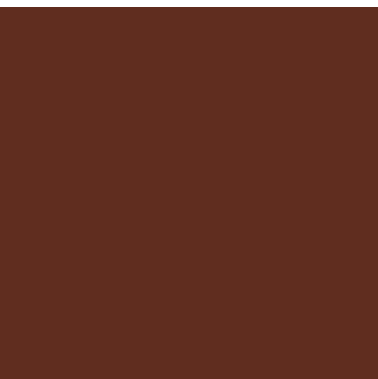
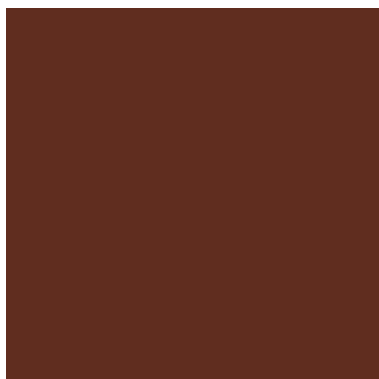


2308<sup>th</sup> Conference

Materials Science & Crystallography 2018



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**APPLIED CRYSTALLOGRAPHY**

November 07-08, 2018 | Atlanta, USA

Keynote Forum

Day 1

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## APPLIED CRYSTALLOGRAPHY

November 07-08, 2018 | Atlanta, USA



### *Ramesh K Agarwal*

*Washington University in St Louis, USA*

#### **Design of metamaterials using transformation physics**

Metamaterials are rationally designed artificial materials composed of tailored functional building blocks densely packed into an effective (crystalline) material. While metamaterials historically are primarily thought to be associated with negative refractive indices and invisibility cloaking in electromagnetism or optics, it turns out that the simple metamaterial concept also applies to many other areas of physics namely the thermodynamics, classical mechanics (including elastostatics, acoustics, fluid dynamics and elastodynamics) and in principle also to the quantum mechanics. This lecture will review the basic concepts and analogies behind the thermodynamic, acoustic, elastodynamic/elastostatic and electromagnetic metamaterials and differences among them. It will provide an overview of the theory, the current state of the art and example applications of various types of metamaterials. The review will also discuss the homogeneous as well as inhomogeneous metamaterial architectures designed by coordinate-transformation-based approaches analogous to transformation optics. The application examples will include laminates, thermal cloaks, thermal concentrators and inverters, anisotropic acoustic metamaterials, acoustic free-space and carpet cloaks and mechanical metamaterials with negative dynamic mass density, negative dynamic bulk modulus, or negative phase velocity. Finally an example of quantum-mechanical matter-wave cloaking will be provided.

#### **Biography**

Ramesh K Agarwal is the William Palm Professor of Engineering at Washington University in St Louis from 1994 to 2001, he was the Sam Bloomfield Distinguished Professor and Executive Director of the National Institute for Aviation Research at Wichita State University in Kansas. From 1978 to 1994, he worked in various scientific and managerial positions at McDonnell Douglas Research Laboratories in St Louis. He became the Program Director and McDonnell Douglas Fellow in 1990. He received PhD in Aeronautical Sciences from Stanford University in 1975, MS in Aeronautical Engineering from the University of Minnesota in 1969 and BS in Mechanical Engineering from Indian Institute of Technology, Kharagpur, India in 1968. He is the author and co-author of over 600 publications and serves on the editorial board of 20+ journals. He has given many plenary, keynote and invited lectures at various national and international conferences worldwide. He is a Fellow of AAAS, ASME, AIAA, IEEE, SAE and SME.

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## APPLIED CRYSTALLOGRAPHY

November 07-08, 2018 | Atlanta, USA



### *Zygmunt Derewenda*

*University of Virginia, USA*

#### **Protein crystallization by mutational surface engineering**

Protein crystallization constitutes a major bottleneck in the high-resolution structural characterization of proteins and their complexes. It is estimated that the probability of obtaining single crystals as a result of screening ranges from less than 1% to 25%, depending on the source and biophysical properties of the target protein or complex. A further complication arises if the crystals lack diffraction quality, impeding high-resolution data collection. Nearly two decades ago we proposed a new approach to protein crystallization based on rational surface engineering to generate surface patches with an enhanced propensity to form crystal contacts. The method relies on the mutational replacement of surface residues with high conformational entropy, such as Lys and Glu/Gln with Ala or other small amino acids. The design of variants with enhanced crystallization propensity is possible using a dedicated server (<http://services.mbi.ucla.edu/SER/>). This methodology, known as Surface Entropy Reduction (SER), has been successfully used in hundreds of studies, not only to obtain crystals of otherwise intractable proteins or complexes, but also to generate new crystal forms with improved diffraction quality allowing to collect X-ray data to much higher resolution than that recorded for the wild-type crystals. In addition, the database of protein crystal structures determined with the help of SER provides interesting insights into the mechanistic aspects of protein crystallization.

#### **Biography**

Zygmunt Derewenda obtained PhD and DSc degrees from the University of Lodz in Poland. His Postdoctoral studies were conducted at the University of York, UK. Prior to joining the faculty of the University of Virginia, where he is currently a Harrison Distinguished Professor of Molecular Physiology and Biological Physics, he was an Associate Professor at the University of Alberta in Edmonton, Canada. He has published more than 150 papers on a range of subjects in structural biology, which were cited over 11,000 times (H-factor 58).

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November 07-08, 2018 | Atlanta, USA



### Georges Denes

Concordia University, Canada

#### When crystallography alone fails, it can use help from tin-119 Mossbauer spectroscopy

Crystallography is unquestionably the most powerful method for obtaining structural data about crystalline solids. However, there are some cases where even the most powerful method can benefit from help from techniques that are not used for structural determination. In the current work, <sup>119</sup>Sn Mossbauer spectroscopy was used to assist crystallography, for finding the tin (II) positions in the unit cell and determine a tin (II) coordination in agreement with both the diffraction data and the tin electronic structure. The first case will show that even high-quality single crystal data do not always guarantee that the right solution will be obtained. A first attempt at the structure of  $\alpha$ -SnF<sub>2</sub> yielded the tin positions with very reasonable R and Rw residuals, 0.23-0.25. However, the fluorine positions could not be found. After many other attempts, the full crystal structure was finally solved 14 years later. The difference in the tin position between the two solutions was that, in the latter, half of the tin atoms were on special sites; however, the tin sublattice was identical. Because the tin sites in the initial solution gave very reasonable residuals, 14 years of efforts were wasted. The presentation will show that this could have been avoided using <sup>119</sup>Sn Mossbauer spectroscopy. This was possible since the spectrum had already been recorded. It will also be shown how Mossbauer spectroscopy can help determine the tin coordination, when combined with powder diffraction data, in the case of disordered structures. The presence of tin(II), disordered with a metal ion in cubic coordination, when diffraction shows there is no lattice distortion and no superstructure, suggests that tin has also a cubic coordination. This would require the tin lone pair to be non-stereo active; however, Mossbauer spectroscopy shows it is stereo active. The same technique helps to suggest an alternate disordered structure in agreement with the X-ray powder diffraction data. Furthermore, <sup>119</sup>Sn Mossbauer spectroscopy was also used to assist diffraction for solving the crystal structure of a compound suffering from an extreme case of preferred orientation. The presentation will show the hurdles faced by diffraction methods alone and how we designed the use of Mossbauer spectroscopy in order to rescue crystallography.

#### Biography

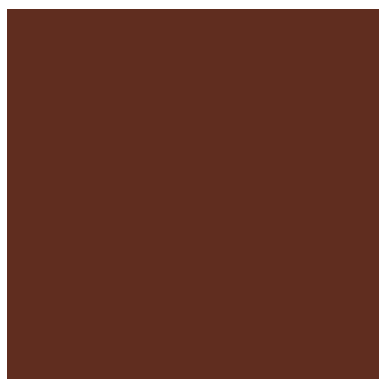
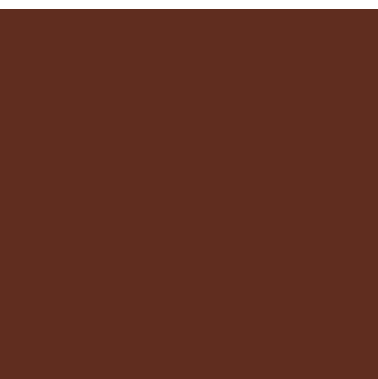
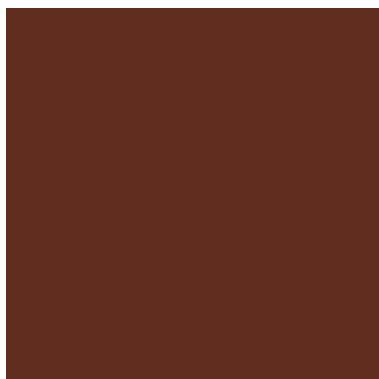
Georges Dénès is a Professor in Department of Chemistry & Biochemistry at Concordia University, Canada. He has completed his PhD at Université de Rennes 1. His research interests are solid state inorganic chemistry. He has been teaching general chemistry, inorganic (main group) chemistry and he has published articles in various journals.

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**APPLIED CRYSTALLOGRAPHY**

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## APPLIED CRYSTALLOGRAPHY

November 07-08, 2018 | Atlanta, USA



### *Masafumi Yamaguchi*

*Toyota Technological Institute, Japan*

#### Overview of solar cell research and development and approaches to automobile applications

Development of high-efficiency solar cell modules and new application fields are very important for further development of PV (photovoltaics) and the creation of new clean energy infrastructure based on PV. For this end, further development of science and technology of PV is necessary. This paper overviews PV R&D activities in Japan as the PV R&D former Project Leader of NEDO and JST. Present status of various solar cells efficiencies under NEDO and JST PV R&D projects are presented. 44.4% for concentrator III-V compound 3-junction solar cell, 37.9% for 1-sun III-V compound 3-junction cell, 26.7% for single-crystal Si cell, 22.9% for CIGS cell and 14.0% for a-Si based 3-junction cell. Efficiency potential of various solar cells is also discussed. Future prospects of PV and our recent approaches towards the creation of “Mobility Society by using Solar Energy” are discussed. Very large-scale installation of PV power systems is needed and thus the development of ultra-high performance, low cost and highly reliable solar cells are very important. In addition, development of low cost and long lifetime batteries, highly reliable and intelligent system technologies such as smart grids is necessary. We are now challenging III-V/Si tandem solar cells. Because III-V/Si tandem solar cells have great potential for high-efficiency, low-cost and light-weight solar cells. Automobile applications by using solar energy are also very important and very attractive. Recently, we have developed high-efficiency (32%) InGaP/GaAs/InGaAs thin-film 3-junction solar cells module with an area of 32cmx32cm and 33% efficiency InGaP/GaAs/Si mechanically stacked 3-junction solar cell. Those are expected to be one of the seeds for solar electric vehicle applications.

#### Biography

Masafumi Yamaguchi is Professor Emeritus at the Toyota Technological Institute (TTI), Nagoya, Japan and Senior Research Scholar of the Research Center for Smart Energy Technology (SET) at the TTI. He is also a Visiting Professor of the Kyushu University and Chairman, Research Committee of the Super High Efficiency Solar Cells, Japan Society for Promotion of Science (JSPS)

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## APPLIED CRYSTALLOGRAPHY

November 07-08, 2018 | Atlanta, USA



### Mark A Zurbuchen

University of California at Los Angeles, USA

#### Topotactic anion exchange in epitaxial films: Synthesis advantages and characterization challenges

**Statement of the Problem:** Despite direct epitaxial deposition/facet-growth of innumerable materials in lab experiments, new lattice-matched buffer (interdiffusion-blocking) layers are desperately needed by the microelectronics industries. There is a need for "substrate agnostic" buffer layer(s) to template epitaxial growth on Si, GaN, Ni and others. Epitaxial templates, particularly ultra-thin oxide layers, have been demonstrated to be excellent epitaxial buffer layers, but the fabrication of epitaxial samples of many materials is frustrated by chemical or lattice mismatch. This talk focuses on a new, better approach to dealing with heterogeneous interfaces. A promising new approach—topotactic anion exchange (TAE) epitaxy. The approach is unique, with two steps—1<sup>st</sup> epitaxial deposition of a precursor layer; and 2<sup>nd</sup> a special gas anneal to exchange the anions in the solid for others; to ultimately yield a highly perfect epitaxial film of the product phase. Opportunities abound, as there are only two criteria to meet: (a) The initial film is formulated to match the surface-symmetry type and lattice parameter of the substrate; (b) A thermal, atmosphere-controlled step initiates the topotactic reaction. Ideally, compositions for TAE layers are chosen with end members commensurate—as the reaction front passes through the solid. Cations are sessile with anions are relatively mobile. Anions are exchanged diffusively; but because the resultant material is a different phase altogether, conversion can dramatically alter the magneto-opto-electrical behaviors of the layers. Characterization requires finesse at the atomic level. The typical anions all have roughly the same atomic mass, making a discernment between the two phases complicated. The results of *ex situ* and *in situ* anion exchange experiments towards an epi buffer for Si and GaN will be presented. Further discussion of analyses thus far will be presented.

#### Biography

Mark A Zurbuchen is an Adjunct Professor in EE and MS&E in the prestigious DRL (Device Research Lab) under the WIN and CEGN Programs and additionally leads the "2D Materials" sub-group and is affiliated with the "Quantum Physics & Devices" sub-group as well. He is a thin film scientist. Electron and X-ray beam methods (XRD, TEM, synchrotron). Expertise in epitaxial films and heteroepitaxial integration. Materials design, thin film deposition, microstructural characterization, crystallography and electrical behavior. 2D materials, oxide electronics, ferroelectrics, dielectrics, multiferroics, superconductors, nano-scale thermal behavior and biomaterials.

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November 07-08, 2018 | Atlanta, USA



### *Dirk M Zajonc*

*La Jolla Institute for Allergy and Immunology, USA*

#### **Design of lipid and peptide antigens for immune cells using X-ray crystallography**

T cells are potent effector cells of the immune system that control infection and tumorigenesis but can also lead to autoimmunity when they respond too strongly to self-antigen. While the majority of T cells are specific to peptides presented by the Major Histocompatibility Complex I and II (MHC I and II) molecules, a small population of T cells respond to lipids when presented by the non-classical MHC I homolog CD1d. Extensive functional and structural data has been accumulated that allows for the design of altered glycolipid ligands that modulate immune responses toward infection and tumorigenesis. We further obtained novel insights into the unconventional presentation of peptides that allows us to design altered peptide ligands with novel functions. The structural basis and functional consequences of both lipid and peptide antigen recognition by the immune system will be discussed.

#### **Biography**

Dirk M Zajonc is an Associate Professor at La Jolla Institute for Allergy and Immunology. He is experienced Associate Professor in Structural Immunology with an interest in characterizing immune responses toward microbial pathogens. He is skilled in Protein Chemistry, including antibodies and recombinant protein production and characterization, molecular biology, biophysics and structural biology. He has strong interest in the interplay between microbial infection, as well as cancer with the immune system. He has published articles in various journals.

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#### **Notes:**