younjin Min²; Christopher Mundy¹; James De Yoreo¹;  
¹Pacific Northwest National Laboratory, WA/USA, ²University of Akron, OH/USA

11:40-12:00  STRUCTURES AND TRANSITIONS IN TUNGSTEN GRAIN BOUNDARIES  
Timofey Frolov¹; Qiang Zhu²; Tomas Oppelstrup¹; Jaime Marian³; Robert Rudd¹;  
¹Lawrence Livermore National Laboratory, USA, ²UNLV, USA, ³UCLA, USA
**Abstract Index**

**Sunday, June 10, 2018 (19:30-21:10)**

**CRYSTALLIZATION BY PARTICLE ATTACHMENT IN BIOMINERALS**

P. Gilbert

Abstract: Crystallization done by living organisms, termed biomineralization, involves biological control over crystal nucleation, growth, and crystal orientation patterns in the final biomineral. Marine biomineralization mechanisms are only beginning to be understood, are often surprising, and important to understand fossils and early life, to explain isotopic signatures, and to predict the fate of biomineralizers in warming, acidifying oceans. In this talk I will describe one mechanism of crystallization by particle attachment [1], which we recently observed in fresh, forming coral skeletons [2], and had previously been observed in mollusk shell nacre [3], in sea urchin spicules [4,5] and teeth [6]. Before attaching, the particles are amorphous [2], they remain amorphous after attachment, when they completely fill three-dimensional space [7]. Finally, crystallinity percolates through the amorphous solid, at the expense of the amorphous precursors, as it random-walks in three-dimensions. Proteins are occluded and slightly disorder the final crystalline biomineral [8].

A. Crystal orientation map of a coral skeleton, demonstrating that the skeleton is formed by particles. B. Model of Crystalline Calcium Carbonate (CCC) biomineral formation, from Amorphous Calcium Carbonate (ACC) nanoparticles. This model is valid for a variety of biomineralizers, including corals, sea urchins, and mollusks. Data and model from ref. [2].

BIOLOGICAL CRYSTALLIZATION OF ULTRAHARD TEETH AND TRANSLATION TO MULTI-FUNCTIONAL MATERIALS
D. Kisailus

Abstract: There is an increasing need for the development of multifunctional lightweight materials with high strength and toughness. Natural systems have evolved efficient strategies, exemplified in the biological tissues of numerous animal and plant species, to synthesize and construct composites from a limited selection of available starting materials that often exhibit exceptional mechanical properties that are similar, and frequently superior to, mechanical properties exhibited by many engineering materials. These biological systems have accomplished this feat by establishing controlled synthesis and hierarchical assembly of nano- to micro-scaled building blocks. This controlled synthesis and assembly require organic that is used to transport mineral precursors to organic scaffolds, which not only precisely guide the formation and phase development of minerals, but also significantly improve the mechanical performance of otherwise brittle materials. In this work, we investigate an organism that have taken advantage of hundreds of millions of years of evolutionary changes to derive structures, which are not only strong and tough, but also demonstrate abrasion resistance. All of this is controlled by the underlying organic-inorganic components. Specifically, we discuss the formation of heavily crystallized radular teeth the chitons[1-4], a group of elongated mollusks that graze on hard substrates for algae. From the investigation of synthesis-structure-property relationships in these unique organisms, we are now developing and fabricating multifunctional engineering materials for energy conversion and storage[5]. We discuss the crystallization of these materials and their subsequent impact on performance.

BARRIER-FREE NUCLEATION OF 2D PHAGE-SELECTED PEPTIDE FILMS ON MOS\textsubscript{2} SURFACES

Abstract: Directed assembly of two-dimensional molecular arrays on crystal surfaces has been widely investigated to reveal the structural and energetic relationships between the substrate and overlying architecture. Progress has been achieved in understanding and controlling their assembly, yet little is known about the mechanism by which they nucleate. Understanding the dominant pathways and formation kinetics would enable precise control over phase and morphology during synthesis of 2D materials. In our study, short peptides were selected for their ability to bind to MoS\textsubscript{2} (0001). We studied nucleation and growth of 2D films of these peptides directly with \textit{in situ} AFM and compared our results to molecular dynamics simulations. We find the peptide arrays exhibit an epitaxial relationship to the underlying hexagonal lattice, but assemble row-by-row from dimeric growth along three equivalent directions. The nuclei are ordered from the earliest stages. Although the final crystals are 2D, due to the 1D nature of the constituent rows, there is no critical size, and the nucleation rate varies linearly with concentration and is finite for all concentrations above the solubility limit. Our results verify long-standing but unproven predictions of classical nucleation theory while revealing the key interactions responsible for ordered assembly.

ROLE OF AMYLOID-LIKE AMELOGENIN NANORIBBONS IN ENAMEL MINERALIZATION
S. Akkineni, S. Engelberth, J. Tao, J. Bonde, S. Habelitz, J. J. De Yoreo

Abstract: Mammalian enamel is a composite with remarkable hierarchical structure made of interwoven apatite crystals, yet to be realized with engineered materials. Amelogenin is the main constituent of the organic matrix in developing enamel. However, during maturation stage, the matrix is enzymatically digested, leaving insufficient evidence to identify the quaternary protein structure-function and the complex crystal growth mechanism upon tooth eruption. Recently, strong \textit{in vivo} and \textit{in vitro} evidence was reported in which amelogenin self-assembles into insoluble, amyloid-like nanoribbons. \textit{In vitro} and \textit{in silico} investigations into the amino acid sequence and amyloid structure predicted that a segment of amelogenin, labelled 14P2, guides amelogenin self-assembly into the cross β-sheet quaternary structure, and also independently forms nanoribbons similar to amelogenin. However, the exact relationship between the amyloid structure of amelogenin and apatite crystal is not yet clear. Preliminary bulk solution crystal growth experiments with recombinant human amelogenin (rH174) and 14P2 in calcium phosphate solutions indicates absence of any apatite associated with the nanoribbons. However, the results suggested a matrix-mediated mineralization mechanism, where amyloid-like nanoribbons promote nucleation only upon interaction with soluble enamel proteins. Using 14P2 as a feasible surrogate for rH174, we developed a surface-chemistry-based self-assembly technique to generate an ordered film of oriented nanoribbons with 3-fold symmetry and
consistent surface coverage across several microns. The ordered 14P2 film was then exposed to continuous flow of supersaturated calcium phosphate solution while nucleation and growth events were recorded with in situ AFM. Analysis of nucleation experiments indicated that mineral particles nucleated, and then grew over time, but the number of particles was relatively low when compared with previous data on nucleation-promoting collagen and amelogenin nanospheres. These preliminary results provide the in situ evidence that 14P2 nanoribbons cannot independently enhance nucleation. The techniques from this study on 14P2 will be subsequently applied to nanoribbons of rH174, and of rH174 and 14P2 sequences extended at the C-terminus with polar amino acids that have high affinity for apatite; the added segment mimics the scenario where soluble proteins are bound to the nanoribbons. For cases that enhance nucleation, surface energies for heterogeneous nucleation will be determined. Upon completion, this study will provide valuable knowledge on the role of insoluble amyloid-like amelogenin and soluble enamel proteins in the crystal growth mechanism of interwoven and oriented apatite crystals.

Monday, June 11, 2018 (09:00-10:30)

CRYSTALLIZATION OF MOLECULAR GLASSES: A CENTRAL ROLE FOR SURFACE DIFFUSION
L. Yu

EXPANDING THE SCOPE OF VIEDMA RIPENING
L. Cuccia

Abstract: The focus of our research centers on conglomerate crystals constructed from achiral building blocks. Three systems were investigated: (i) A classic example of chiral inclusion compounds are the numerous clathrates of tri-o-thymotide (TOT). Regardless of the crystal packing, all of TOT’s conglomerate clathrates owe their chirality to a unique three-bladed propeller conformation with restricted rotation of the single bonds of the 12-membered macrocycle (*i.e.* an atropisomer). (ii) Conglomerate co-crystals formed from achiral molecules, for example tryptamine with various achiral carboxylic acids, are chiral due solely to their asymmetric molecular arrangement in the crystal structure. (iii) Conglomerate crystals, such as decacyclene and hippuric acid, that exhibit mesoscale twisting, where enantiomorphous crystals are expected to twist in opposite directions. Attrition-enhanced deracemization of conglomerate crystals was first demonstrated by Viedma in 2005 with sodium chlorate and is now widely known as ‘Viedma ripening’. This simple yet effective method for chiral amplification of conglomerate crystals has spawned great interest from both practical and fundamental perspectives. Numerous examples of Viedma ripening in conglomerate crystal systems, with either chiral or achiral building blocks, have since been explored. Herein, the scope of Viedma ripening is further widened with examples (i), (ii) and (iii).

POLYMORPHIC PHASE TRANSFORMATIONS OF ACTIVE PHARMACEUTICAL INGREDIENTS DURING EXTRUSION INTO CRYSTALLINE SOLID DISPERSIONS
V. Lopez-Mejias, T. Stelzer, J. Hernandez Espinell

Abstract: The inadvertent occurrence of polymorphic transformations of active pharmaceutical ingredients (APIs) during manufacturing has been shown to be detrimental to the US health and economy. For APIs that display poor solubility, and hence, dissolution limited behavior, polymorphism, particle size, and surface area have a direct impact on the quality and efficacy of the final drug product. In recent years, hot melt extrusion (HME) has emerged as an alternative technology to conventional tableting for the solid dosage formulation of drug products. However, studies aiming to understand and control polymorphism during the processing of APIs by HME are very limited, when compared to other unit operations. One might argue that this scarcity originates from the recent emergence of HME, the contrastingly large interest in gaining insights into the stabilization of amorphous solid dispersions (ASDs), and the prevalent notion that APIs displaying polymorphism should not be formulated into crystalline solid dispersions (CSDs) using HME. The latter is unsubstantiated and limits the use of HME to a narrow set of APIs. Moreover, it presents a critical issue to be addressed if there is prospect of implementing HME as a formulation strategy in continuous industrial settings. Recent studies demonstrate the feasibility of HME as an alternative continuous formulation strategy to produce CSDs, while improving the dissolution, an advantage often attributed to ASDs. Yet, their full potential has not been achieved due to the lack of understanding of how the crystalline state behaves during the conditions required for HME. The present work aims to develop control strategies for polymorph selection that would help to identify design spaces for the production of CSDs using HME. Specifically, this work demonstrates that flufenamic acid (FFA), one of the most polymorphic APIs known, thus far, can be processed using temperature-
simulated HME with polyethylene glycol (PEG) as polymeric carrier. At temperatures above the transition point of FFA forms III and I (42 °C), the induction time of the polymorphic phase transformation is longer than the average reported residence time in conventional HME processes (5 min). Moreover, it was demonstrated that thorough understanding of the thermodynamic and kinetic design spaces for the PEG-FFA system leads to polymorphic control in the produced CSDs. Ultimately, this study helps to generate an understanding of the processing needs of CSDs, and hence, lead to the broader application of HME as a continuous formulation strategy for CSDs containing APIs presenting polymorphism, which represents about 80% of all APIs.

Monday, June 11, 2018 (11:00-12:00)

EARLY ONSET OF KINETIC ROUGHENING DUE TO FINITE STEP WIDTH IN HEMATIN CRYSTALLIZATION
P. G. Vekilov, K. Olafson, J. D. Rimer

Abstract: Crystallization is an example of a highly non-equilibrium process, in which the flows of mass and energy are governed by dynamic structures comprising a two-dimensional interface between adjacent three-dimensional semi-spaces. During crystal growth, the structure of its interface with the growth medium dictates the molecular mechanism of solute incorporation, the response of the growth dynamics to temperature and composition gradients, the action of impurities and dopants, and, ultimately, the crystal perfection. Interfaces that are smooth at equilibrium may become rough during growth at elevated supersaturation. We observed a smooth to rough transition during the growth of hematin crystals from a biomimetic mixed organic-aqueous solvent. Hematin crystallization is the main pathway employed by malaria parasites to sequester toxic hematin, released during hemoglobin digestion; its inhibition is considered the most successful target for antimalarial drugs. We show that the transition occurs at a supersaturation significantly lower than that predicted by published criteria. Moreover, surface roughness varies non-monotonically with supersaturation and the rate constant for rough growth is slower than that resulting from nucleation and spreading of layers. We attribute these unexpected behaviors to the dynamics of step growth dominated by surface diffusion and the loss of identity of nuclei separated by less than the step width w. We put forth a general criterion for the onset of kinetic roughening using was a critical lengthscale. The slow growth in the rough growth regime may relate to the high efficacy of antimalarial drugs that inhibit hematin layer growth by introducing negative feedback between elevated hematin concentration and crystal growth rate that enables accumulation of hematin and parasite demise.

L-CYSTINE CRYSTAL GROWTH INHIBITION BY TAILOR-MADE ADDITIVES
A. Shtukenberg, L. N. Poloni, J. P. Lee-Thorp, R. V. Kohn, M. D. Ward

Abstract: Crystallization of excess L-cystine in the kidneys, known as cystinuria, is a chronic and painful pathology that affects 20,000 Americans, for which there are no adequate therapies. Recently our lab proposed a new approach to prevent L-cystine stone formation by inhibiting crystallization by tailor-made additives [J. Rimer et al. Science, 2010, 330, 337-341]. Here we
analyze the mechanism of growth inhibition using bulk crystallization, optical and electron microscopy, *in situ* atomic force microscopy (AFM), and molecular mechanics simulations. Among the 31 unique tailor-made additives evaluated, L-cystine diesters and diamides were found to be the most effective inhibitors. Relatively strong inhibition required preservation of the L-cystine molecular backbone and replacement of terminal hydroxyl groups with relatively small, hydrophobic groups. L-cystine growth inhibition by tailor-made additives on the {0001} face occurs via Cabrera-Vermilyea step pinning mechanism. Quantitative discrepancies between the step velocities predicted using the Cabrera-Vermilyea model and those measured from experimental data were successfully resolved by accounting for the chaotic arrangement of stoppers over the crystal surface and their finite lifetime. The amount of inhibitor incorporated by L-cystine crystals, estimated from kinetic data, suggests that imposter binding to the {0001} face is less probable than binding of L-cystine solute molecules, whereas imposter binding to {10-10} faces is comparable to that of L-cystine molecules. These estimates were corroborated by calculated binding energies from molecular mechanics simulations. This work was supported primarily by the NYU MRSEC Program of the National Science Foundation (NSF) under Award Number DMR-1420073.

### Monday, June 11, 2018 (19:30-21:10)

**THEORETICAL AND COMPUTATIONAL ADVANCES IN SOLUTE PRECIPITATE NUCLEATION**

B. Peters

Abstract: Nucleation is an activated process by which the first stable embryo is born to initiate a phase transition. Experimental and computational studies of nucleation are difficult because, at any moment in time, the critical nuclei have extremely small populations that exist only as ephemeral species before the onset of growth. In addition, nucleation often occurs heterogeneously on sites with unknown characteristics. I will discuss our recent work on LaMer burst nucleation, where theoretical consideration suggest that essentially all of the individual nucleation events occur *homogeneously*. A simple model suggests that the nucleation kinetics can be extracted from particle size distribution data and from the maximum solute concentration during the LaMer burst. These findings suggest a powerful route to homogeneous nucleation kinetics that have long eluded other experiments. On the simulation front, there are now several rare events methods that can compute the nucleation rates for single component processes like freezing. In contrast, solute precipitate nucleation continues to pose major challenges. I will present a new seeded simulation approach for solute precipitate nucleation along with a detailed analysis of factors that influence the accuracy of the estimated rates.

**PREDICTING THE FORMATION OF INCLUSION-TYPE SILICON PHASES: INSPIRED BY THE ANALOGY BETWEEN SILICON AND WATER**

T. Li, Y. Bi, E. Xu, T. A. Strobel
Abstract: Despite being chemically distinct, water and silicon belong to the same group of “tetrahedral materials” for their common structural motif where atoms/molecules are tetrahedrally coordinated. In this contribution, I will show how such structural analogy may be exploited to help guide prediction and synthesis of new energy materials. Through performing high-throughput computer modeling, we find that unconventional silicon phases spontaneously nucleate from liquid silicon in the presence of noble gases under high pressure and high temperature. In particular, a medium-sized noble gas, e.g., Ar, can trigger the nucleation and growth of inert-gas silicon clathrate, a structural analog of methane hydrate; whereas a small noble gas such as helium is able to induce the formation of an unconventional, inclusion-type compound Si$_2$He, which bears strong resemblance to “filled ices”. Importantly, both novel silicon phases are predicted to exhibit a direct or quasi-direct electronic band gap, a desirable electronic property for energy applications. The formation of both phases is attributed to the same thermodynamic and kinetic rationale that explains the crystallization of gas hydrate. Our findings thus strongly suggest a viable experimental synthesis route for these silicon phases using noble gases at high pressure.

STRUCTURE AND COLLECTIVE DYNAMICS OF BOEHMITE ORIENTED AGGREGATION

Abstract: Although orientation-dependent forces governing crystallization by particle attachment have been reported, their scaling with particle anisotropy and solution chemistry remains unknown. Accordingly, the collective dynamics of systems exhibiting oriented attachment remain difficult to predict, particularly for non-spherical particles. In this context, we investigated the structure and dynamics of boehmite aggregation as a function of solution pH and ionic strength. Cryogenic transmission electron microscopy showed that boehmite platelets assemble by oriented attachment on (010) planes. The coagulation rate constants obtained from dynamic light scattering span both the reaction-limited and diffusion-limited regimes. We use simple scaling arguments, calculations of stability ratios, and rotational/translational diffusivities of irregular particle shapes to rationalize the effects of orientation on the early stages of aggregation. Using Monte Carlo simulations, we found that a nanoscale geometric parameter, namely the contact area between two attaching platelets, has a determining impact on the emerging macroscale aggregates and explains their unusually high fractal dimensions.

TRYING A DIFFERENT APPROACH TO THE FREEZING OF LIQUID WATER
Fundamentals of Crystal Growth
C. A. Knight

Abstract: Ice consists of tetrahedrally bonded water molecules, and growing in water it exhibits only basal facets. On ice’s three low-index interfaces, half of the molecules have all four bonds
in the ice structure and the rest have three, with one “dangling” into the liquid. Growing the ice structure with successive molecules, the first of a new layer has only one bond to ice. On the prism interfaces the second molecule always produces a two-molecule island fixed in the ice structure. However on a basal face a second molecule bonded to the first cannot bond to the original crystal surface, but makes a two-molecule tail into the liquid. This probably has a very short lifetime on an equilibrium surface compared to the two-molecule island on a prism interface, which necessarily propagates the ice structure. Further growth at the two orientations once an island is large enough to be viewed as bounded by steps. The idealization of growth used is rather drastic, but this finding provides an intriguingly simple, geometric explanation of growth facets forming only on the basal face (and with an extremely small critical supercooling); and also for other aspects of the ice growth difficult to describe within the word-count limit. The (unexpected) realization that a two-molecule “island” on a basal interface is not a template for further growth of a new layer leads one to wonder about nucleation theory applied to crystals. The further growth of the ice structure cannot be molecule by molecule, but requires larger-scale reorganization. For the homogeneous nucleation of ice, how big must a water cluster be before it can be a template for growth of the ice structure? One does not know, but certainly considerably more than four molecules, the formal content of ice’s unit cell. It appears that homogeneous nucleation of a crystal may involve two distinct barriers, one arising from interfacial energy, and the other the initiation of the crystal structure itself. If so, either could be the dominant barrier, and the use of homogeneous nucleation theory to estimate the interfacial energy of ice in water, as often is done, might be misleading.

Tuesday, June 12, 2018 (09:00-10:40)

EPITAXIAL GROWTH OF HBN ATOMIC LAYERS ON COPPER VIA HETEROGENEOUS PYROLYSIS: ATOMIC-SCALE GROWTH MECHANISMS
B. Narayanan, C. V. Ciobanu, G. Siegel, M. Snure, S. C. Badescu

Abstract: Two-dimensional hexagonal boron nitride (hBN) has emerged as a promising insulator for applications in nano-electronic devices, tunneling barriers, and atomically thin capacitors. These applications require synthesis of large area, uniform, and high-quality atomic layers of h-BN. More importantly, a precise (and reproducible) control over the number of hBN layers as well as their orientation is crucial for enhancing performance of these low-dimensional devices. Until now, growth of hBN on metal substrates has been primarily achieved via chemical vapor deposition from a single precursor (e.g., borazine); this yields monolayers of hBN, limited by the catalyzing effect of the metal substrates. Here, we depart from this paradigm, and demonstrate close control over the growth of mono-, bi-, and trilayers of hBN on copper using triethylborane and ammonia as independent sources of boron and nitrogen. Our density functional theory (DFT) calculations and reactive force field molecular dynamics illustrate that the growth of hBN beyond the first layer is enabled by the activation of ammonia through heterogeneous pyrolysis with boron-based radicals at the surface. The as-grown hBN layers are in registry with each other and assume a perfect or near perfect epitaxial relation with the substrate. Additionally, our atomic force microscopy (AFM) show a moiré superstructure in the first hBN layer with an
apparent height modulation and lateral periodicity of $\sim$10 nm; this is unexpected, since the moiré pattern of hBN/Cu(111) does not have a significant morphological corrugation. Our DFT calculations reveal that this unusual AFM response is associated with a spatially modulated interface dipole layer. These findings will be discussed in the context of developing new methods for growing 2D materials, particularly for applications in which control over the number of layers and their alignment is essential.

Hanchen Huang, Title: TBD

CONGRUENTLY MELTING PEROVSKITE SOLID SOLUTIONS
V. Fratello, L. Boatner, H. Dabkowska, A. Dabkowski

Abstract: If a crystal material is non-congruent, has a high liquidus temperature, contains volatile ingredients and the material is desired in a thin film, multilayer or superlattice, then epitaxy is the required growth method. Good epitaxial growth typically requires a high-quality substrate that is a structural and lattice-parameter match to the film. Perovskites include the most common minerals in the earth’s crust, but also comprise technologically important materials that are ferroelectric, electrooptic, ferromagnetic, ferrimagnetic, antiferromagnetic, multiferroic, piezoelectric, pyroelectric, paraelectric, magnetoresistive, colossal magneto resistive (CMR), magneto optic, photovoltaic, photoluminescent, insulating, conducting, semiconducting, superconducting, ferroelastic, magnetostrictive, catalytic, etc. Researchers have developed complex perovskite multilayer thin films for potential device applications ranging from spintronics to ferroelectric transistors. However, there are currently limits on the available substrates for film growth with substrates such as strontium titanate, potassium tantalate and the rare earth scandates being small in size, high in cost and limited in availability. Above 0.3865 nm in the primitive perovskite unit cell lattice parameter, there are no commercial perovskite substrates and there are not even any experimental substrates available in the important range of 0.403-0.416 nm. A class of low-cost perovskite solid solutions has been identified that are congruently melting at a temperature minimum indifferent point and that have a cubic structure with no structural phase transition – i.e., qualities that make them more useful as substrates. In fact, there are a few relevant compounds already reported in the literature – including the technologically important perovskite substrate material lanthanum strontium aluminum tantalate. While having two phases in equilibrium at a point seems to violate the usual expression of Gibbs’ phase rule, a more detailed look shows that this is thermodynamically possible if the coefficient matrix has a zero determinant. It requires an uncommon balancing of various terms of the free energy for the required condition. The factors that have been found to produce such a congruently melting minimum cubic perovskite solid solution include a common ion(s) among the end members, similar sized ions, similar melting temperatures (within 300°C) and, most profoundly, a Goldschmidt tolerance factor $T$ close to unity, preferably 0.98-1.02. This contributes to a thermodynamic energy minimum, and it was found to shift the position of the minimum melting composition to optimize $T$. Six new compositions have now been identified with cubic lattice parameters from 0.3872 to 0.4071 nm. Attempts to characterize these materials further and to grow single crystals are ongoing.
TITANIA NANOPARTICLE CRYSTAL GROWTH WITHIN POLYMER-CARBON NANOFIBER MATRICES
L. Cruz, D. Kisailus

Abstract: Titanium dioxide is known to be one of the most widely used photocatalytic material due to its strong oxidation potential. However, many TiO$_2$ photocatalytic systems are particulate in nature, which necessitates a recollection process that hinders their efficiency, increases cost, and limits their widespread application. Anchoring these nanoparticles on surfaces or within three-dimensional matrices would be beneficial. Here, we impregnate TiO$_2$ within a polymer matrix and subsequently investigate its diffusion, crystal growth and phase transformations upon annealing. The effects temperature, atmosphere, and polymer structure on the growth and phase transformation of the TiO$_2$ nanoparticles within this carbonaceous matrix are discussed. Subsequent photodegradation of organic analytes are performed.

Tuesday, June 12, 2018 (11:00-12:00)

IN SITU SCANNING TUNNELING MICROSCOPY STUDIES OF GROWTH AND STRUCTURE OF HEXAGONAL BORON NITRITE MONOLAYERS ON PD(111)
P. Arias, A. Abdulslam, A. Ebnonnasir, C. V. Ciobanu, S. Kodambaka

Abstract: Two-dimensional (2D) layered hexagonal boron nitride (hBN) is an insulator, isostructural to graphene, and is considered an ideal dielectric for a variety of 2D layer based nanoelectronic devices. In contrast to free-standing hBN layers, substrate-supported hBN can be metallic, semiconducting, or insulating, depending on the chemistry and electronic structure of the hBN/substrate interface. Control over these properties hinges on the ability to grow high-quality, wafer-scale hBN crystals. hBN layers are commonly grown on transition-metal substrates and the hBN layer structures, as well as their interactions with the transition-metals have been fairly well characterized. However, relatively few studies have investigated (i) the mechanisms underlying the growth of the hBN layers and (ii) influence of hBN domain orientation (with respect to the substrate) on its electronic properties. Using in situ ultra-high vacuum scanning tunneling microscopy (UHV STM), we investigated the chemical vapor deposition (CVD) kinetics of hBN on Pd(111). STM images are acquired during CVD of borazine as a function of substrate temperature, borazine flux, and deposition time. We observe the nucleation and growth of chemisorbed borazine islands on the Pd surfaces. Furthermore, we investigated the surface structure of hBN domains on Pd(111) using STM, scanning tunneling spectroscopy (STS), and density functional theory (DFT) calculations. STM images acquired from the hBN/Pd(111) sample reveal moiré patterns with at least four different periodicities corresponding to four rotational domains of hBN. From the STM images, we measured the surface corrugations in each of the moiré patterns and found that the corrugation amplitude Dz depends on the tunneling bias and increases with increasing l. We suggest that Dz is a measure of hBN-Pd(111) interaction strength and attribute the higher corrugation amplitudes to stronger interactions between the hBN domains and the Pd(111). We expect that similar approach could be used to investigate growth kinetics and orientation-dependent interactions in other substrate-supported 2D layers as well as in 2D layered heterostructures.
GROWTH MECHANISM OF FIVEFOLD-TWINNED AG NANOWIRES IN SOLUTION
Functional Materials
K. Fichthorn, X. Qi

Abstract: There has been significant emphasis recently on the synthesis of fivefold-twinned Ag and Cu nanowires, which are considered to be excellent candidates for transparent conductors in flexible and stretchable electronic devices. A fundamental understanding of nanowire growth is important in achieving optimal syntheses. Nanowires grow from fivefold-twinned seeds and our work shows that likely shapes for these structures include \{111\} end facets and “notches”, \{100\} side facets, and \{110\} facets between the notches and the ends, as shown in the figure. We find that the density of islands on the \{111\} facets of growing wires is lower than that on \{100\} facets and that islands are likely to nucleate on \{111\} facets near \{110\}-\{111\} facet boundaries. Our climbing-image nudged-elastic band calculations of diffusion barriers based on embedded-atom method potentials indicate that diffusion in the \{111\} notches and on the \{110\} “steps” is significantly faster than diffusion on \{100\} facets. Thus, these structures become “superhighways” that channel atom diffusion to the wire ends to increase wire aspect ratios. Small islands facilitate trapping of atoms on \{111\} facets, as indicated in the figure. We use finite Markov chains to model nanowire growth and to predict net atom fluxes from nanowire sides to the ends. These simulations predict anisotropic nanowires similar to those seen experimentally.

![Image](image_url)

(a) (b)

THE ROLE OF SOLUTION COMPLEXATION IN THE HYBRID ORGANIC-INORGANIC PEROVSKITE CRYSTALLIZATION PATHWAY

Abstract: Hybrid organic-inorganic perovskites (HOIPs), such as CH$_3$NH$_3$PbI$_3$, have attracted much attention for use in inexpensive, high-performance solar cells. Control over HOIP thin-film
morphology, which is essential to achieve consistent solar cell efficiencies, requires a fundamental understanding of the crystal nucleation and growth mechanisms and kinetics. Previous work has established that multiple different crystalline precursors form during film growth. Our current work seeks to establish a link between the solution complexation chemistry and the first crystalline phase to appear during HOIP thin-film growth. Density functional theory (DFT) studies have shown that the enthalpy of solvation of the lead salt (e.g., PbI₂ in dimethylsulfoxide) and the binding energy between one solvent molecule and one HOIP cluster (e.g., CH₃NH₃PbI₃ monomer) vary significantly as a function of the solvent. However, there is still little understanding of how the solvation of the lead salt affects the formation of crystalline precursor phase(s). Based upon computational predictions, we have performed in situ X-ray diffraction studies during film annealing to better understand the role of the solvent, and the associated solvent-solute coordination interactions, in directing the HOIP crystallization pathway. We have found that in weakly coordinating solvents, a crystalline precursor to the HOIP forms at early times, whereas strongly coordinating solvents can suppress the formation of this precursor phase. Our results strongly suggest that solution complexation plays an important role in determining the crystallization pathway of HOIPs. Moreover, we have observed variations in the solid-state transformation dynamics among the studied weakly coordinating solvents, which might be due to differences in precursor phase structure.

---

**Tuesday, June 12, 2018 (19:30-20:50)**

**MULTI-STEP PATHWAYS IN DNA SELF-ASSEMBLY**  
W. M. Jacobs

Abstract: Single-stranded DNA oligonucleotides can self-assemble into complex, multicomponent structures. However, current protocols often suffer from low yields or require long assembly times. One strategy for overcoming these limitations is to optimize the initial nucleation step of these multicomponent, self-assembly reactions. I shall discuss how a combination of in situ dynamic light scattering experiments and computer simulations of DNA 'brick' nucleation and growth have led to progress in this direction. By designing multi-strand precursors that assemble at high temperatures, it is possible to modify the critical nucleus that is required to initiate structure growth. This approach broadens the range of conditions over which self-assembly occurs and, consequently, can dramatically improve the final yield of correctly formed structures. Because it is only necessary to modify a small portion of a target structure to optimize its yield, this strategy provides a practical route for improving the speed and accuracy of self-assembly in biomolecular and colloidal systems where the interactions between subunits can be programmed.
ENGINEERING AND IN SITU CHARACTERIZATION OF DNA CRYSTAL JOINING, HEALING AND SELECTIVE MELTING
R. Schulman

Abstract: The ability to design synthetic DNA crystal structure and assembly kinetics and the ease of characterizing DNA crystal structure make them a unique laboratory for crystal growth studies. We have used DNA tile nanotubes to hierarchical crystallization, crystal healing and selective crystal melting in situ. By carefully controlling supersaturation we have found it is possible to build “living crystals” that can continually assemble by both monomer growth and joining, form large crystals with no major defects and heal when defects are introduced. Analytical studies following the same crystal over time using fluorescence microscopy can explain these behaviors and their rates using simple models.

STRUCTURAL DEVELOPMENT AND BIOMINERALIZATION OF THE MANTIS SHRIMP DACTYL CLUB
N. Yaragh, J. Kosacki, A. Fernandez, M. Zhernenkov, R. Wuhrer, P. Zavattieri, D. Kisailus

Abstract: Mantis shrimp are aggressive marine crustaceans well known for their rapid and powerful hunting strategies, deploying hammer-like fists called dactyl clubs to strike and kill prey with tremendous force and speed. The success of the dactyl appendage in mitigating damage from repeated impacts can be attributed to its multi-regional composite architecture, featuring amorphous and crystalline forms of biogenic carbonated calcium phosphate templated by alpha-chitin fibers that are likely co-localized with acidic peptides. Here we investigate formation and biomineralization pathways of the dactyl club through ultrastructural and chemical characterization of clubs extracted at various stages of the molt cycle. A combination of electron microscopy, electron/synchrotron diffraction, and spectroscopic analyses are used to characterize crystallinity, phase, morphology, and orientation of organic and inorganic constituents. Such studies will provide insight to the assembly of alpha-chitin fiber architectures as well as the nucleation and growth of biogenic calcium phosphate that yields domains of either amorphous mineral, randomly oriented single crystalline nanoparticles or highly textured apatite nanorods.

Wednesday, June 13, 2018 (19:30-20:50)

UNIVERSAL BACKBONE CONFORMATION IN PEPTOID POLYMER CRYSTALS
S. Xuan, D. Greer, N. Balsara, R. Zuckermann

Abstract: How do polymer crystals differ from small molecule crystals? With the recent advent of sequence-defined peptoid polymer chemistry, we can now readily synthesize molecularly pure, peptoid polymers, with precision, atomic control of their molecular structure. This allows us to systematically explore how the chemical structure of a polymer chain effects its ability to crystallize and pack into well-defined assemblies. It allows us to explore the impact of molecular weight on molecular crystallization. Here we used X-ray scattering and cryo-TEM to examine a series of crystalline, sequence-defined peptoid diblock copolymers, where we varied the main
chain length, side chain chemistry and size, terminal groups and monomer composition. The peptoids assemble into both 2D and 3D lattices, depending on solvent conditions, allowing a variety of characterization tools to be used to elucidate the molecular structure and packing configuration. Interestingly we found that in over 22 crystalline peptoid polymers reported in the literature, all of them likely share a similar packing motif, where the chains are extended, and the backbones are in an all-cis conformation. This common structural motif over a wide variety of structures, suggests favorable backbone-backbone interactions resulting in chain alignment, and provides great opportunities to engineer these crystals by using synthesis to introduce point mutations to introduce specific function.

CONTROLLING SILICA BINDING AND TITANIA PRECIPITATION WITH SOLID-BINDING PROTEINS

F. Baneyx

Abstract: Solid binding proteins are genetically engineered chimera that incorporate one or more combinatorially-selected solid-binding peptides (SBPs) within specific locations of their framework. These macromolecules have emerged as powerful tools to study the fundamentals of biotic-abiotic interactions because they allow for the presentation of SBPs within solubilizing and structurally defined contexts. They have also proven useful for the assembly of hybrid architectures that harness the “built-in” function and topology of the host scaffold, and for controlling the nucleation, growth and morphology of inorganic phases. Focusing on derivatives of the green fluorescent protein modified with one or more metal oxide binding peptides that have been rationally mutated, I will discuss how SBP sequence, structure, and valency influence the kinetics and thermodynamics of silica binding, and the amount, crystallography and catalytic activity of titania precipitated from soluble precursors.

CONTROLLED SYNTHESIS OF HIGHLY-BRANCHED PLASMONIC GOLD PARTICLES THROUGH PEPTOID ENGINEERING

C. Chen

Abstract: Inspired by peptide- and protein-controlled formation of hierarchical inorganic nanostructures in nature, many biomimetic approaches have been developed for the preparation of nanostructured inorganic materials. These approaches are attractive because they generate complex, functional nanomaterials under mild aqueous synthetic conditions. The unique integration of bio- and inorganic nanomaterials has demonstrated superior performance. Despite the advances in developing biomimetic approaches, the rules of designing sequence-defined molecules that lead to the predictable synthesis of inorganic nanomaterials are unknown. Herein we report the design of sequence-defined peptoids for controlled synthesis of highly-branched plasmonic gold particles. By engineering peptoid sequences and investigating resulting particle formation mechanisms, we developed a rule of thumb for designing peptoids that predictively enabled the morphological evolution from spherical to spherical coral-shaped nanoparticles. Through a combination of hyperspectral UV-Vis absorption micro-spectroscopy and three-photon photoemission electron microscopy, we demonstrate that the individual coral-shaped gold nanoparticles exhibit a plasmonic enhancement as high as $10^5$ fold. This research significantly
advances our ultimate vision of predictive bio-inspired materials synthesis using sequence-defined synthetic molecules that mimic proteins and peptides.

Wednesday, June 13, 2018 (11:00-12:00)

IN SITU STUDIES OF THE NUCLEATION AND GROWTH OF NANOCRYSTAL SUPERLATTICES

Y. Yu, C. Orme

Abstract: In situ studies of the nucleation and growth of nanocrystal superlattices Yixuan Yu, Dian Yu, Norman Su, Jeff Urban, Christine A. Orme. Lawrence Livermore National Laboratory, 7000 East Avenue, Livermore, CA 94550, USA. University of California, Los Angeles, Los Angeles, CA 90095, USA. Lawrence Berkeley Lab, Berkeley, CA, USA. Ordered ensembles, also known as superlattices, have been formed with a large variety of nanocrystals. The structure of nanocrystal superlattices have been extensively studied and well documented; however, their assembly process is poorly understood. In this work, we demonstrate an in situ space-time-resolved small angle X-ray scattering (SAXS) measurement and use it to probe the assembly of nanocrystal superlattices driven by electric fields. The field controls the nanocrystal flux making the deposition process akin to vapor deposition. Beyond simply depositing films, we demonstrate that flux control allows us to systematically change the nucleation density and growth rates. We use nickel and silver nanocrystals to show that films can grow either via a layer-by-layer or by an island formation mechanism. We show that the ligands play a central role in determining whether nanocrystals assemble into thin films or colloidal crystals. This level of control allows us to tune the correlation length, which we expect to have advantages for fundamental studies and to benefit device performance. Work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

DIRECT OBSERVATION OF NUCLEATION FLUCTUATIONS WITH IN SITU AFM

B. A. Legg, M. D. Baer, Y. Min, C. J. Mundy, J. J. De Yoreo

Abstract: Classical nucleation theory (CNT) predicts that nucleation of crystals from solution requires a population of sub-critical molecular clusters that form through dynamic statistical fluctuations. These clusters are expected to occur in any solution, and their observation would provide direct confirmation of the classical nucleation theory. However, these clusters have been extraordinarily difficult to observe, due to their scarcity and their transitory nature. Here, we introduce high-speed in-situ atomic force microscopy (AFM) as a method for directly imaging subcritical clusters of aluminum hydroxide at a mica-water interface. With this technique, we are able to determine the size-distribution of subcritical clusters and track the fluctuations of individual clusters over time. When imaging a cleaved mica surface in the presence of AlCl₃ aqueous solutions, we observe single-molecule adsorbates. Based on concentration-dependance, streaming-potential measurements, and ab-initio molecular dynamics, we conclude that the adsorbates are surface-bound hydrated aluminum-ions, and that the surface promotes hydrolysis of these ions. When the solution saturation is increased, we find a population of dynamic
molecular clusters emerges, with sizes of up to 4.0 nm\(^2\). The concentration of clusters drops off exponentially with size, in general agreement with the size-dependant free energy of cluster formation predicted by CNT. The clusters also fluctuate in size in a manner that is consistent with CNT. Further increases in supersaturation leads to growth of a monolayer of crystalline aluminum hydroxide through cluster-coalescence. We arrive at a description of the nucleation pathway in which the surface enhances nucleation rates by concentrating a dense-liquid layer of aluminum at the mica-water interface, and that classical cluster fluctuations occur within this layer. However, the high concentrations of clusters favors a late-stage crystal growth pathway that is dominated by cluster coalescence, rather than ion-by-ion addition.

---

**STRUCTURES AND TRANSITIONS IN TUNGSTEN GRAIN BOUNDARIES**

T. Frolov, Q. Zhu, T. Oppelstrup, J. Marian, R. E. Rudd

Abstract: Tungsten is a structural material with many advantageous properties such as high thermal conductivity, high melting temperature, mechanical strength at elevated temperatures, and resistance to surface sputtering. Tungsten is known to be susceptible to embrittlement. Below its ductile-brittle transition temperature, pristine tungsten undergoes fracture by cleavage with essentially no plasticity prior to failure. At higher temperatures, recrystallization takes place, and grain boundary (GB) embrittlement is the dominant fracture mode. Radiation damage also affects tungsten’s failure properties. Predictive modeling of recrystallization and deformation of polycrystalline W relies on the accurate description of the W GBs. The goal of this work is to use atomistic modeling to investigate the structure of bcc W GBs and potential effects of point defects and elevated temperatures. Accurate prediction of GB structure and possible transitions using atomistic modeling are important for strategies that aim to improve properties of materials. While grain boundaries created by the γ- surface method as a union of two perfect half crystals have been studied extensively, it is known that the method has limitations and does not always predict the correct ground states. In this work, we use a newly developed computational tool, based on the USPEX structure prediction code, to perform a grand-canonical search of grain boundaries in bcc metals. We find new ground states and multiple phases that cannot be described using the conventional structural unit model. We use molecular dynamics simulations to investigate high-temperature structures of these boundaries and transitions induced by absorption of point defects and relevant to recrystallization. This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.
You are invited to the beautiful mountains of Colorado for the 19th International Conference on Crystal Growth and Epitaxy (ICCGE-19) and the 17th International Summer School on Crystal Growth (ISSCG-17), to be convened over two weeks in July-August, 2019. ICCGE will be held at the Keystone Resort and Conference Center, featuring modern, comfortable accommodations and the largest conference center in the Rocky Mountains. ISSCG will take place at a companion location to be determined.

These triennial meetings, organized under the auspices of the International Organisation for Crystal Growth (IOCG), are the premier forums for the world’s crystal growth communities. The International Summer School on Crystal Growth will feature world-renowned scholars delivering tutorials on the fundamentals and practice of crystal growth. The International Conference on Crystal Growth and Epitaxy will provide a forum for the presentation and discussion of recent research and development activities in crystal growth and will feature all aspects of bulk crystal and epitaxial thin film growth; sessions will integrate fundamentals, experimental and industrial growth processes, characterization, and applications.

The technical program will include both oral and poster sessions, as well as plenary and invited talks to provide a complete picture of the latest developments in the fields. The official language of the conference will be English. Conference proceedings will be reviewed and published in a special issue of the Journal of Crystal Growth.

The magnificent setting of the Rocky Mountains and the American West will provide multiple opportunities for recreation and enjoyment of nature for the conferees and their families before and after, as well as during the conference. There will be a full social program and vendor exhibit together with the technical sessions.

Organizing Committee:

**ICCGE Co-Chair**
Vincent Fratello  
*Quest Integrated, Inc.*

**Program Co-Chair**
Christine Wang  
*Lincoln Laboratory, MIT (ret.)*

**ISSCG Co-Chair**
Thomas Kuech  
*University of Wisconsin*

**ICCGE Co-Chair**
Jeffrey Derby  
*University of Minnesota*

**Program Co-Chair**
Peter Schunemann  
*BAE Systems*

**ISSCG Co-Chair**
Joan Redwing  
*Penn State University*

Inquiries: AACG@comcast.net  *  www.crystalgrowth.org