The 42nd Condensed Matter and Materials Meeting

Wagga Wagga, NSW
30th January – 2nd February 2018

Conference Handbook

Australian and New Zealand Institutes of Physics

42nd Annual Condensed Matter and Materials Meeting

Charles Sturt University, Wagga Wagga, NSW
30th January – 2nd February, 2018

CONFERENCE HANDBOOK

2018 Organising Committee

Chair: Jennifer MacLeod
Program Committee Chair: John Bell
Treasurer: Josh Lipton-Duffin
Committee members: Nunzio Motta
Soniya Yambem, Maksym Rybachuk (Griffith Uni)

School of Chemistry, Physics and Mechanical Engineering

Queensland University of Technology (QUT)

CONTENTS

Front Cover Image:

This scanning electron microscope (SEM) image shows a thin film of titanium on Si(100) at ~35000X magnification. This sample was prepared and imaged as part of PVB304, the undergraduate capstone physics unit offered at QUT.

Courtesy: Dr Jennifer MacLeod (Queensland University of Technology)

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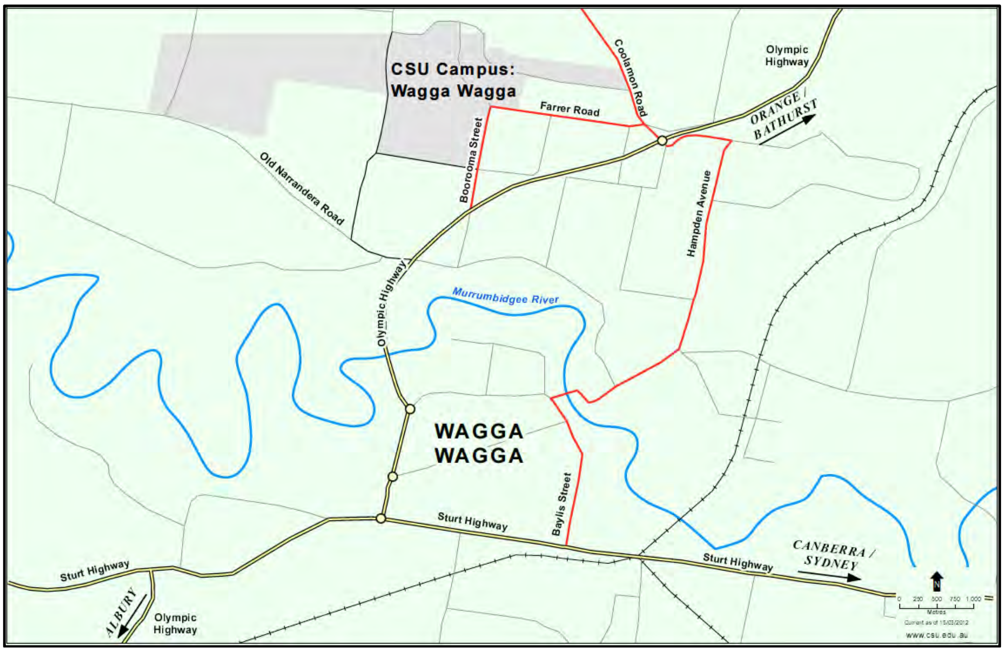
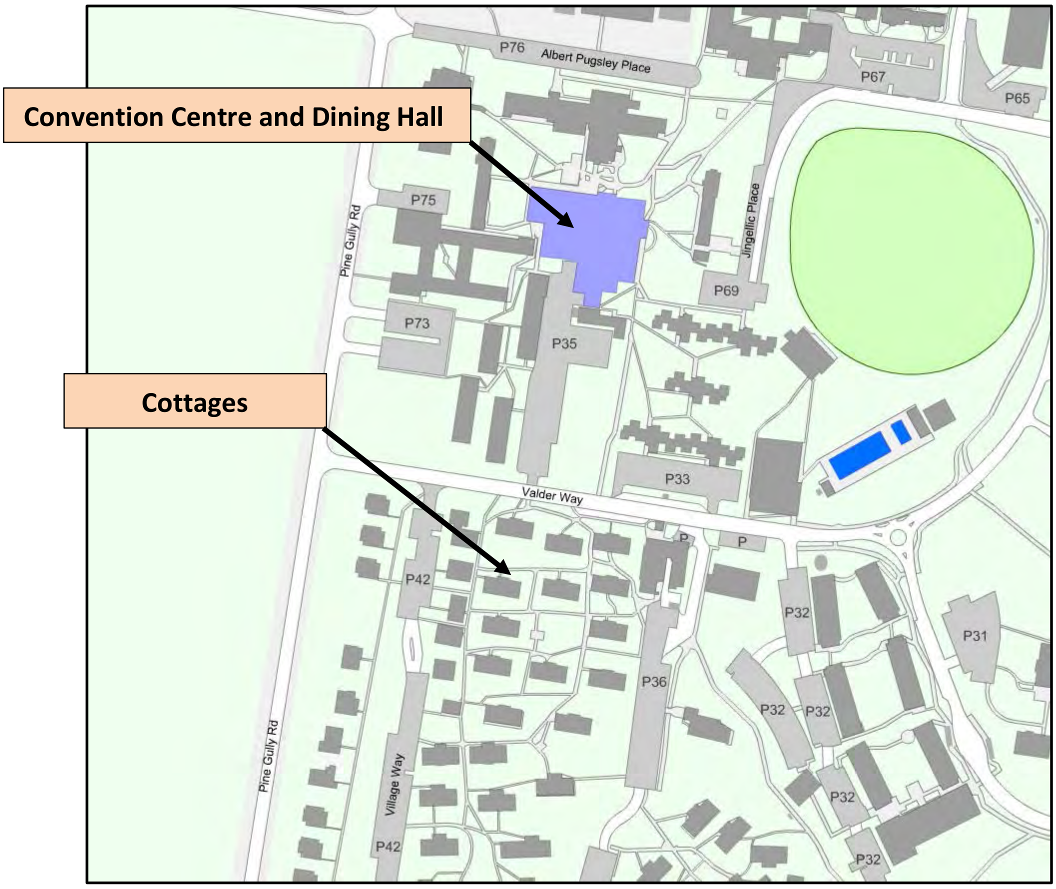
MAPS

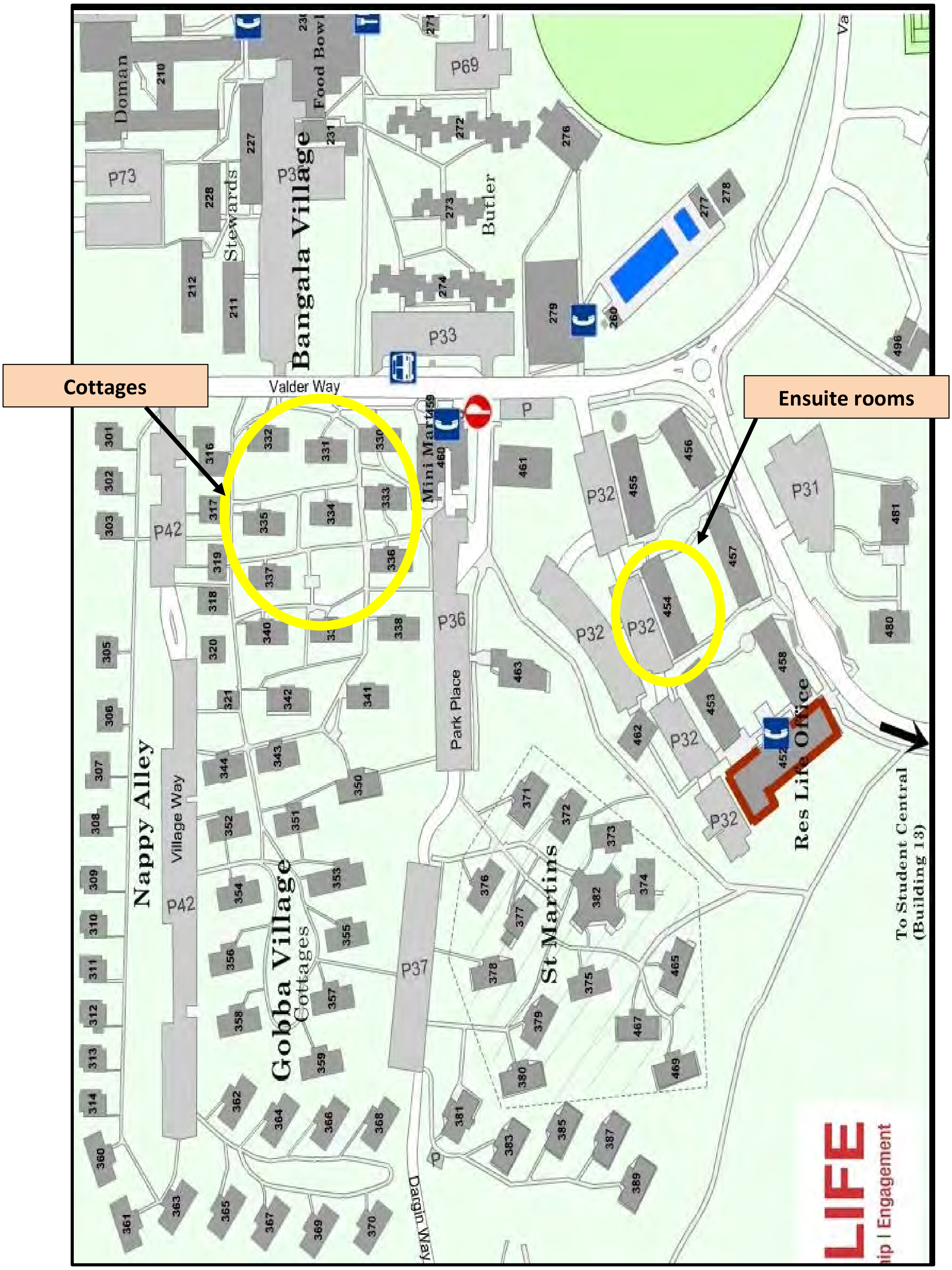
Wagga Wagga and the location of the Charles Sturt University campus



Location of Convention Centre and cottage accommodation



Detailed map of accommodation



THE CMM GROUP

Welcome to the “Wagga” community

Just by attending the annual Condensed Matter and Materials (CMM) Meeting you are a member of the CMM topical group of the Australian Institute of Physics (AIP). However, when you are renewing your AIP membership (or joining for the first time), please indicate your association with the CMM topical group by ticking the appropriate box. There are no additional forms or membership fees involved.

Take a look at the CMM Group web site

It can be accessed from the AIP national web site (www.aip.org.au) by clicking the drop-down tag “BRANCHES AND GROUPS” at the top of page and then selecting “CONDENSED MATTER AND MATERIALS (CMM)”.

Alternatively, you can go directly to http://cmm-group.com.au/

Take some time to glance through the images of participants and activities from previous meetings that can be found in the “Past Wagga Years, tributes” section of the site.

Please share your favourite “Wagga” experiences

If you have some special group images of you and colleagues, interesting events and stories from previous "Waggas", please share them with us by passing them on to Glen Stewart (g.stewart@adfa.edu.au) who will have them incorporated into the “Past Wagga Years, tributes” section of the CMM Group web site. Please include in your e-mail the year of the meeting and the names of those “Waggarites” you are able to identify in the images.

1978

2002

PHOTOS FROM WAGGA 2017

ATTENDEE INFORMATION

Scientific Program:

All poster sessions and lectures will be held at the Convention Centre. Chairpersons and speakers are asked to adhere closely to the schedule for the oral program. A PC laptop computer and data projector, overhead projector, pointer and microphone will be available. Please check that your presentation is compatible with the facilities provided as early as possible. Posters should be mounted as early as possible. Please remove your Wednesday session posters by early Thursday morning and your Thursday session posters by the close of the program on Friday.

Logistics:

Please wear your name tag at all times. Registration and all other administrative matters should be addressed to the registration desk or a committee member. For lost keys or if locked out of your room from 09:00 to 17:00, contact the Events Office for assistance 6933 4974; after hours, contact the Accommodation and Security Office near the corner of Valder Way and Park Way or phone them at 6933 2288. **Delegates must check out of their rooms on Friday morning before 10:00am.**

Meals, Refreshments and Recreational Facilities:

CSU is currently renovating the Convention Centre, which may cause some changes to the locations for Meeting events. Please pay attention to posted signs and announcements from the Meeting organisers.

All meals will be served in the "Food Bowl" dining room at Atkins Hall, except the Conference Dinner on Wednesday 31st January, which will be held in the Convention Centre. Your conference name tag will be required in order to obtain your meals from the Food Bowl.

Morning and afternoon tea will be served each day, as indicated in the timetable. Coffee and tea-making facilities are also available in the Common Room of each residence. In addition, on arrival on Tuesday afternoon and for the poster sessions, drinks will be available from the Conference Bar.

The swimming pool and the adjacent gymnasium and squash courts are available for the use of Meeting attendees. A wide range of facilities such as exercise bikes, table tennis and basketball are available in the gymnasium. Access to these facilities is covered by your registration fee. The pool opening hours are 11am to 9pm every week day and 11am to 6pm weekends. The gym is open 6am to 9pm every day.

CSU Contact Numbers:

Events Office Phone	(02) 6933 4974
Campus Security	1800 931 633

Wireless Internet:

Available onsite through eduroam.

EXHIBITORS

scitek

total vacuum solutions

www.scitek.com.au
Address: 4/12 Chaplin Dr, Lane Cove NSW 2066
Phone:(02) 9420 0477
Contact: Tobias Schappeler
Email: tobias@scitek.com.au

www.ezzivacuum.com.au
Address: 1 Dalmore Dr, Scoresby VIC 3179
Phone: 1800 463 994
Contact: Dr Adil Adamjee
Email: adil@ezzivacuum.com.au

ezzi vision

Vacuum & Thin Film Technology

www.ezzivision.com.au

http://vac.agency/
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c/o Australian Nuclear Technology Org.
Lucas Heights, NSW 2234
Phone: 61439130430
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VSA

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Tuesday 30-01-2018	Wednesday 31-01-2018		Thursday 01-02-2018		Friday 02-02-2018	
	07:30 Breakfast		07:30 Breakfast		07:30 Breakfast	
	08:45 Conference Opening		08:45 TM1 Julie Cairney	NANOMAT. CHARACTERISATION	08:45 FM1 Liangzhi Kou	QUANTUM SYSTEMS
	09:00 WM1 Gail Iles	MAGNETIC SYSTEMS I				
			09:15 TM2 Aldritt Madathiparambil		09:15 FM2 Tokuei Sako	
	09:30 WM2 Clemens Ulrich		09:30 TM3 Joseph Schuyt		09:30 FM3 Robin Guehne	
	09:45 WM3 Carlos Torres-Torres		09:45 TM4 Nitish Kumar		09:45 FM4 Dimi Culcer	
	10:00 WM4 Mary Clare Sison Escaño		10:00 TM5 Annalena Wolff		10:00 FM5 Sven Rogge	
	10:15 CONFERENCE PHOTO					
	10:30 Morning Tea		10:30 Morning Tea		10:30 Morning Tea	
	11:00 WN1 Raimundo Lora-Serrano	MAGNETIC SYSTEMS II	11:00 TN1 Agustin Schiffrin	SURFACE SCIENCE	11:00 FN1 Cathy Foley	SUPERCONDUCTIVITY
	11:30 WN2 Kirrily Rule		11:30 TN2 Jonathan Bradford		11:30 FN2 Antony Jones	
	11:45 WN3 Trevor Finlayson		11:45 TN3 Gunther Andersson		11:45 FN3 Ben Mallett	
	12:00 WN4 Wai Tung (Hal) Lee		12:00 TN4 Stephan Rachel		12:00 FN4 Sebastian Wolf	
	12:15 WN5 Julie Karel		12:15 TN5 Josh Lipton-Duffin		12:15 Awards and Closing	
	12:30 Lunch		12:30 Lunch		12:30 Lunch	
14:00 Registration	14:00 WA1 Nicola Gaston	EMERGING MATERIALS I	14:00 TA1 Dmitri Golberg	EMERGING MATERIALS 2		
	14:30 WA2 Chunmei Zhang		14:30 TA2 Iolanda Di Bernardo			
	14:45 WA3 Konstantin Firestein		14:45 TA3 Andriy Yakymovych			
	15:00 WA4 Madhav Prasad Ghimire		15:00 TA4 Joseph Fernando			
	15:15 WA5 Maryam Abyazisani		15:15 TA5 Thomas Raeber			
	15:30 WA6 Brenton Cook		15:00 TA6 Kimal Wasalathilake			
	15:45 WA8 Muhammed Azeem		15:45 TA7 Xi Shi			
16:00 Registration and Welcome Reception	16:00 Afternoon Tea and Poster Session 1 (WP)		16:00 Afternoon Tea and Poster Session 2 (TP)			
18.00 Dinner			18.00 Dinner			
	18:30 Conference Dinner After-Dinner Talk Cathy Foley 22:00					
19:30 Wine Tasting 21:00			19:30 Trivia Night Lindsay Davis Cup 22:00			

MAGNETIC SYSTEMS I

Session Chair: John Bell (Queensland University of Technology)

WM1 Wednesday, January 31 INVITED 9:00

Research projects at RMIT in Physics, Space and Beyond!
Gail N. Iles
Physics, School of Science, RMIT University, Melbourne, VIC 3000, Australia

WM2 Wednesday, January 31 9:30

Stability and Scaling Behavior of the Spin Cycloid in $BiFeO_3$ Thin Films
Clemens Ulrich
School of Physics, The University of New South Wales, Sydney, Australia

WM3 Wednesday, January 31 9:45

Optical Kerr Effect Exhibited by Platinum and Gold Nanoparticles Measured by Time-Resolved Self-Diffraction
C. Torres-Torres
Sección de Estudios de Posgrado e Investigación, Escuela Superior de Ingeniería Mecánica y Eléctrica Unidad Zacatenco, Instituto Politécnico Nacional, México, 07738, México

WM4 Wednesday, January 31 10:00

Magnetic Behavior of As-antisite Defect in Low-temperature GaAs from First-principles Bandstructure with Spin-orbit Interaction
M.C. S. Escaño
Department of Applied Physics, University of Fukui, 3-9-1 Bunkyo, Fukui 910 8507, Japan

Wednesday, January 31 10:15

CONFERENCE PHOTO

MAGNETIC SYSTEMS II

Session Chair: Garry McIntyre (ANSTO)

WN1 Wednesday, January 31 INVITED 11:00

On the physical properties of the magnetically frustrated system $BaTi_{1/2}Mn_{1/2}O_3$, a spin liquid candidate
R. Lora-Serrano
Univ. Fed. de Uberlândia, Instituto de Física, 38400-902, Uberlândia-MG, Brasil

WN2 Wednesday, January 31 11:30

Chemical disorder in a frustrated J_1/J_2 quantum spin chain material
K. C. Rule
Australian Nuclear Science and Technology Organisation, Locked bag 2001, Kirrawee DC, NSW 2232

WN3 Wednesday, January 31 11:45

Solitons and Martensitic Phase Transformations

T.R. Finlayson

School of Physics, University of Melbourne, Vic 3010, Australia

WN4 Wednesday, January 31 12:00

Polarised Neutrons for Material Science Research at ANSTO

W.T. Lee

Australian Centre for Neutron Scattering, Australian Nuclear Science and Technology Organisation, Lucas Heights, New South Wales 2234, Australia

WN5 Wednesday, January 31 12:15

Uncovering Berry: The Role of Topology in the Anomalous Hall Effect of Amorphous Ferromagnetic Fe-Si and Antiferromagnetic Mn3Ge

J. Karel

Department of Materials Science and Engineering, Monash University, Clayton, Victoria

EMERGING MATERIALS I

Session Chair: Iolanda Di Bernardo (University of Rome/ANU)

WA1 Wednesday, January 31 INVITED 14:00

Designing Superatomic Assemblies

Nicola Gaston

The MacDiarmid Institute for Advanced Materials and Nanotechnology, Department of Physics, the University of Auckland, Private Bag 92019, Auckland 1010 New Zealand

WA2 Wednesday, January 31 14:30

Computational Discovery and Design of Novel Dirac Materials

Chunmei Zhang

School of Chemistry, Physics and Mechanical Engineering, Queensland University of Technology, Gardens Point Campus, QLD 4001, Brisbane, Australia

WA3 Wednesday, January 31 14:45

Al based composite materials reinforced with BN, AlN and AlB_2

K.L. Firestein

School of Chemistry, Physics and Mechanical Engineering, Queensland Universityof Technology (QUT), Brisbane, Queensland 4000, Australia

WA4 Wednesday, January 31 15:00

Cleavage Energies of Layered Materials: $Bi_{14}Rh_3I_9$, Bi2TeI, β-Bi_4I_4 and 2H-MX_2

Madhav Prasad Ghimire

IFW Dresden e. V., Helmholtzstraße 20, D-01069 Dresden, Germany

CMPRC Butwal, Butwal-11, Rupandehi, Nepal

WA5 Wednesday, January 31 15:15

Growth of one-dimensional polymers through on-surface reactions
M. Abyazisani
School of Chemistry, Physics and Mechanical Engineering, Queensland University of Technology (QUT), Brisbane, Queensland 4000, Australia

WA6 Wednesday, January 31 15:30

The limit of superelasticity of glassy carbon following compression
B.A. Cook
School of Science, RMIT University, Melbourne, VIC, Australia

WA7 Wednesday, January 31 15:45

Direct energy gap in light rare earth nitrides: EuN and SmN
Muhammad Azeem
Department of Applied Physics and Astronomy, University of Sharjah, Sharjah 27272, United Arab Emirates

NANOMATERIALS CHARACTERIZATION

Session Chair: Dmitri Golberg (Queensland University of Technology)

TM1 Thursday, February 1 INVITED 8:45

Minerals at the atomic scale – new frontiers in atom probe tomography
J. M. Cairney
The Australian Centre for Microscopy and Microanalysis, The University of Sydney
New South Wales 2006 Australia

TM2 Thursday, February 1 9:15

Optically Stimulated Luminescence and 2-D Dosimetry using Fluoroperovskites
A.S. Madathiparambil
School of Chemical and Physical Sciences, Victoria University of Wellington, PO Box 600, Wellington 6140, New Zealand

TM3 Thursday, February 1 9:30

Fluoroperovskites as Radiation Dosimeter Materials
J.J. Schuyt
School of Physical and Chemical Sciences, Victoria University of Wellington, PO Box 600, Wellington 6140, New Zealand

TM4 Thursday, February 1 9:45

Defect Mechanisms in BaTiO3-Bi*M*O3 (*M* = metal) Ceramics
Nitish Kumar
Materials Science, Oregon State University, USA
Materials Science and Engineering, The University of New South Wales, Sydney, Australia

TM5 Thursday, February 1 INVITED 10:00

Ion Microscopy: From Ion Solid Interactions to Real World Applications
Annalena Wolff
Institute for Future Environments, Queensland University of Technology (QUT), Brisbane, Queensland 4000, Australia

SURFACE SCIENCE

Session Chair: Jennifer MacLeod (Queensland University of Technology)

TN1 Thursday, February 1 INVITED 11:00

On-Surface Synthesis of Trinuclear Coordination Nanostructures
A. Schiffrin
School of Physics & Astronomy, Monash University, Clayton, Victoria 3800, Australia
ARC Centre of Excellence in Future Low-Energy Electronics Technologies, Monash University, Clayton, Victoria 3800, Australia

TN2 Thursday, February 1 11:30

Lateral graphene/h-BN heterostructures from chemically converted epitaxial graphene on SiC (0001)
J. Bradford
School of Chemistry, Physics & Mechanical Engineering, Queensland University of Technology, Brisbane, Queensland 4000, Australia

TN3 Thursday, February 1 11:45

Electronic Structure of Titania Surfaces Modified by Au Clusters
G. G. Andersson
Flinders Centre for NanoScale Science and Technology, Flinders University, Australia

TN4 Thursday, February 1 12:00

Charge order in a frustrated two-dimensional atom lattice
Stephan Rachel
School of Physics, University of Melbourne, Parkville, Victoria, Australia

TN5 Thursday, February 1 12:15

The role of halogens in on-surface Ullmann polymerization
Josh Lipton-Duffin
Institute for Future Environments and School of Chemistry, Physics & Mechanical Engineering, Queensland University of Technology, Brisbane, Queensland 4000, Australia

EMERGING MATERIALS II

Session Chair: Julie Cairney (University of Sydney)

TA1 Thursday, February 1 INVITED 14:00

Boron Nitride Nanotubes, Nanoparticles and Nanosheets
D. Golberg
School of Chemistry, Physics and Mechanical Engineering, Queensland University of Technology (QUT), Brisbane, Queensland 4000, Australia

TA2 Thursday, February 1 14:30

NanoPorous Graphene: topology vs. doping effects
I. Di Bernardo
Physics Department, Spienza Università di Roma, Roma, Italy.
School of Chemistry, Physics and Mechanical Engineering, Queensland University of Technology (QUT), Brisbane, Queensland 4000, Australia

TA3 Thursday, February 1 14:45

Density and Molar Volume of AlCoCrCuFeNi high-entropy alloy family
A. Yakymovych
Department of Metal Physics, Ivan Franko National University of Lviv, Lviv 79005, Ukraine.
Department of Inorganic Chemistry – Functional Materials, Faculty of Chemistry, University of Vienna, Vienna 1090, Austria.

TA4 Thursday, February 1 15:00

Three Component Hybrid Nanostructures of Pt-Au-ZnO with Enhanced Photocatalytic Properties
J.F.S. Fernando
School of Chemistry, Physics and Mechanical Engineering, Queensland University of Technology (QUT), Brisbane, Queensland 4000, Australia

TA5 Thursday, February 1 15:15

Switching, transport and junction characteristics of an all-carbon memristor
T. J. Raeber
School of Science, RMIT University, GPO Box 2476V, VIC 3001, Melbourne, Australia

TA6 Thursday, February 1 15:30

Investigation of mechanical and electrical properties of 3D porous graphene hydrogels
K.C. Wasalathilake
School of Chemistry, Physics and Mechanical Engineering, Science and Engineering Faculty, Queensland University of Technology (QUT), Brisbane, Queensland 4000, Australia

TA7 Thursday, February 1 15:45

Fatigue Mechanisms in Lead-free BNT-BT-KNN Piezoceramics
Xi Shi
School of Science, Materials Science and Engineering, UNSW, Sydney, NSW 2052, Australia

QUANTUM SYSTEMS

Session Chair: Agustin Schiffrin (Monash University)

FM1 Friday, February 2 INVITED 8:45

Electronic-mechanical coupling in 2D Dirac materials
Liangzhi Kou
School of Chemistry, Physics and Mechanical Engineering, Queensland University of Technology (QUT), Brisbane, Queensland 4000, Australia

FM2 Friday, February 2 9:15

Angular electron correlation dynamics in two-dimensional quantum dots in strongly correlated and completely uncorrelated regimes
Tokuei Sako
Laboratory of Physics, College of Science and Technology, Nihon University,
7-24-1, Narashinodai, Funabashi, Chiba 274-8501, Japan.
Graduate School of Quantum Science and Technology, Nihon University

FM3 Friday, February 2 9:30

Extraordinary Magnetic Field Independent NMR Linewidths Observed in Bi_2Te_3 Topological Insulator Nanoparticles
R.Guehne
The MacDiarmid Institute for Advanced Materials and Nanotechnology, SCPS, Victoria University of Wellington, PO Box 600, Wellington 6140, New Zealand.
Robinson Research Institute, Victoria University of Wellington, PO Box 33436,
Lower Hutt 5046, New Zealand.
Felix Bloch Institute for Solid State Physics, University of Leipzig, Linnéstrasse 5,
04103 Leipzig, Germany

FM4 Friday, February 2 9:45

Quantum kinetic theory of magneto-transport in topological materials
Dimitrie Culcer
School of Physics and Australian Research Council Centre of Excellence in Future Low-Energy Electronics Technologies, UNSW Node,
The University of New South Wales, Sydney 2052, Australia

FM5 Friday, February 2 INVITED 10:00

Engineered quantum matter
S. Rogge
Centre for Quantum Computation and Communication Technology, School of Physics, The University of New South Wales, Sydney, New South Wales 2052, Australia

SUPERCONDUCTIVITY

Session Chair: Kirrily Rule (ANSTO)

FN1 Friday, February 2 INVITED 11:00

One HTS Josephson Junction - An Array of Applications: Has anything come from HTS devices in the last 32 years?

C.P. Foley
CSIRO Manufacturing, P.O. Box 218 Lindfield, NSW 2070, Australia

FN2 Friday, February 2 11:30

Manipulation of the critical current density in $YBa_2Cu_3O_7$ thin films by artificial defects

A. Jones
Institute for Superconducting and Electronic Materials, University of Wollongong, Northfields Avenue, Wollongong, NSW 2522, Australia.
CSIRO Manufacturing, 36 Bradfield Rd, Lindfield, Australia

FN3 Friday, February 2 11:45

Superconductor Sandwiches

B.P.P. Mallett
The Photon Factory, School of Chemistry and Department of Physics, The University of Auckland, Auckland, New Zealand.

FN4 Friday, February 2 12:00

Unconventional superconductivity in 2D systems from repulsive electron-electron interactions

Sebastian Wolf
School of Physics, University of Melbourne, Parkville, VIC 3010, Australia

WEDNESDAY POSTER SESSION

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WP01 Wednesday, January 31 16:00 – 18:00

Mössbauer and Magnetic Properties of Non-Stoichiometric Strontium M-type Hexaferrites Prepared by the Solid State Reaction Method
A. Septiani
School of Physical, Environmental and Mathematical Sciences, University of New South Wales, Canberra, 2600, Australia

WP02 Wednesday, January 31 16:00 – 18:00

In situ monochromator alignment on ANSTO's thermal spectrometer, TAIPAN
C. Sutton
Australian National University, Canberra, Australia
Australian Nuclear Science and Technology Organisation, Lucas Heights, NSW 2234 Australia

WP03 Wednesday, January 31 16:00 – 18:00

The magnetic structures of RTi_2Ga_4 (R= Er, Ho and Dy)
Hatem Saad
School of Physical, Environmental and Mathematical Sciences, The University of New South Wales, Canberra, ACT 2600

WP04 Wednesday, January 31 16:00 – 18:00

Investigation of the Magnetic and Crystal Field Excitations in the Orthorhombically Distorted Perovskites $TbVO_3$ and $CeVO_3$
J. O'Brien
School of Physics, University of New South Wales, Sydney NSW 2052, Australia

WP05 Wednesday, January 31 16:00 – 18:00

Recent upgrades to ANSTO's thermal neutron spectrometer, TAIPAN
K.C. Rule
Australian Nuclear Science and Technology Organisation, Lucas Heights, NSW 2234 Australia

WP06 Wednesday, January 31 16:00 – 18:00

Hot Isostatic Pressing of Ceramics, Glass and Glass-Ceramics for Immobilisation of Intermediate- and High-Level Nuclear Waste
E. R. Vance
ANSTOsynroc, Locked Bag 2001, Kirrawee DC, NSW 2232, Australia

WP07 Wednesday, January 31 16:00 – 18:00

Structural, Magnetic Phase Transitions and Magnetocaloric Effect in $Sm_{1-x}R_xMn_2Ge_2$
N. F. Makmor
School of Physical, Environmental and Mathematical Sciences, The University of New South Wales, Canberra, ACT 2600

WP08 Wednesday, January 31 16:00 – 18:00

Size-driven ferroelectrics in 2D pseudo-spin model
Se-Hun Kim
Faculty of Science Education and Educational Science Research Institute, Jeju National University, Jeju 63243, Korea

WP09 Wednesday, January 31 16:00 – 18:00

Magnetocaloric $Mn(Co_{1-x}Ni_x)Ge$ - Structural and magnetic transitions
Stewart J. Campbell
School of Physical, Environmental and Mathematical Sciences, UNSW Canberra at the Australian Defence Force Academy, ACT 2610

WP10 Wednesday, January 31 16:00 – 18:00

Determination of the Crystal Field Levels in TmV_2Al_20
W.D. Hutchison
School of Physical, Environmental and Mathematical Sciences, The University of New South Wales, Canberra, ACT, 2600, Australia

WP11 Wednesday, January 31 16:00 – 18:00

Investigation on the Nature of the Verwey Transition in Cu-doped Fe_3O_4
Y. Kareri
School of Physics, University of New South Wales, 2052 NSW, Australia.

WP12 Wednesday, January 31 16:00 – 18:00

Spin dynamics of quasi-one-dimensional spin-ladder system SrCa13Cu24O41 in the long-range magnetic ordering state
Guochu Deng
Australian Nuclear Science and Technology Organisation, New Illawarra Road, Lucas Heights NSW 2234, Australia

WP13 Wednesday, January 31 16:00 – 18:00

Magnetic Interplay of Mn and Yb Sites in $YbMn_2Si_2$ – Crystal Field and Electronic Structure Studies
Stewart J. Campbell
School of Physical, Environmental and Mathematical Sciences, UNSW Canberra at the Australian Defence Force Academy, Canberra, ACT 2610

WP14 Wednesday, January 31 16:00 – 18:00

The Cold-Neutron Triple-Axis Spectrometer SIKA at OPAL

Guochu Deng
Australian Nuclear Science and Technology Organisation, New Illawarra Road, Lucas Heights NSW 2234, Australia

WP15 Wednesday, January 31 16:00 – 18:00

New Sample Environment Projects and Developments at the Australian Centre for Neutron Scattering

N. Booth
Australian Nuclear Science and Technology Organisation, New Illawarra Road, Lucas Heights NSW 2234, Australia

THURSDAY POSTER SESSION

Sponsored by

TP01 Thursday, February 2 16:00 – 18:00

Structure changes in SAC 305 solder joints with nanosized Ni and Ni-Sn additions during the thermal treatment

A. Yakymovych

Department of Metal Physics, Ivan Franko National University of Lviv, Lviv 79005, Ukraine.
Department of Inorganic Chemistry – Functional Materials, Faculty of Chemistry, University of Vienna, Vienna 1090, Austria

TP02 Thursday, February 2 16:00 – 18:00

Reassessment of the Oxidation State of Iron in MORB Glasses
(Based on an Alternative Interpretation of Reference Mössbauer Spectra)

G.A. Stewart

School of PEMS, UNSW, ADFA, Canberra, Australia

TP03 Thursday, February 2 16:00 – 18:00

Effect of Na excess and cation disorder on voltage and capacity of NaxRuO3 as Na ion battery cathode

M.H.N. Assadi

Center for Computational Sciences, University of Tsukuba, Tennodai 1-1-1, Tsukuba, Ibaraki 305-8577, Japan

TP04 Thursday, February 2 16:00 – 18:00

Unravelling the Iron Coordination in the Mössbauer Spectra of SFCA

J.D. Cashion

School of, Physics and Astronomy, Monash University, Melbourne, Vic. 3800 Australia

TP05 Thursday, February 2 16:00 – 18:00

Strain mechanisms in lead-free piezoelectric BNT-BT under the influence of an applied electric field

Kai-Yang Lee

Institute for Applied Materials, Karlsruhe Institute of Technology, Karlsruhe, Germany

TP06 Thursday, February 2 16:00 – 18:00

Structure and dynamics in photovoltaic metal hydrides
K. Chea
College of Science, Engineering & Health, RMIT University, Melbourne, Australia.

TP07 Thursday, February 2 16:00 – 18:00

Investigating and tuning the pore structure of graphitic supercapacitor electrodes.
Michael Horn
School of Chemistry, Physics and Mechanical Engineering, Queensland University of Technology (QUT), Brisbane, Queensland 4000, Australia

TP08 Thursday, February 2 16:00 – 18:00

Quasi Free-Standing Graphene Growth on FIB-Patterned 3C-SiC Nanostructures
Mojtaba Amjadipour
School of Chemistry, Physics and Mechanical Engineering, Science and Engineering Faculty, Queensland University of Technology, QLD, Australia

TP09 Thursday, February 2 16:00 – 18:00

Synthesis and Characterization of Covalent Organic Frameworks as Thin Films
N. Turangan
School of Chemistry, Physics and Mechanical Engineering, Queensland University of Technology (QUT), Brisbane, Queensland 4000, Australia

TP10 Thursday, February 2 16:00 – 18:00

^{209}Bi NMR Study of Topological Insulator Bi_2Se_3 Single Crystals
R. Guehne
The MacDiarmid Institute for Advanced Materials and Nanotechnology, SCPS, Victoria University of Wellington, PO Box 600, Wellington 6140, New Zealand.
Robinson Research Institute, Victoria University of Wellington, PO Box 33436, Lower Hutt 5046, New Zealand.
Felix Bloch Institute for Solid State Physics, Leipzig University, Linnéstrasse 5, 04103 Leipzig, Germany.

TP11 Thursday, February 2 16:00 – 18:00

Mechanical Characterisation of Soft Tissue: Investigation of Tear Resistance of Multi-fibrous Soft Tissue
Satcha Foongkajornkiat
School of Chemistry, Physics, and Mechanical Engineering, Queensland University of Technology (QUT), Brisbane, Queensland 4000, Australia

ABSTRACTS
OF
ORAL PRESENTATIONS

Research projects at RMIT in Physics, Space and Beyond!

Gail N. Iles[a]

[a] *Physics, School of Science, RMIT University, Melbourne, VIC 3000, Australia*

The physics department at RMIT is home to five ARC centres of excellence in the fields of biophotonics, quantum computing, electronics, exciton science and artificial intelligence. The RMIT Microscopy and Microanalysis facility is a linked lab of the Australian Microscopy, and Microanalysis Facility. The School of Engineering hosts the MicroNano Research Facility and the Advanced Manufacturing Precinct with over 20 3D printers capable of both plastic and metal printing.

Emerging, cross-disciplinary research projects are as follows; a) construction of a nanoparticle device to investigate magnetic nanoparticle formation in simulated microgravity, b) manufacture of 3D magnetic devices for racetrack memory, c) investigation and manufacture of thin, lightweight materials for the protection of humans from radiation in lunar orbit and d) design, construction and launch of a microgravity experiment into space to investigate scientific phenomena and implement complex systems engineering principles.

Connections formed through teaching undergraduate physics and aerospace engineering students will lead to the formation of a research group skilled in implementing space projects and this will form the basis of the new ‘Physics with Space Science’ degree to be offered within the next three years at RMIT.

The state-of-the-art infrastructure at RMIT in engineering and physics will allow these projects to be realised and will engage students and staff across a number of disciplines.

Stability and Scaling Behavior of the Spin Cycloid in $BiFeO_3$ Thin Films

S. R. Burns[1], D. Sando[1], J. Bertinshaw[2], L. Russell[2], X. Xu[3,4], R. Maran[1], S. J. Callori[2,5], V. Ramesh[1], J. Cheung[1], S. A. Danilkin[5], G. Deng[5], W. T. Lee[5], S. Hu[1], L. Bellaiche[3,4], Jan Seidel[1], Nagarajan Valanoor[1] & Clemens Ulrich[2]

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[2]*School of Physics, The University of New South Wales, Sydney, Australia*
[3]*Department of Physics, University of Arkansas, Fayetteville, Arkansas 72701, USA*
[4]*Institute for Nanoscience and Engineering, University of Arkansas, Arkansas 72701, USA*
[5]*Australian Centre for Neutron Scattering, Australian Nuclear Science and Technology Organisation, Lucas Heights, New South Wales 2234, Australia*

Multiferroic materials demonstrate excellent potential for next-generation multifunctional devices, as they exhibit coexisting ferroelectric and magnetic orders. Bismuth ferrite ($BiFeO_3$) is a rare exemption where both order parameters exist far beyond room temperature, making it the ideal candidate for technological applications. To realize magnonic devices, a robust long-range spin cycloid with well-known direction is desired, since it is a prerequisite for the magnetoelectric coupling. Despite extensive investigation, the stabilization of a large-scale uniform spin cycloid in nanoscale (<300 nm) thin $BiFeO_3$ films has not been accomplished. Using neutron diffraction we were able to demonstrate cycloidal spin order in 100 nm $BiFeO_3$ thin films which became stable through the careful choice of crystallographic orientation and control of the electrostatic and strain boundary conditions during growth [1]. Furthermore, Co-doping, which has demonstrated to further stabilize the spin cycloid, did allow us to obtain spin cycloid order in films of just 50 nm thickness, i.e. films thinner than the cycloidal length of about 64 nm. Interestingly, in thin films the propagation direction of the spin cycloid has changed and shows a peculiar scaling behavior for thinnest films. We were able to support these observations by Monte Carlo theory based on a first-principles effective Hamiltonian method. Our results therefore offer new avenues for fundamental research and technical applications that exploit the spin cycloid in spintronic or magnonic devices.

[1] J. Bertinshaw, *et al.*, Nature Com. **7**, 12664 (2016).

Optical Kerr Effect Exhibited by Platinum and Gold Nanoparticles Measured by Time-Resolved Self-Diffraction

C. Torres-Torres[a], J. Bornacelli[b], R. Rangel-Rojo[c] and A. Oliver[b]

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[c] *Depto. de Óptica, Centro de Investigación Científica y de Educación Superior de Ensenada A.P. 360, Ensenada, B.C., 22860, México.*

The impact of plasmonic phenomena in quantum and all-optical applications has been importantly empowered by nonlinear optical properties at the nanoscale. Ultrafast nonlinear optical parameters exhibited by metallic nanoparticles are able to modulate phase and irradiance conditions related to nanophotonic signals [1]; besides, single-photon devices based on sharp selective energy transfer processes can be derived from Surface Plasmon Resonance interactions in low-dimensional systems [2]. The main result presented in this work concerns to the temporal dynamics exhibited by polarization-selectable third-order nonlinear optical effects in gold and platinum nanoparticles. The first-order of diffraction generated by a degenerated two-wave mixing was numerically and experimentally analyzed to identify the physical mechanism responsible for an induced birefringence in the samples. Comparative nanocomposites were separately nucleated by using gold and platinum ion-implantation in silica plates. The advantages of different resonant behavior of the nanostructures, together to the possibility for controlling multi-photonic signals by pico- and femto-second pulses were highlighted. The authors kindly acknowledge the financial support from IPN, CICESE, DGAPA-UNAM IN108217 and CONACyT through grants 222485 and CB-2015-251201.

[1] C. Torres-Torres, L. Tamayo-Rivera, R. Rangel-Rojo, R. Torres-Martínez, H. G. Silva-Pereyra, J. A. Reyes-Esqueda, L. Rodríguez-Fernández, A. Crespo-Sosa, J. C. Cheang-Wong and A. Oliver, *Nanotechnology* **22(35)**, 355710 (2011).

[2] J. Bornacelli, C. Torres-Torres, H. G. Silva-Pereyra, L. Rodríguez-Fernández, M. Avalos-Borja, J. C. Cheang-Wong and A. Oliver, *Methods Appl. Fluoresc.*, **5**, 025001 (2017).

Magnetic Behavior of As-antisite Defect in Low-temperature GaAs from First-principles Bandstructure with Spin-orbit Interaction

M.C. S. Escaño[a], Y. Osanai[b] and M. Tani[b]
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[b] *Research Center for Development of Far-Infrared Region, University of Fukui, 3-9-1 Bunkyo, Fukui 910-8507, Japan.*

Study of defect's nature in wide-gap semiconductor such as GaAs can give light into its use as THz detector/emitter. In low-temperature GaAs (LT-GaAs), a two-step photon absorption via mid-gap states is proposed to explain the LT-GaAs-based photoconductive antenna's detection of THz radiation when probed with 1.55μm probe laser [1]. So far, within first-principles, the defect's magnetic and electronic properties using realistic defect concentration (1.0-1.3%) and within the broken-inversion symmetry of GaAs is still lacking. Here, density functional theory (DFT) calculations on a 216-atom GaAs bulk using hybrid exchange correlation functionals are conducted. The symmetry is accounted for by including spin-orbit (SO) interaction via projector augmented wave method [2]. We found that at the level of DFT+SO, a 1.46eV band-gap and 0.337eV split-off band at Γ are obtained in agreement with resonant Raman scattering (1.43eV, 0.341eV) [3]. Among the defects tested: As-antisite (As_{Ga}), Ga-antisite (Ga_{As}) and Ga-vacancy (Ga_{vac}), only the As_{Ga} leads to a mid-gap state. Spin-resolved bandstructure of the GaAs with As_{Ga}, reveals a paramagnetic nature of the defect, in agreement with electron spin resonance studies. The non-split behavior of the mid-gap state is due to induced tetrahedral symmetry when a Ga atom is replaced by As. Also, the state arises from localized charge density within the As tetrahedra and not solely on As_{Ga}, as commonly thought.

[1] M. Tani, K.S. Lee and X. C. Zhang, *Appl. Phys. Lett.*, **77**, 1396 (2000).
[2] M.C Escaño, H. Kasai, M. Tani, *J. Vac. Soc. Jpn.* (in press).
[3] P. Kusch, S. Breuer, M. Ramsteiner, L. Geelhaar, H. Reichert, and S. Reich, *Phys. Rev. B.* **86**, 075317 (2012).

On the physical properties of the magnetically frustrated system $BaTi_{1/2}Mn_{1/2}O_3$, a spin liquid candidate.

F. A. Garcia[a], R. Lora-Serrano[b], M.R. Cantarino[a], R. P. Amaral[b], E. C. Andrade[c], S. Brauninger[d], R. Sarkar[d], H. Luetkens[e], C. Baines[e].

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Important examples of materials hosting a ground state determined by dimensionality are the spin dimers forming valence bound solid (VBS). For some materials, site occupancy disorder and/or defects will lead to the appearance of *orphan* spins. The latter can be diluted in the lattice, and usually interact by means of an effective exchange much lower than the first neighbors' interaction. At sufficient low temperatures (T), this interaction, however small, may lead to the formation of a spin liquid (SL) state, which will present many unusual magnetic properties [1]. In this ongoing research, we explore the magnetism of the disordered double perovskite $BaTi_{1/2}Mn_{1/2}O_3$ (BMTO), which we have presented as a magnetically frustrated system where magnetic Mn^{4+} dimers, trimers and orphan spins coexist and create different energy scales of correlations [2]. This scenario is supported by macro- and microscopic structural and magnetic data in a large T interval ($0.5\ K \leq T \leq 1000\ K$). No long-range order is observed down to 0.2 K, though $\theta_{CW}<0$ suggest antiferromagnetic correlations. Recent low T heat capacity, magnetization under applied magnetic fields ($T = 0.2$ K, $H = 9$ T), and µSR data strongly suggest evidence that BMTO is a suitable candidate to host a SL ground state [3]. I will present the BMTO system, our main results and discuss some aspects of the challenging Physics involved.

[1] L. Balents, *Nature* **464**, 199 (2010).
[2] F. A. Garcia *et al*., *Phys. Rev. B* **91**, 224416 (2015).
[3] M.R. Cantarino *et al*. In preparation.

Chemical disorder in a frustrated J_1/J_2 quantum spin chain material

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[b] *School Of Physics, Northfields Ave, University of Wollongong, NSW, 2522*

Recently a new one-dimensional (1D) quantum spin chain system has been synthesised: catena-dichloro(2-Cl-3Mpy)copper(II), [where 2-Cl-3Mpy=2-chloro-3-methylpyridine]. We shall refer to this compound as **cd-Cu**. Preliminary calculations and bulk magnetic property measurements indicate that this system does not undergo magnetic ordering down to 1.8K and is a prime candidate for investigating frustration in a J_1/J_2 system (where the nearest neighbour interactions, J_1, are ferromagnetic and the next nearest neighbour interactions, J_2, are antiferromagnetic) [1]. Calculations predicted 3 possible magnetic interaction strengths for J_1 below 6meV depending on the orientation of the ligand [2]. For one of the predicted J_1values, the existence of a quantum critical point is implied.

A deuterated sample of **cd-Cu** was produced at the National Deuteration Facility and the excitations measured using the PELICAN TOF spectrometer. Scattering was weak from this sample, but indicated the most likely scenario involves an average of the 3 possible magnetic excitations in this material, rather than the random array of exchange interactions as predicted by Herringer et al., [2]. This may indicate the possibility of tuning the chemical structure to favour a system which may exhibit a quantum critical point.

[1] T. Hamada et al., J. Phys Soc. Jpn, **57** 1891-1894 (1988); T. Hamada et al., **58** 3869 (1989);
[2] S.N. Herringer et al., Chem Eur J. **20**, 8355-8362 (2014)

Solitons and Martensitic Phase Transformations

T.R. Finlayson[a] and A. Saxena[b]

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[b] *Los Alamos National Laboratory, Los Alamos, NM 87545, U.S.A.*

A model for the dynamical behaviour of coherent interfaces and modulated structures based on topological solitons was introduced by Barsch and Krumhansl (B&K) and applied to the twins accompanying martensitic transformations [1]. For wave propagation in the principal symmetry directions in a cubic crystal, B&K obtained the phonon dispersion relations

$$\rho_0\omega_\lambda^2(\mathbf{k}) = c_\lambda(\hat{\mathbf{k}})\mathbf{k}^2 + d_\lambda(\hat{\mathbf{k}})\mathbf{k}^4 \tag{1}$$

where $c_\lambda(\hat{\mathbf{k}})$ are the second-order elastic constants associated with mode λ and propagation direction, $\hat{\mathbf{k}} = \mathbf{k}/k$. The $d_\lambda(\hat{\mathbf{k}})$ are linear combinations of strain gradient coefficients. B&K further showed [1] that for a wave vector along a high symmetry direction, it was more instructive to consider the truncated series

$$\rho_0\omega_\lambda^2(\mathbf{k}) = A_\lambda(\hat{\mathbf{k}})[\sin(\pi\zeta/2)]^2 + B_\lambda(\hat{\mathbf{k}})[\sin(\pi\zeta/2)]^4 \tag{2}$$

Here ζ is the wave vector in reciprocal lattice units, $A_\lambda(\hat{\mathbf{k}})$ is proportional to $d_\lambda(\hat{\mathbf{k}})$ and $B_\lambda(\hat{\mathbf{k}})$ is a linear combination of $c_\lambda(\hat{\mathbf{k}})$ and $d_\lambda(\hat{\mathbf{k}})$. Phonon dispersion data available at the time [2], were used to illustrate the soliton model. Based on Equation (2), an analysis of the phonon frequencies, ν, for the $[\zeta\zeta0][\zeta\bar{\zeta}0]$ branch, via $[\nu/\sin(\pi\zeta/2)]^2$ versus $[\sin(\pi\zeta/2)]^2$, resulted in two, straight-line sections, the slopes of which are related to the strain-gradient coefficient and the intercept corresponded to the ultrasonic velocity for a crystal of similar composition [3]. Similar analyses more recently using $[\zeta\zeta0][\zeta\bar{\zeta}0]$ data sets from several In-Tl crystals of different compositions, show very similar behaviour. A discussion of the B&K soliton model will be presented and an interpretation of the results found for In-Tl crystals will be suggested.

[1] G.R. Barsch and J.A. Krumhansl, *Proc. Int. Conf. on Martensitic Transformations (1992)*, eds. C.M. Wayman and J. Perkins (Monterey Inst. of Adv. Studies, 1993) p 53.

[2] T.R. Finlayson, M. Mostoller, W. Reichardt and H.G. Smith, *Solid State Commun.* **53**, 461 (1985).

[3] D.J. Gunton and G.A. Saunders, *Solid State Commun.* **14**, 865 (1974).

Polarised Neutrons for Material Science Research at ANSTO

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[a] *Australian Centre for Neutron Scattering, Australian Nuclear Science and Technology Organisation, Lucas Heights, New South Wales 2234, Australia.*

Polarised neutron scattering can definitively identify magnetic structures and dynamics, and separate the structural signal and the spin-incoherent scattering in hydrogen-rich materials. At ANSTO, our project to incorporate this capability to a wide suit of instruments is coming to fruition. User research experiments using polarised neutrons have recently been carried out to study multiferroic and magnetostrictive materials on the TAIPAN thermal triple-axis spectrometer and WOMBAT high-intensity diffractometer, and from an earlier time, magnetic multilayers on the PLATYPUS reflectometer. One of the first round of user research has been published. We have now also completed the deployment and test on the PELICAN cold neutron chopper spectrometer, QUOKKA SANS instrument and SIKA cold triple-axis spectrometer. Condensed matter research experiments will be carried out on those three instruments in the first half of 2018. The ECHIDNA high-resolution diffractometer is the next instrument to acquire this capability. Our development focus is now on providing user support to plan experiment, reduce data and analyse data: Rather than a surveying technique, a polarised neutron experiment is often done in the regions of interest identified using unpolarised neutron measurements. The type of polarizer and analyser (often polarised Helium-3 based) would affect what and how the measurements will be done. And polarised neutron data reduction and analysis would add a level of complexity to the process. This presentation will provide an overview of the capabilities available, some of the experiments that had been carried out to illustrate how material research can utilize polarised neutrons and the key factors to consider in planning an experiment and reducing the data.

Uncovering Berry: The Role of Topology in the Anomalous Hall Effect of Amorphous Ferromagnetic Fe-Si and Antiferromagnetic Mn_3Ge

J. Karel[a], A.K. Nayak[b], J. E. Fischer[b], B. Yan[b], J. Kübler[b], S.D. Bouma[c], C. Bordel[c], C. Felser[b] and F. Hellman[c]

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[b] *Max Planck Institute for Chemical Physics of Solids, Dresden, Germany*
[c] *Physics Department, University of California Berkeley, Berkeley, California*

The consideration of topology has recently led to the emergence of new exotic physics. Since its discovery, the Berry phase has helped explain diverse phenomena in condensed matter physics, with perhaps one of the most important breakthroughs being the reinterpretation of the intrinsic contribution to the anomalous Hall effect (AHE) in ferromagnets in terms of a Berry phase curvature in momentum space. Recent theoretical predictions have further suggested that the Berry phase can also give rise to an AHE in antiferromagnets with non-collinear spin structures. [1]

This talk will examine the role of the Berry phase on the AHE in both amorphous ferromagnets and noncolinear antiferromagnets. It will be shown that the anomalous Hall conductivity (σ_{xy}), when suitably normalized by magnetization and number of charge carriers, is independent of the longitudinal conductivity in a series of amorphous Fe-Si thin films. This observation suggests a primary dependence on an intrinsic mechanism, which is remarkable because it indicates a local atomic level description of a Berry phase, resulting in an intrinsic AHE in a system that lacks lattice periodicity. [2] The second part of the talk will discuss the emergence of the AHE in the noncolinear antiferromagnet, Mn_3Ge. The AHE in ferromagnets generally scales with the magnetization, meaning that an antiferromagnet with no net magnetization should not exhibit an AHE. It will be shown that not only does Mn_3Ge exhibit an AHE but one that is comparable to that of ferromagnetic metals. Theoretical calculations will demonstrate that this effect originates from a non-vanishing Berry curvature, arising from the chiral spin structure. [3]

[1] Chen *et al.*, *Phys. Rev. Lett.* **112**, 017205 (2014).
[2] Karel *et al.*, *Europhys. Lett.* **114,** 57004 (2016).
[3] Nayak *et al.*, *Science Advances* **2,** e1501870 (2016).

Designing Superatomic Assemblies

Nicola Gaston

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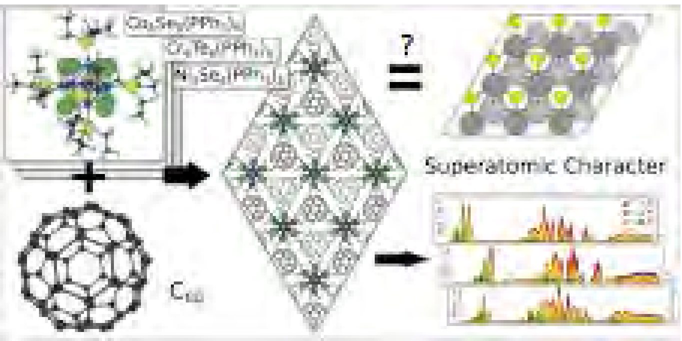
Inspired by recent progress in the synthesis of cluster assembled solids, and the theoretical description of globally delocalized electronic structure of nanoscale building blocks – superatoms – we address the question to what extent the three new materials $[Co_6Se_8(PEt_3)_6][C_{60}]_2$, $[Cr_6Te_8(PEt_3)_6][C_{60}]_2$, and $[Ni_9Te_6(PEt_3)_8]C_{60}$, upon forming bulk compounds, imitate atomic analogues.

The concept of superatoms for describing atom-imitating clusters is very intriguing since it allows chemists to apply chemical intuition – a useful tool for predicting new materials – when it comes to inter-cluster reactions. Thus, we systematically study the lattice structure, the intercluster binding, and the electronic structure by density functional theory and assess their superatomic features. We show that collective properties emerge upon bulk formation, which promotes arguments for the formation of solids in which the constituent clusters have a superatomic character, allowing for solid-state concepts to become relevant.

Finally, we present principles for the design of novel assemblies created from tunable superatoms [1] and methods for the prediction of their electronic properties [2]. We also propose an extension of the superatomic concept to include tunable transition metal clusters, which have long been neglected but which allow for the incorporation of tunable magnetic states [3].



[1] J. Schacht & N. Gaston. Chem. Phys. Chem. **17**, 3237 (2016).
[2] L. Hammerschmidt, J. Schacht, & N. Gaston. Phys. Chem. Chem. Phys. **18**, 32541 (2016).
[3] J. T. A. Gilmour, L. Hammerschmidt, J. Schacht, & N. Gaston. J. Chem Phys. **147** (15), 154307 (2017).

Two-dimensional C_3B/C_3N Van der Waals Heterostructure: Built-in Electric Field, Band Opening/Inversion and Enhanced Photocurrent Production by Strong Electron Coupling

Chunmei Zhang[1], Yalong Jiao[1], Tianwei He[1], Steven Bottle[1], Thomas Frauenheim[2] and Aijun Du[1,]*

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Two-dimensional (2D) van der Waals (vdW) heterostructures (HTS) allow the combination of properties from a variety of 2D materials and represent the fundamental platform for important solid-state device fabrication. However, the interlayer electron coupling is often governed by relatively weak long-range vdW interactions, thereby limiting practical applications. Herein, based on density functional theory, we demonstrate that an effective electron coupling can be created in 2D C_3B/C_3N vdW HTS. Monolayer C_3B and C_3N, which have been fabricated in recent experiments, are p- and n-typed doped large gap semiconductors, respectively. However, the formed vdW HTS exhibits novel Dirac fermion as presented in this work. Additionally, a large interlayer built-in electric field is generated in this HTS, leading to an intrinsic band inversion between p_z orbital of B and N atoms. A simple tight-binding model with the nonzero interlayer hopping parameters is constructed and can well reproduce the electronic band structure. Compared to isolated C_3B and C_3N, the 2D C_3B/C_3N vdW HTS is very optically active with enhanced photocurrent production and displays broadened absorbance spectrum from the near infrared to the ultraviolet region. Our results demonstrate the importance of electron coupling in the modulation of materials properties of 2D vdW HTS and suggest a practical strategy to realize a strong electron coupling toward the realistic applications in nanoelectronics and photonics.

Al based composite materials reinforced with BN, AlN and AlB2

K.L. Firestein[a], A. E. Steinman[b], S. Corthay[b], A.M. Kovalskii[b], A.T. Matveev[b],
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For many years metal matrix composites (MMC) continue to attract interest in both scientific and industrial fields. The combined effect of a ductile metallic matrix and a strong reinforcing phase allows for achievement of properties unreachable for traditional alloys. In our previous works [1, 2] we showed that utilization of BN nano- and microparticles as reinforcing phase in Al-based composite materials resulted in significant increase of material strength. In work [2] powder mixtures were obtained using ball milling technique, which led to formation of additional phases on the Al – BN interphase: AlB2 and AlN. The aim of the present work is to investigate the specific influence of AlN, AlB2 and BN nanophases and their combination on the mechanical properties of the final Al-MMCs.

The composites were fabricated by combination of high-energy ball milling and spark plasma sintering techniques. To form desired reinforcing phases in-situ during ball milling, powders of Al, BN, B and Li3N were used as source materials. The structures of powder mixtures and composite materials were studied by scanning and transmission electron microscopy. The influence of reinforcing phase content (1, 3, 5, and 7 wt%) on the tensile strength was investigated. In addition, the tensile tests at 500 °C were performed. X-ray and EDX analysis demonstrated that B and Li3N particles react with Al with formation of AlB2 and AlN during high-energy ball milling and sintering processes.

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Cleavage Energies of Layered Materials: $Bi_{14}Rh_3I_9$, Bi_2TeI, β-Bi_4I_4 and 2H-MX_2

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In recent years weakly bonded layered systems have become important for the manufacturing of two-dimensional materials. Precise knowledge of the interlayer bonding allows to understand in detail the exfoliation process in these compounds. Cleavage energies are crucial in this respect. Here we report the cleavage energies and electronic properties of the weak topological insulators (TIs) $Bi_{14}Rh_3I_9$, Bi_2TeI and β-Bi_4I_4, as well as of 2H-transition metal dichalcogenides (MX_2 where M=Mo, W and X=S, Se, Te) determined by means of density functional theory calculations. Our calculations reproduce the experimentally measured value of cleavage energy of graphite, E_c (graphite) = 0.37 Jm^{-2} [1], which we use as a benchmark. Based on this, we calculate the cleavage energies of the three weak TIs and 2H-MX_2 systems. We find that all energies are smaller than 2×E_c of graphite. The obtained values suggest the possibility of exfoliation of individual layers in these materials.

MPG thanks the Alexander von Humboldt Foundation for financial support through HERMES program.

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Growth of one-dimensional polymers through on-surface reactions

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We present an investigation of the surface-confined growth of one-dimensional (1D) covalently interlinked polymers on metal surfaces formed through decarboxylative coupling of isophthalic acid (IPA) and 3,5 pyridinedicarboxylic acid (PDC). The reactions were studied by x-ray photoemission spectroscopy (XPS).

Recently, Gao *et al.*[1] reported successful decarboxylative coupling facilitated via a three-step process. A schematic overview of the reaction pathway for IPA is shown in Fig.1.

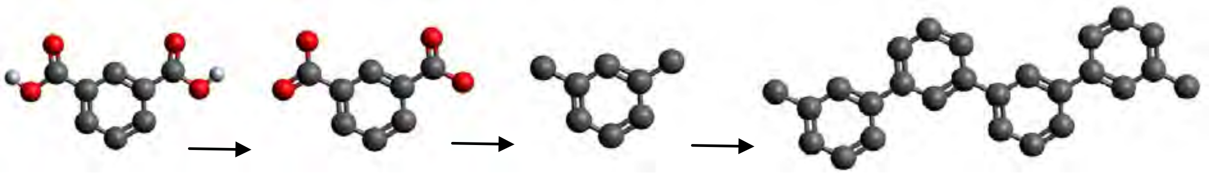

Figure 1.Schematic overview of the expected chemistry. The arrows indicate annealing, and each step should occur at a higher temperature than the previous one.

IPA and PDC were deposited on Cu (111) followed by annealing a range of temperatures up to 300 °C, and the reactions were studied by XPS. The molecular structure can be inferred from the evolution of the C1s core level, where the signatures of dehydrogenation and decarboxylation are clearly evident [2]. XPS showed deprotonation and decarboxylation are completed upon annealing at 230° C and 270° C, respectively. The decarboxylation approach can be applied to many other carboxyl-terminated molecules to produce tailored 1D and 2D polymers with broad potential in nanotechnology. Such systems might be of central importance to develop future electronic and optoelectronic devices with high quality active materials, besides representing model systems for basic science investigations.

Acknowledgements

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The limit of superelasticity of glassy carbon following compression

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Glassy carbon (GC) is a predominately sp^2 bonded disordered carbon material which is temperature resistant up to ~3000°C making it a non-graphitizing carbon and is superelastic meaning that it retains its original structure following compression [1]. The pressure limits for these properties are not known. In this study, the structural changes in GC after compression in a diamond anvil cell at room temperature are investigated. Figure 1(a) shows a transmission electron microscopy (TEM) image of uncompressed GC showing its tangled graphitic microstructure (red circle). Also shown is a selected area diffraction pattern (SADP) (inset) which can be indexed to graphite. Figure 1(b) shows an image of a GC sample recovered after compression to 45 GPa. The tangled graphitic microstructure of GC has clearly changed with the SADP (inset) showing strong permanent orientation of graphitic layers as indicated by the strong {002} arcs oriented parallel to the high stress direction. These TEM results along with measurements obtained from Raman spectroscopy reveal that the threshold for permanent structural change in GC occurs at ~40 GPa. We propose that this pressure also represents the limit to the non-graphitizing and superelastic properties of GC.

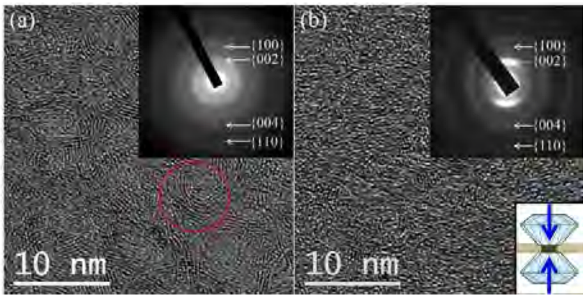

Figure 1. TEM images and SADPs (indexed to graphite) of (a) uncompressed GC and (b) GC following compression to 45 GPa. The compression direction is shown by arrows.

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Direct energy gap in light rare earth nitrides: EuN and SmN.

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Due to their proximity in the periodic table, the light rare earth metals, samarium and europium, are of particular interest because of their antiparallel L and S moments according to Hund's rule. On the optical energy gaps, there are a few reports for SmN and EuN. The energy gap as obtained from X-ray absorption and emission (XAS/XES) Spectra[1] of SmN thin films is 1.5 eV, noticeably larger than the 0.70 eV of bulk SmN crystals.[2] The theoretically estimated direct gap at the X point is 0.81 eV and an indirect gap at Γ-X is 0.48 eV when T>TC [2]. Similarly for EuN, experimental values of Eg = 0.76 eV and 0.90 eV are appreciably different from the theoretical value of 1.20 eV.

The direct energy gap for SmN and EuN is determined for the first time by transmittance and reflectance spectra for polycrystalline thin films at room temperature. SmN shows a direct optical energy gap at 1.2±0.05 eV and for EuN the energy gap value is 0.90±0.05 eV. Both samples show large effects due to free carriers in the subgap region. The fundamental absorption edge for SmN coincides with that of DyN indicating that both materials have similar electronic structure. For the case of EuN, a QSGW band structure calculation engineered to the experimentally determined energy gap value predicts a semiconducting ground state for EuN.

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Minerals at the atomic scale – new frontiers in atom probe tomography

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Atom probe tomography is a powerful microscopy technique that provides beautiful three-dimensional ‘maps’ that show the position and elemental species of tens of millions of atoms in a given volume within a material, with a resolution on par with the most advanced electron microscopes. It has seen widespread use for the characterisation of bulk metals and alloys, but new developments in specimen preparation and the use of lasers to enable the study of less conducting materials have now made it applicable to the study of a much wider range of material types.

Our atom probe techniques, originally driven by the needs of researchers investigating structural materials, has proven useful in other disciplines. This presentation will include recent work with geoscientists that provides information to more accurately date zircon, i.e., to determine the age of rocks. Atom probe data, reveals that the lead (Pb) used to date the mineral can diffuse through regions of the rocks that have experienced deformation events [1]. This information is essential for accurate geochronological dating, showing that measurements from deformed areas of zircon are not as robust as previously thought.

The presentation will also cover work undertaken in collaboration with dental researchers to provide the first-ever atom maps from human dental enamel, the decay of which affects 60-90% of children and nearly 100% of adults worldwide. The results provided the first direct evidence for the presence of a proposed amorphous Mg-rich calcium phosphate phase that plays an essential role in governing the properties of teeth [2]. The impact of these findings are expected to be wide-reaching: Treatments to avoid decay will be designed to protect against the dissolution of this specific amorphous phase, mechanical models will incorporate the true properties of the binding phase and research into methods to remineralise teeth will be able to incorporate a better understanding of how enamel forms.

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Optically Stimulated Luminescence and 2-D Dosimetry using Fluoroperovskites

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There is a need for development of new dosimeter materials for applications like radiotherapy and 2-D imaging for medical diagnostics. This can be achieved by using tissue equivalent $NaMgF_3$ that is known to exhibit optically stimulated luminescence (OSL) when doped with Eu and Mn [1,2]. Hence they have the potential to be developed as a suitable material for 2 D imaging in radiotherapy and medical diagnostics.

In this work, we present the OSL and dose characterization of Mn doped $NaMgF_3$ and X-ray imaging of 2D dosimetric plates of Eu doped $NaMgF_3$ using a CCD camera. OSL is observed from different percentages of Mn doped $NaMgF_3$ by exciting at 397 nm. The dose response is observed to be linear for lower dose ranges. Films of Eu doped $NaMgF_3$ are prepared by grinding them and formulating a paint which are coated on to Perspex sheets. X-ray imaging of the films are made after exposing them to different doses of x-ray by using the CCD camera. The stimulation is by using an ultrabright blue LED with a peak wavelength of 465 nm which is in the range of wavelengths that stimulate OSL from the active material of the imaging plates. The resolution of the imaging plates are measured by using a standard test grid of lead lines of varying spatial frequency and the sensitivity and inhomogeneities of the films are also studied. Thus, it establishes the possibility to use Mn doped $NaMgF_3$ as an OSL dosimeter in the linear range of the dose response and demonstrates the potential of Eu doped $NaMgF_3$ films to be developed as a 2D dosimeter.

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Fluoroperovskites as Radiation Dosimeter Materials

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There is a need for new radiation dosimeter materials, particularly in the field of radiotherapy. Fluoroperovskites (ABF_3) have great potential as novel optics-based dosimeters because they are known to display optically stimulated luminescence (OSL), radioluminescence (RL), and thermoluminescence (TL) when doped with luminescent ions [1,2]. RL and OSL-based dosimeters are particularly advantageous since they allow the dose rate and total dose to be monitored, respectively [1-3]. However, OSL measurements erase the dose information and this makes it difficult to monitor cumulative doses. Furthermore, high energy irradiation produces Cerenkov radiation, which affects uncertainty when RL is used to record dose rates.

This talk presents the results of studies on bulk and nanoparticle $NaMgF_3$ and $KMgF_3$ doped with luminescent ions (Eu, Mn and Sm). Optical absorption, RL, TL, OSL, and conductivity measurements were made before, during, and after exposure to x-ray irradiation. RL is observed that increases with the dose rate and is independent of dose history for nanoparticles after a predose. Optical absorption occurs after irradiation due to point defects that result in OSL and TL. F-centre/Mn complexes are observed and we show that they can be used to provide non-destructive measurements of the total and cumulative doses. Radiation-induced conductivity is seen during irradiation that can be used to record the dose rate. This is especially useful for high energy irradiations where Cerenkov light can be a problem in RL-based dosimeters. Thus, we show that the fluoroperovskites have potential as radiation dosimeters operating in all-optical and electronic modes.

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Defect Mechanisms in $BaTiO_3$-BiMO_3 (M = metal) Ceramics

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Addition of BiMO_3 to $BaTiO_3$ (BT) helps improve their properties for energy storage applications across length scales. This is intimately related to their underlying defect mechanisms and transport properties, which are not well-understood. On adding BiMO_3 to BT, the resistivity values are often improved significantly (>2 orders of magnitude) and there is a simultaneous shift to n-type conduction from p-type for BT. Using a specific BiMO_3, *i.e.* $Bi(Zn_{1/2}Ti_{1/2})O_3$ (BZT), several prospective candidates for this n-type behavior in BT-BZT were investigated such as loss of volatile cations, oxygen vacancies, bismuth present in multiple valence states and precipitation of secondary phases. Combined x-ray and neutron diffraction, prompt gamma neutron activation analysis and electron energy loss spectroscopy suggested much higher oxygen vacancy concentration in BT-BZT ceramics as compared to BT alone. X-ray photoelectron spectroscopy and x-ray absorption spectroscopy did not suggest presence of bismuth in multiple valence states. At the same time, using transmission electron microscopy, some secondary phases were observed, whose compositions were such that they could result in effective donor doping in BT-BZT ceramics. Using experimentally determined thermodynamic parameters for BT and slopes of Kröger-Vink plots, it has been suggested that an ionic compensation mechanism is prevalent in these ceramics instead of electronic compensation. These defects have an effect of shifting the conductivity minimum in Kröger-Vink plots to higher oxygen partial pressure values in BT-BZT ceramics as compared to BT, resulting in a significantly higher resistivity values in air atmosphere and an n-type behavior. This provides an important tool to tailor transport properties and defects in BT-BiMO_3 ceramics, to make them better suited for dielectric or other applications.

Ion Microscopy: From Ion Solid Interactions to Real World Applications

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Ion microscopy is an exciting and emerging technology with a vast range of applications from materials characterization to nanostructuring. The talk will start off with an introduction to FIB/SEMs, which combine a gallium Focused Ion Beam (FIB) and a Scanning Electron Microscope (SEM). FIB/SEMs are a versatile tool for materials analysis and nanostructuring and are most commonly used to reveal internal sample structures at high resolution (cross-sectioning), to reconstruct a 3D model of the sample via a slice and view process and to prepare TEM-lamellas (sections) or samples for Atom Probe Tomography at precisely selected points within the sample which cannot be achieved by other techniques. In addition, FIB/SEMs are commonly used to fabricate nanoporous arrays or plasmonic devices [1-3]. The first part of the talk will conclude with a discussion about the ion solid interactions and the most commonly found process induced artefacts and ways to avoid them. The presentation will then focus on introducing the more recent Helium/Neon Ion Microscopy (HIM) which excels at high resolution surface imaging of conductive and non-conductive samples while outperforming the Focused Ion Beam (FIB) at sub 10nm structuring [4].

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On-Surface Synthesis of Trinuclear Coordination Nanostructures

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Multimetallic complexes are molecular compounds composed of organic ligands coordinated with several metal atoms. These systems exhibit chemical and electronic properties that allow for a vast range of applications, in particular in the area of catalysis [1]. Yet, their synthesis remains challenging. On-surface supramolecular chemistry – a bottom-up approach driven by noncovalent interactions between molecules and atoms on a surface – allows for the design of atomically precise organic and metal-organic nanomaterials [2], whose morphology, properties and functionalities can differ dramatically from those of compounds obtained via conventional synthetic chemistry.

Here, I will describe the bottom-up synthesis of one-dimensional coordination nanostructures on a noble metal surface, where the coordination motif is based on an iron-terpyridine interaction borrowed from functional metal-organic complexes used in photovoltaic and catalytic applications. By a combination of low-temperature scanning tunneling microscopy (STM) and spectroscopy, STM manipulation, non-contact atomic force microscopy and density functional theory, I will show that the metal-ligand coordination motif consists of coplanar head-to-head terpyridine groups linked via a linear tri-iron cluster. This unusual metal-organic structure not been observed from conventional solution-based synthetic chemistry methods, and is enabled by the bottom-up on-surface synthesis, opening the door to novel pathways for the engineering of nanomaterials with tailored electronic, catalytic and magnetic functionalities.

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Lateral graphene/h-BN heterostructures from chemically converted epitaxial graphene on SiC (0001)

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Graphene has attracted a great deal of interest due to its remarkable properties, but as a zero-bandgap semimetal its full potential for next generation electronic devices is yet to be realized. Unlocking its potential for future applications in nanoelectronics will depend critically on the development of novel approaches to introducing a bandgap while preserving carrier mobility. In-plane heterostructures of graphene and its insulating analogue, h-BN, have been predicted to allow tuning of the bandgap and carrier mobility according to the carbon concentration [1]. Such hybrid structures have previously been synthesized by CVD on metal foils, and patterned using photolithography/reactive ion etching followed by a second growth step, before transfer onto insulating substrates [2].

In this research lateral graphene/h-BN heterostructures are grown on directly on 6H- and 4H-SiC (0001) by topological conversion of epitaxial graphene. Graphene can be chemically converted to h-BN upon heated exposure to ammonia (NH_3) and boric acid (H_3BO_3) vapors, and the concentration of h-BN can be controlled by limiting the reaction time [3]. By x-ray photoelectron spectroscopy (XPS) and scanning tunneling microscopy (STM), we observe the substitution of h-BN domains in the epitaxial graphene layer. The reaction nucleates at defects or functionalized carbon atoms which we confirm by Raman spectroscopy. This technique allows the growth of semiconducting hybrid atomic layers with tunable properties directly on a substrate suitable for device fabrication.

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Electronic Structure of Titania Surfaces Modified by Au Clusters

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Metal clusters with a size of less than 100 atoms are suitable for modifying the electronic properties of semiconductor surfaces. [1, 2] In order to avoid agglomeration of the metal clusters and in order to retain their specific electronic structures, the coverage of the surface with metal clusters has to be kept below 10%. The main challenges in this field are a) to maintain the size and thus the properties of the metal clusters and b) to determine the electronic structure of the clusters.

The first challenge is considered as one of the main challenges in the field of surface modification with metal clusters can be addressed by introducing defects on the metal oxide surface, specifically oxygen vacancies. The second challenge can be addressed by using experimental techniques which are exclusively sensitive for the electronic structure of the outermost layer. Metastable Induced Electron Spectroscopy (MIES) is such a technique and has been used successfully to determine the change in electronic structure due to the deposition of Au clusters. Applying techniques such as singular value decomposition, the changes of the electronic structure can even be quantified. [2]

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Charge order in a frustrated two-dimensional atom lattice

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The triangular lattice of localised electrons is the canonical example for a geometrically frustrated spin arrangement. As a consequence, strong local Coulomb interactions lead to a competition of antiferromagnetic order and spin liquid behaviour. However, when longer-ranged Coulomb interactions become relevant, charge order can emerge. Thus, contingent on the competing energy scales, an even richer phase diagram must be expected. Yet, candidate material are rather limited. Here we show that Sn/Si(111) [1] and Pb/Si(111) are excellent realisations of an extended Hubbard model. In our study of the Pb atom lattice on silicon using scanning tunneling microscopy, we detect a charge-ordered state not previously known. We employ an extended variational cluster approach to determine the full interacting phase diagram, which finds charge order driven by longer-ranged interactions, and in competition with magnetic order. By exploiting the tunability of correlation strength, hopping parameters and bandfilling, this material class represents a promising platform to search for exotic states of matter, in particular, for chiral topological superconductivity.

[1] Li *et al.*, Nat. Commun. **4**, 1620 (2013).

The role of halogens in on-surface Ullmann polymerization

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Ullmann coupling is commonly used to form surface-confined one- and two-dimensional conjugated structures from haloaryl derivatives. This methodology is simple and can be reliably tracked by photoelectron spectroscopy and scanning probe microscopy.[1] However, the halogen atoms that control the reaction also influence the reaction rate and topology of the products, even when they act as spectators that do not participate in the chemistry. We demonstrate this effect using five different 1,4-dihalobenzene molecules containing chlorine, bromine, and iodine deposited on Cu(110) using scanning tunneling microscopy, fast-X-ray photoelectron and near edge X-ray absorption fine structure spectroscopies.

The influence of the halogens can be understood by a kinetic model that describes the motion of both the organic precursors[2] and the detached halogen atoms hosted on the surface as a function of the reaction temperature. We find distinct diffusion barriers for the different halogen species, and these diffusing byproducts exert a significant influence on the growth of the polymers. Producing polymers from on-surface Ullman coupling is therefore critically influenced by the choice of capping species and this must be taken into consideration when designing novel materials.

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Boron Nitride Nanotubes, Nanoparticles and Nanosheets

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Boron nitride (BN) nanomaterials are well known counterparts of the famous Carbon (C) ones. Nanotubes, nanoparticles are graphene-like nanosheets are similarly form in this system and have been found to be very promising for diverse practical applications due to the unique combination of electrical insulation, oxidation resistance, high thermal conductivity, huge tensile strength and Young's modulus, superb hydrophobicity and lubricant properties [1-8].

In this presentation I will detail many functional properties of these nanostructures, in many occasions first measured using original methods of *in situ* high resolution transmission electron microscopy (HRTEM) [3-6].

An overview of originally developed synthetic techniques of BN nanostructures and thorough analysis of their physical, mechanical and chemical properties will be followed by the illustration of most recent examples of their applications in polymer and metal matrix composites, water purifiers, drug carriers, hydrogen accumulators, photocatalysts, light sensitizers, and optical and magnetic components [7-11].

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NanoPorous Graphene: topology vs. doping effects

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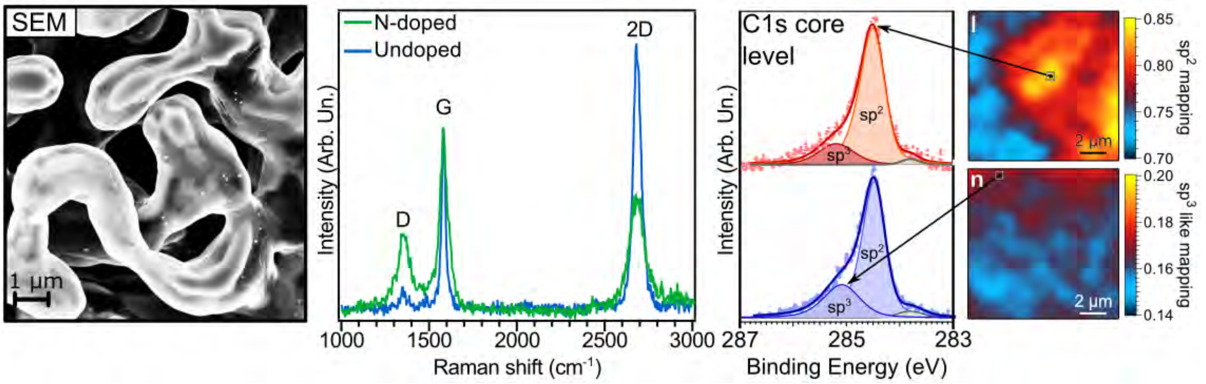
The spatial arrangement of the honeycomb carbon network in graphene-based materials has a deep impact on their properties, for example the chirality of carbon nanotubes affects their conductance, the stacking between the carbon planes influences the carrier mobility etc. Compacting graphene into three-dimensional (3D) architectures in order to minimize the volume and increasing the surface area, while maintaining its very two-dimensional (2D) properties, is a current challenge. A viable method to synthesise graphene in 3D nanostructures is chemical vapour deposition (CVD) on Ni-based nanotemplates, leading to nanoporous graphene (NPG) with high interconnectivity, low defect density, hundreds of μm thickness and tunable pore size, spanning from 50 nm to 1 μm [1,2].

We present herewith an experimental study of the topological and N-doping effects on the electronic/vibrational structure and on the lattice network, for these bicontinuous 3D graphene architectures, composed by thousands of separated but interconnected graphene layers. A careful, spatially-resolved spectroscopic analysis carried of by state-of-the-art facilities (nano-photoemission and micro-Raman) allows the disentanglement of the different effects that the insertion of heteroatoms and the radius of curvature have on the NPG properties, ascertaining the homogeneity of the structure [3].



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Density and Molar Volume of AlCoCrCuFeNi high-entropy alloy family

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Continuous search of new inorganic materials with promising properties to replace existing conventional ones in the industry has been leading to the development of alloys with unique compositions, such as metal matrix composites (MMCs), nanostructured metal(metal oxide)/polymer composites, and high-entropy alloys (HEAs). It is quite complicated to predict the structure and properties of such materials due to the lack of experimental data related to interactions between structural constituents in those under different conditions. This essential prerequisite has been encouraging a blazing fast increase in articles related to these topics, especially HEAs.

The main goal of the present study was to receive a set of reliable thermophysical data (density, molar volume) of the liquid phase of the AlCoCrCuFeNi HEA and their sub-system alloys. For experimental investigation, samples were prepared by arc-melting method. The measurements were performed using an electromagnetic levitation facility designed for optical dilatometry. The excess molar volume was calculated based on the experimental density values of the investigated alloys and data of those for pure liquid metals, previously measured by ourselves Furthermore, the integral enthalpy of mixing of the AlCoCrCuFeNi alloy family was calculated based on Miedema's model. A good agreement between the excess molar volume and the integral enthalpy of mixing was obtained.

Three Component Hybrid Nanostructures of Pt-Au-ZnO with Enhanced Photocatalytic Properties

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Hybrid nanostructures are synthesized by combining two or more distinct nanomaterials into a single system. Such heterostructures often manifest synergistic effects between the connected components leading to useful multifunctional properties. In this work, we report a Pt@Au-ZnO type three component hybrid nanomaterial with novel photocatalytic properties. The photocatalytic properties were measured by monitoring the degradation of an organic dye molecule under UV illumination (365 ± 10 nm). It has been reported previously that Au-ZnO particles have better photocatalytic properties compared to bare ZnO nanoparticles. We found that Pt@Au-ZnO hybrid particles inherit superior photocatalytic properties compared to Au-ZnO particles. Most importantly, in the presence of Pt@Au-ZnO catalyst, modulation of the UV light (on/off) during the photocatalytic reaction did not influence the direction of the dye molecule degradation reaction. However, in the presence of Au-ZnO nanoparticles, reversion of the degradation reaction was noted upon turning off the UV light. Pt@Au-ZnO nanomaterials will be highly desirable for photocatalytic systems that utilize natural solar radiation as the light source, where fluctuations in light intensity can be expected. Synthesis, characterization (TEM, STEM, EDX and XPS), measurements and analysis of photocatalytic properties of Pt@Au-ZnO and Au-ZnO hybrid nanoparticles with different Au nanoparticle sizes will be presented.

Switching, transport and junction characteristics of an all-carbon memristor

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The electrical and structural characteristics of memristors fabricated wholly from carbon were studied. Utilising a through-film device structure, lower resistance sp^2-rich contacts are separated by a higher resistance, sp^3-rich layer forming a tri-layer amorphous C device. Deposited via filtered cathodic vacuum arc and thermal evaporation, devices were defined by photolithographic patterning, enabled by the moderate deposition temperature (<100°C). Current through the devices was limited by interface barrier(s) at low applied bias (1 V). Increasing the applied bias (4 V) resulted in an onset of reversible and repeatable bipolar switching between high and low resistance states (HRS/LRS). The switching phenomena was attributed to bias-dependent variation of the interface barrier(s). When testing the resistive states via a non-perturbative read voltage, the resistance of the LRS was approximately two orders of magnitude less than the recorded value for the HRS. Memristors made entirely from carbon will enable devices that have the potential to be biocompatible, largely chemically inert and thermally stable. Such devices could be fabricated for biological and electronic applications.

Investigation of mechanical and electrical properties of 3D porous graphene hydrogels

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As a 3D porous carbon monolith, graphene hydrogel (GH) has attracted increasing attention in various applications like energy storage devices, pollutant adsorption, catalysis, and tissue engineering. Among different synthesis methods of GHs, hydrothermal reduction demonstrates an advantage over others as it is a water-only simply routine producing reduced graphene oxide (rGO) with less impurity. Self-assembly and reduction play an important role in determining the final structure and properties of GHs. However there is a lack of understanding of the nature of the linkage (covalent or π-π stacking) between graphene sheets that causes the hydrogel formation and how self-assembly affects the properties. In this study, we have investigated the influence of the reduction degree and the bonding mechanism of graphene sheets on morphology, and mechanical and electrical properties. The effects of pH value on self-assembly of GHs, in terms of electrostatic repulsion force between GO sheets were examined.

Fatigue Mechanisms in Lead-free BNT-BT-KNN Piezoceramics

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Bismuth alkali piezoceramics such as $(Bi_{1/2}Na_{1/2})TiO_3$–$BaTiO_3$–$(K_{1/2}Na_{1/2})NbO_3$ (BNT-BT-KNN) are exciting alternatives to replace PZT ($Pb(Zr_{1-x}Ti_x)O_3$), as they exhibit high strain values and are attractively lead-free. Unlike PZT-based ceramics, their macroscopic strain is generated through electric field-induced phase transitions between relaxor and ferroelectric states, and reversibility of the transitions is dependent on temperature and composition of ceramics. Therefore, as a first step, the electric field-temperature (E-T) phase diagrams have been generated for some BNT-BT-KNN ceramics, which exhibit different relaxor behaviors under ambient conditions. Even though strain mechanisms are relatively well-understood in these ergodic and non-ergodic relaxors, the understanding of piezoelectric fatigue behavior in them is below the desired levels. Herein, fatigue measurements performed under varying frequencies and temperatures have been shown and the results are dependent on the relaxor nature under a given fatigue environment. This study is expected to enhance the understanding of fatigue mechanisms in these ceramics and help design more reliable lead-free piezoelectric devices.

Electronic-mechanical coupling in 2D Dirac materials

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The discovery and exploration of graphene has stimulated intensive research in recent years, leading to the identification and study of a wide range of two-dimensional (2D) materials that exhibit a rich variety of novel structural, electronic, catalytic, and mechanical properties. We report findings of an extraordinary combination of unusual mechanical and electronic properties in hydrogenated borophene, known as borophane[1], from first-principles calculations. This novel 2D material has been shown to exhibit robust Dirac transport physics[2]. Our study unveils that borophane is auxetic with a surprising negative Poisson's ratio stemming from its unique puckered triangle hinge structure and the associated hinge dihedral angle variation under a tensile strain in the armchair direction. Our results also identify borophane to be ferroelastic with a stress-driven 90-degree lattice rotation in the boron layer, accompanied by a remarkable orientation switch of the anisotropic Dirac transport channels.

On the other hands, 2D topological insulators possess the helical metallic edge states, which exhibit interesting Dirac cone feature. We have demonstrated several feasible approaches to turn the graphene into strong topological insulators.

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Angular electron correlation dynamics in two-dimensional quantum dots in strongly correlated and completely uncorrelated regimes

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Recent advances in nanotechnology have allowed us to fabricate nanoscale tiny objects on semiconductor surfaces in which a small number of electrons are confined in a quasi-zero-dimensional potential. These systems have been known as semiconductor quantum dots or artificial atoms, since their electronic properties can be controlled artificially by changing the confinement strength etc. In such finite few-body systems the correlation contribution to the total energy can differ significantly such as from 1 percent, similar to the case of the ground state of the Helium atom, to as large as more than 20 percent depending on the size of their size and shape [1]. Therefore, their wave functions particularly in the highly correlated regime are many-body in nature. In order for these systems to be used for practical applications such as in quantum computation, single-photon detectors, etc., their nature of the correlated wave functions need to be clarified.

In the present study we have focused on the two-dimensional circular-symmetric quantum dots and studied the angular correlation of the confined electrons relying on the full configuration interaction wave functions supplemented by high angular momentum basis functions [2,3]. The two-electron angle density distributions [4] have been calculated for different spin states of the low-lying singly-excited states. The results show strong angular dependences not only in the correlated regime but also in the *uncorrelated* regime where the correlation energy is negligibly small. The origin of these strong angular dependences will be discussed on the basis of the probability density distributions in the internal space.

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Extraordinary Magnetic Field Independent NMR Linewidths Observed in Bi_2Te_3 Topological Insulator Nanoparticles

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There is considerable interest in understanding the fundamental physics in topological compounds that display exotic phenomena including metallic surfaces while the bulk is insulating. The most prominent representatives of three dimensional topological insulators are the binary systems Bi_2Se_3 and Bi_2Te_3 [1]. In 2016, we showed that the ^{77}Se nuclear magnetic resonance (NMR) in Bi_2Se_3 is governed by an exotic electronic spin susceptibility of Bloembergen-Rowland (BR) type giving rise to an unusually strong indirect dipole coupling among distant nuclei mediated by bulk electrons [2].

In this report we present the results from ^{125}Te NMR measurements from 7 T to 17.6 T on Bi_2Te_3 single crystals, micron sized powders, and nanopowders. The ^{125}Te results are the same as found by ^{77}Se NMR on Bi_2Se_3 where there are huge magnetic field independent NMR linewidths that are essentially doping independent (BR). A similar result is found for micron sized powders. But when grinding the material to very fine powders with dimensions on the 10's on nm scale we find that the field independent linewidth increases dramatically, which has not been reported in the literature. Possible effects leading to this extraordinary observation will be discussed.

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Quantum kinetic theory of magneto-transport in topological materials

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Topological materials, such as topological insulators, Weyl semimetals, and strongly spin-orbit coupled semiconductors, have attracted considerable attention due to their potential in spin electronics and quantum computation. Their strong spin-orbit coupling gives rise to a host of observable inter-band coherence effects such as the spin- and anomalous Hall effects, spin-orbit torques, a minimum conductivity and chiral anomalies in magneto-transport. I will first discuss a general quantum kinetic theory of linear response to an electric field which can be applied to solids with arbitrarily complicated band structures and includes the inter-band coherence response and the Bloch-state repopulation response on an equal footing [1]. One of the principal aims of our work is to enable extensive transport theory applications using computational packages constructed in terms of maximally localized Wannier functions. I will demonstrate that the inter-band response in conductors consists primarily of two terms: an intrinsic contribution due to the entire Fermi sea that captures, among other effects, the Berry curvature contribution to wave-packet dynamics, and an anomalous contribution caused by scattering that is sensitive to the presence of the Fermi surface. The Berry phase correction to the density of states in a magnetic field in semiclassical wavepacket dynamics appears as an intrinsic contribution to the density matrix in linear response to a magnetic field. I will subsequently discuss the magneto-transport of Weyl metals that results from chiral anomalies, i.e., positive magneto-conductances quadratic in magnetic field associated with the presence of separate Fermi surface pockets surrounding distinct Weyl points. Our theory explicitly accounts for the dependence of chiral anomalies on weak inter-pocket scattering, and demonstrates that the chiral anomaly only partially survives disorder scattering even in the limit of extremely weak inter-pocket scattering [2]. Finally I will focus on the the charge conductivity of 2D hole systems, which displays strong signatures of the spin-orbit interaction. The Hall coefficient in a weak perpendicular magnetic field contains a contribution of second order in the spin-orbit interaction and non-linear in the carrier number density, which at high densities represents as much as 20% of the total signal. An appropriate experimental setup with top and back gates can lead to a direct electrical measurement of the spin-orbit constant [3]. I will end with a summary of potential future applications of our approach.

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Engineered quantum matter

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Atomic-scale engineering reached the level of control where single-atom devices can be reproducibly fabricated with high yield [1]. This talk focuses on the progress of single dopant atom placement in the context of engineered quantum matter. Silicon offers a particularly interesting platform for single dopants because when isotopically purified it acts as a "semiconductor vacuum" for spins. This leads to extraordinary coherence [2] that is used to realise donor atom based qubits [3]. Spatially resolved tunnelling experiments reveal the spectrum and quantum state image of such qubits [4]. These measurements grant access to the wavefunction of donors in the silicon lattice that exhibited quantum interference processes reflecting the valley degrees of freedom inherited from the silicon "semiconductor vacuum". This interference process makes it possible to pinpoint the dopants to their exact position in the lattice [5] that is essential in the evaluation of engineered quantum matter. Finally, a first step towards engineered quantum matter in for form of atomic chains was taken where interacting dopants were employed to simulate a two-site Hubbard Hamiltonian at low effective temperatures with single-site resolution. Quasi-particle tunnelling maps of spin-resolved states with atomic resolution reveal interference processes from which the entanglement entropy and Hubbard interactions are quantified [6].

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One HTS Josephson Junction - An Array of Applications: Has anything come from HTS devices in the last 32 years?

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The discovery of high temperature superconductors (HTS) thirty two years ago was heralded with great anticipation to enable a broad range of potential applications. However applications of HTS electronics are dependent on high quality Josephson junctions that have controllable transport parameters with high reproducibility in YBCO. A number of different technologies for junctions have been developed with a few (bicrystal, ion beam bombardment and step edge junctions) being effective. Based on these junctions, a number of device applications have been successfully deployed and in some cases commercialised. Starting with devices with no junctions such as filters for telecommunications, single junctions such as in bow-tie antennas and RF SQUIDs, two junctions for DC SQUIDs for magnetometers, gradiometers and a number of different detectors such for terahertz and most recently arrays of thousands of SQUIDs for SQIFs. This talk will overview the development of the HTS Josephson junctions in YBCO with a view to what is needed to achieve mass market application and adoption. Then I will review the most successful applications of HTs devices in filters, magnetometers and gradiometers for mineral exploration, metal in food detection, biomedical, defence and array antennas. The talk will finish with the need for standards and the ability to model devices to enable commercial foundry manufacture enabling the realisation of the thirty year dream.

Manipulation of the critical current density in $YBa_2Cu_3O_7$ thin films by artificial defects

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The current-carrying ability can be effectively enhanced by introducing certain ‘intelligent’ defects within the material. These defects can also give rise to other practically and scientifically appealing effects, such as current rectification, flux quantum filtering, and an inhomogeneous response to external magnetic field. One such defect is the controlled removal of the superconductor through optical lithography and ion beam etching. This gives a worse resolution than the traditional electron beam lithography, but comes with certain advantages. Optical lithography is much cheaper and also a quicker procedure, making it more desirable for industry, if the required improvements are obtained. Using these techniques, not only an improvement in the critical current density has been found, but also current ratcheting. With holes as large as 2-3μm, the vortex will be pinned to the edge of the superconductor and the hole. Pinning of the vortices can be modified by simply changing the shape of the hole. Furthermore, an improvement to the ratchet effect has been proposed and partially implemented by manipulating the ion beam angle on the bridge. This gives a bridge with varying thickness across the width, and correspondingly changes the pinning potential (hence J_C). Simulations of this setup suggest great potential for applications.

Superconductor Sandwiches

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When we sandwiched a high-temperature superconductor between two layers of specific Manganite last year, we discovered a that the superconductor adopts a startling new ground state [1]. This `superconductor sandwich' exhibit many unusual effects; an exotic granular-superconductor that transitions in a strong magnetic field to a ‘customary’ superconductor. Here, we highlight how we used state-of-the-art THz ellipsometry (Fig. 1) in conjunction with synchrotron-based x-ray studies and transport measurements to reveal the ground-state nature of our superconductor sandwiches. We'll also present some ways we think other spectroscopic probes could be used to elucidate the physics behind these unusual effects. Aside from being a fascinating system to study in its own right, the discovery provides a novel way to study the physics of high-temperature superconductors. It is also a great example of the surprising and useful behaviours that can be realised at engineered interfaces.

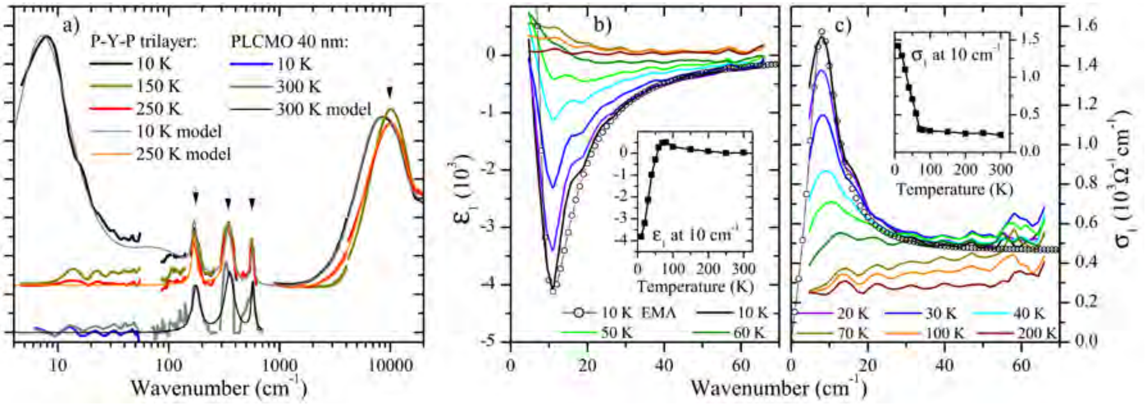

Figure 1: The optical conductivity measured by ellipsometry of the Superconductor-Manganite sandwich, from the THz to near UV. The superconductor layer is 7 nm thick, each of the Manganite layers 20 nm thick. The large peak around 10 cm^{-1} and low temperature is evidence of the unusual granular-superconductor.

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Unconventional superconductivity in 2D systems from repulsive electron-electron interactions

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Superconductivity usually arises from a phonon-mediated attractive interaction between the conducting electrons which leads to the formation of Cooper pairs. There are, however, several superconducting materials that behave differently, in particular the high temperature and topological superconductors. The *unconventional* superconductivity in these materials arises primarily from repulsive electron-electron interactions.

Here, we apply a weak-coupling renormalization group (RG) method to compute the superconducting groundstates of several paradigmatic 2D lattices with tunable parameters. Among the different superconducting groundstates we find chiral topological superconductivity with p+ip and d+id pairing symmetry. Applications to materials are also discussed.

ABSTRACTS
OF
POSTER PRESENTATIONS

Mössbauer and Magnetic Properties of Non-Stoichiometric Strontium M-type Hexaferrites Prepared by the Solid State Reaction Method

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The present work is focused on the study of the magnetic properties of M-type hexaferrites with differing iron content, both directly and via hyperfine interactions using ^{57}Fe Mössbauer spectroscopy. M-type hexaferrites are versatile materials that are utilised in data recording, microwave devices and as permanent magnets [1]. The non-stoichiometric strontium M-type hexaferrites $SrFe_{12-x}O_{19-\delta}$ with x = -0.50, -0.25, 0.25, 0.50, 0.75 and 1.00 have been prepared using the solid state reaction method with double step-sintering at 1200°C. X-ray diffraction patterns show generally good phase purity as quantified by Rietveld refinement. Residual α-Fe_2O_3 of 1.2 wt. % and 4.2 wt. % was noted for x = -0.25 and -0.50.

Hysteresis curves were obtained at room temperature using a Physical Properties Measurement System (PPMS-ACMS) and the values of the saturation magnetisation were derived using the ‘approach to saturation’ law [2]. The hyperfine parameters, obtained from ^{57}Fe Mössbauer spectroscopy, are discussed in terms of the distribution of Fe^{3+} sites in light of the differing iron contents.

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In situ monochromator alignment on ANSTO's thermal spectrometer, TAIPAN

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TAIPAN is the thermal triple axis spectrometer at ANSTO and also hosts an alternate secondary spectrometer called the Be-filter. Both instruments use a common graphite monochromator (PG002) to select a single wavelength or energy of the neutrons. By rotating the monochromator with respect to the incident beam of neutrons from the reactor, the energy of the neutrons from the monochromator can vary between 5-70 meV. The PG002 monochromator is made from 63 individual crystals of highly oriented pyrolytic graphite and the neutrons are scattered from the 002 lattice planes. The benefit of separate crystals is that they can be oriented to allow for vertical focusing of the neutron beam, or horizontal focusing or double focusing, depending on the experimental requirements.

Recent measurements at TAIPAN have indicated that the crystals may not be well aligned on the double focusing mechanism, leading to broad peaks that indicate an increased mosaicity. We will present our work to develop a rapid *in situ* laser alignment-checking procedure for the 63-crystal TAIPAN graphite monochromator. Due to the small aperture, translation, rotation and tilt of the laser, as well as rotation and tilt of the monochromators would be needed, which will involve derivation of the geometrical mathematics, construction from what we have available of a stage with the large translations needed, testing *ex situ*, then *in situ*.

The magnetic structures of RTi_2Ga_4 (R= Er, Ho and Dy)

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The first study of magnetism in the RTi_2Ga_4 system was reported by Ghosh et al. in 1993 [1] who observed unusual magnetic behaviour, leading them to conclude that these compounds exhibit the effects of mixed Ferro/Antiferromagnetic exchange, possibly with spin-glass behaviour. Interestingly, they observed a rather rapid increase in coercivity with decreasing temperature. In 2001, Abe et al. [2] studied a single-crystal of $ErTi_2Ga_4$ and showed that this compound is a ferromagnet oriented along the [100] direction, with quite strong magnetic anisotropy.

We have carried out high-resolution neutron diffraction measurements to determine the magnetic and crystal structural parameters and magnetic ordering temperatures of the RTi_2Ga_4 (R=Er, Ho and Dy) compounds. These compounds crystallise in the tetragonal $YbMo_2Al_4$-type structure with the I4/mmm (#139) space group. These compounds are confirmed to be ferromagnetic. The Dy and Ho magnetic moments order within the tetragonal basal plane whereas the ordering of the Er moments is along the c-axis.

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Investigation of the Magnetic and Crystal Field Excitations in the Orthorhombically Distorted Perovskites $TbVO_3$ and $CeVO_3$

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Inelastic neutron scattering experiments have been performed on a series of vanadates, in particular $TbVO_3$ and $CeVO_3$, to categorise the crystal field and magnetic excitations. The vanadates crystallize in the 3-dimesnional perovskite structure (space group P*bnm*), which is characterized by a network of corner sharing, distorted VO_6 octahedra. The Tb/Ce ions are located in an open cage created by the VO_6 octahedra. C-type antiferromagnetic order sets in below the Néel temperatures of $T_N = 110$ K and 124 K, respectively [1-4].

The temperature dependence of the neutron scattering data did indicate a hitherto unobserved shift of the crystal field excitations energies at low temperatures. In order to determine to origin of these shifts we have used point-charge calculations to determine the energies of the crystal field excitations. After confirming that the calculated energies were in agreement to the experimentally measured values we have modeled both scenarios, the effect of the crystallographic phase transition at about 136 K and the effect of the internal magnetic field below the magnetic phase transition temperature. The obtained data did provide valuable insight to the detailed interplay and competition between magnetic order and crystal field excitations.

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Recent upgrades to ANSTO's thermal neutron spectrometer, TAIPAN

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TAIPAN is the thermal neutron spectrometer located at the reactor face of Australia's OPAL reactor (ANSTO). TAIPAN hosts two interchangeable secondary instruments; the triple-axis spectrometer (TAS) and the Beryllium-filter spectrometer - which is a high-throughput, low-energy, band-pass filter spectrometer. The TAS option has been operating in the user program since 2010 whilst the Be-filter is a newer addition, which began operating in 2015. TAIPAN is renowned for its versatility and high neutron flux which has allowed the TAS to successfully measure a broad range of samples including single crystals, powders, thin films, and co-aligned multi-crystal arrays [1,2]. While the TAS option is used mostly to study structural and magnetic excitations in materials, the Be-filter spectrometer is used to measure vibrational density of states from mainly powder samples [3].

TAIPAN has recently undergone some significant upgrades to improve the accessible momentum and energy range of both the TAS and the Be-filter spectrometers. Four key features have been modified to improve performance: a new sapphire filter translation stage mechanism has been installed to allow epithermal neutrons to pass to the monochromators; a new Cu-200 double-focussing monochromator has been installed to allow monochromatic scattering of neutrons up to 160 meV; a new tertiary shutter and snout have been designed to improve the signal to noise ratio and reduced background outside the instrument enclosure; and finally the accessible momentum transfer has been increased by re-designing the enclosure and expanding the available instrument range of motion.

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Hot Isostatic Pressing of Ceramics, Glass and Glass-Ceramics for Immobilisation of Intermediate- and High-Level Nuclear Waste

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Different classes of nuclear wastes are briefly described, together with an idea of the required qualities of the processed waste for geological disposal. The main Synroc project at ANSTO these days is immobilisation of the upcoming ~5000L/yr intermediate-level waste from the production of the ^{99}Mo radiopharmaceutical and this has been demonstrated inactively by hot isostatic pressing (HIP) a glass at full scale, together with showing its resilience to compositional variations of 10% for all main components, minor impurities and HIP temperature and pressure. Other work deals with HIP immobilisation of zirconolite-based glass-ceramics for surplus PuO_2 immobilisation, glass-ceramics and ceramics for U-rich legacy ANSTO ^{99}Mo intermediate-level and low-level waste, immobilisation of pyroprocessing fluoride-salt waste, spent power plant fuel, refractory glasses and CuI .

Structural, Magnetic Phase Transitions and Magnetocaloric Effect in $Sm_{1-x}R_xMn_2Ge_2$

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Rare earth-based intermetallic compounds attract special attention due to their potential for various applications. One important application is as magnetocaloric materials essential for magnetic refrigeration [1]. The $SmMn_2Ge_2$ compound usually forms in the $ThCr_2Si_2$ structure (space group *I*4/*mmm*) with the layered nature of this crystal structure leading to strong dependence of the magnetic interactions on the interplanar and intraplanar interatomic Mn-Mn distances [2]. There is potential in this system for enhancement of the magnetocaloric effect (MCE) because the layered nature allows the control of the intrinsic magnetism via inter and intraplanar separations of the Mn and Sm atoms in turn controlling the large magnetisation due to ferromagnetic coupling between the Mn and Sm sublattices below the Sm ordering temperature [3].

In this report, the influence of substitution of other heavy rare earths (R = Dy, Ho and Er) for Sm in terms of magnetism, lattice parameter, and MCE are discussed. The structural properties of the $Sm_{1-x}R_xMn_2Ge_2$ series compounds have been investigated in detail using X-ray diffraction, both laboratory and synchrotron measurements over the temperature range 12 to 450 K. While magnetic properties were explored via magnetic susceptibility in the range 0 to 310 K and differential scanning calorimetry (DSC). The MCE effect has also been quantified with magnetisation isotherms recorded to a maximum field of 5.0 T from which magnetic entropy changes are derived.

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Size-driven ferroelectrics in 2D pseudo-spin model

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We performed Monte Carlo simulation of the pseudo-spin Ising model in a two-dimensional ferroelectric system. The Metropolis method was employed by studying the size dependence of dielectric properties along the electric-field direction and the internal energy of the two-dimensional ferroelectric system. The critical phenomena in the vicinity of the phase transition temperature were considered by the scaling function obeying the values of critical exponents in view of the large-scale lattice.

Magnetocaloric $Mn(Co_{1-x}Ni_x)Ge$ - Structural and magnetic transitions

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The structural and magnetic properties of MnCoGe-based alloys have been studied extensively in recent years due to their potential application as magnetic cooling materials based on the magnetocaloric effect (MCE). The $Mn(Co_{1-x}Ni_x)Ge$ series is of particular interest as magnetic transitions in the range 275 K to 345 K generally coincide with a martensitic structural transition T_M, with such an overlap then allowing scope for the formation of magneto-structural transitions (ferromagnetic orthorhombic to paramagnetic hexagonal) and hence an associated large MCE [*e.g.* 1].

Neutron diffraction, magnetisation and x-ray experiments on $Mn(Co_{1-x}Ni_x)Ge$ compounds (x = 0.12 to 1.00) have demonstrated magnetic structures ranging from ferromagnetic for $x < 0.50$ to non-collinear spiral antiferromagnetic for $x > 0.55$ at low temperature (*e.g.* 5 K). T_M is found to decrease initially with increasing Ni content and then increase. First-order magneto-structural transitions are observed in $Mn(Co_{1-x}Ni_x)Ge$ samples for $\sim 0.20 < x < \sim 0.65$ with the presence of ferro-/antiferro-magnetic structures in $Mn(Co_{1-x}Ni_x)Ge$ allowing investigation of both direct and inverse magnetocaloric effects. Our results (including the magnetic phase diagram for $Mn(Co_{1-x}Ni_x)Ge$) are discussed in terms of the increase of valence electron concentration on substitution of Ni ($3d^8 4s^2$) for Co ($3d^7 4s^2$) in the orthorhombic phase, leading to expansion of the unit cell and redistribution of the valence electrons [2].

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Determination of the Crystal Field Levels in TmV_2Al_{20}

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The interest in compounds of the RM_2Al_{20}-type (R = lanthanide, M = transition metal) in recent years reflects the fascinating physical and magnetic properties on display at low temperatures. For example, in PrV_2Al_{20} and $PrTi_2Al_{20}$ the phenomena reported include a quadrupolar Kondo effect [1] and superconductivity [2]. Central to such systems is the cubic symmetry of the Pr^{3+} site inducing a non-magnetic ground state in the ion. As a hole analogue of the PrV_2Al_{20} compound, TmV_2Al_{20} has been investigated in the hope of observing similar phenomena at low temperatures. At last year's 'Wagga' we reported that we had determined the Tm^{3+} crystal field parameters W = 0.42(1) and x = -0.63(1) [3] (based on the Lea, Leask and Wolf formalism [4]) for TmV_2Al_{20} using inelastic neutron scattering on PELICAN at the OPAL reactor, Lucas Heights. However, the line shapes found were extremely broad Lorentzians, indicative of a coupling of crystal field states to conduction electrons, 'smearing out' the energy required for transitions. Here, we report more recent developments: Tm^{3+} electron spin resonance results together with modelling of physical properties lead to the conclusion that there is a small local distortion away from cubic symmetry.

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Investigation on the Nature of the Verwey Transition in Cu-doped Fe_3O_4

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Magnetite (Fe_3O_4), the oldest known magnet, is still a hotly debated material in scientific research, due to its complex magnetic, electronic and transport properties. One of the most interesting physical phenomena associated with Fe_3O_4 is the occurrence of a metal-insulator transition at ~120 K (T_V), the so-called Verwey transition, which is associated to a charge ordering below T_V, accompanied with a structural transition from the cubic phase to the monoclinic phase. However, due to the twinning of crystal domain, the detailed crystallographic structure is not fully solved yet and different charge ordered and bond-dimerized ground states have been proposed. In order to overcome this problem, we have investigated Cu-doped Fe_3O_4 and have determined the stability range of the Verwey phase in the phase diagram of $Fe_{1-x}Cu_xFe_2O_4$.

Using neutron diffraction and high resolution X-ray synchrotron diffraction we have investigate both the crystallographic and magnetic structure of Cu-doped Fe_3O_4 ($Cu_xFe_{3-x}O_4$ with $x = 0$ to $x = 0.95$) in order to elucidate the effect of doping on the Verwey transition. Data obtained from both complementary diffraction techniques indicate that the Verwey transition temperature and the magnetic structure, in particular the magnetic moment remains unchanged up to highest doping levels of 75% Cu-substitution. The large stability range of the Verwey phase is a surprising result and did require a systematic investigation. The analysis of our high resolution X-ray synchrotron diffraction data in combination with the neutron diffraction data did allow us to extract detailed information on the precise doping mechanism, for example if the Cu-ions are placed on tetrahedral or octahedral sites in the spinel structure. The obtained diffraction data provide therefore valuable information on the charge order transition, i.e. the Verwey transition.

Spin dynamics of quasi-one-dimensional spin-ladder system $SrCa_{13}Cu_{24}O_{41}$ in the long-range magnetic ordering state

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$Sr_{14-x}Ca_xCu_{24}O_{41}$ is a quasi-one-dimensional magnet, which consists of two sublattices: spin ladder and spin chain, forming an incommensurate crystal structure along the *c* axis, namely, the ladder leg or chain direction.[1] The highly Ca-doped compounds undergo a superconducting phase transition under hydrostatic pressure ~ 3GPa, which is really intriguing since the hole-doped even-leg spin-ladder system was theoretically predicted as superconductors by charge-pairing mechanism through antiferromagnetic interaction on the rungs of spin ladders. In the previous study, we discovered that all compounds with different Ca content have a singlet ground state with a spin-gap ~ 32meV.[2] In the highly Ca-doped sample $SrCa_{13}Cu_{24}O_{41}$, a long-range magnetic ordering takes place at ~ 4.2K. Interestingly, the singlet spin-liquid state and the long-range magnetic ordering coexist in this compound.[3] In this study, we further investigated its spin dynamics in the ordered phase by using inelastic neutron scattering on PELICAN and SIKA at OPAL. We observed the gapless spin-wave excitation, dispersive along the *a* and *c* axes but nondispersive along the *b* axis, indicating the nature of a 2D magnet. A dynamic model has been proposed to fit the experimental data, indicating three major exchange interactions along rungs (J_R), legs (J_L) and between neighbor ladders (J_{Inter}). This study helps us to understand the origin of the spin liquid ground state in this low-dimensional magnet, in which hole-doping should be attributed to induce the long-range magnetic ordering due to the disorder-induced order effect.

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Magnetic Interplay of Mn and Yb Sites in $YbMn_2Si_2$ – Crystal Field and Electronic Structure Studies

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The layered RT_2X_2 series of compounds (R = rare-earth, T = 3*d*, 4*d* transition metal, X = Si, Ge) of bct $ThCr_2Si_2$–type structure (*I4/mmm*) is one of the most widely studied systems in condensed matter and materials science [*e.g.* 1]. Yb-based compounds are of particular interest with their intermediate valence character leading to a wide range of unusual physical and magnetic properties. Following investigation of the magnetic dynamics of YbT_2Si_2 for non-magnetic T = Ni, Co and Fe [2], we investigated $YbMn_2Si_2$ to explore the interaction between the crystal field excitations of Yb atoms and the magnetic ordering of Mn atoms by thermal inelastic neutron scattering [3]. Here we extend these studies of crystal field splitting of $YbMn_2Si_2$ to high resolution (800 μeV and a dynamic range of ~14 meV; PELICAN, OPAL) over the temperature range 5-65 K.

The results have been analysed in terms of a crystal field model above and below T_{N2}, the temperature at which the collinear antiferromagnetic structure AF*il* (T_{N1} = 526(4) K > T > T_{N2} = 32(2) K) transforms to the low temperature structure below T_{N2} in which the magnetic cell is doubled along the *c*-axis [*e.g.* 3]. Density functional theory with a Hubbard correction (DFT+U method) was used to model $YbMn_2Si_2$. A key finding is that the 4f electron U_{eff}-parameter in this compound needs to be negative to stabilise the trivalent state of $YbMn_2Si_2$ with the strength of these interactions reflected in contraction of the lattice parameter.

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The Cold-Neutron Triple-Axis Spectrometer SIKA at OPAL

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SIKA is a high-flux cold-neutron triple-axis spectrometer funded by Ministry of Science and Technology of Taiwan and currently being operated by National Synchrotron Radiation Research Center. It is located on the OPAL reactor face at the Australian Nuclear Science and Technology Organization (ANSTO). Its incident energy ranges from 2.6meV to 30meV with the highest flux at ~8meV. SIKA is equipped with a multiplexing analyzer consisting of an array of 13 PG crystal blades, a multi-wire detector, a single detector and a diffraction detector.[1] The most frequently-used single-detector mode and the multi-Q constant-E_f mode are demonstrated by using the standard samples, namely, MnF_2 and Pb single crystals, respectively. The spin-wave excitation of MnF_2, the phonon dispersion of thermoelectric material SeSn [2], the spin dynamics of the spin-glass system $(Ni_{0.40}Mn_{0.60})TiO_3$[3], and other experimental data from SIKA are demonstrated as examples of SIKA's capabilities and performance. The spin-wave excitation was observed in the quasi-one-dimensional spin-ladder compound $SrCa_{13}Cu_{24}O_{41}$,[4] indicating the low background of SIKA. These results indicate that SIKA is a highly-flexible cold triple-axis spectrometer with reasonably low background.

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New Sample Environment Projects and Developments at the Australian Centre for Neutron Scattering

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The sample environment team at the Australian Centre for Neutron Scattering (ACNS) has been recently awarded funding for the design, building and commissioning of a new superconducting split-coil magnet, a fast cooling closed cycle cryostat and a new type of closed cycle dilution refrigerator.

The new magnet design is complicated by the need to serve two separate classes of instruments: small angle scattering and time of flight. The new magnet will have active magnetic shielding and an asymmetric coil design to allow experiments with polarised neutrons. The fast cooling cryostat is planned to be a compact closed cycle dry cryostat (1.5 K to 800 K). The aim is to halve the system and sample cooling time of similar systems to be comparable to the performance of traditional wet cryostats without the commensurate consumption of non-renewable helium gas. The closed cycle dilution refrigerator will have high cooling power and a very large sample space allowing a new class of experiments with neutrons at ultra-low temperature.

Also presented is the development of line of sight cryogenic sample sticks to allow optical excitation of the sample and gas or vapour delivery sticks for in situ neutron experiments. These sample sticks are used currently in the available top loading cryostat buts will be available in due time for the new cryostats discussed above.

Structure changes in SAC 305 solder joints with nanosized Ni and Ni-Sn additions during the thermal treatment

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Over the past decade the nanostructured Sn-Ag-Cu (SAC) solders have been in discussion as a possible next generation of lead-free solders in electronic packaging. Due to an efficiency-enhancing effect of metal nanoparticles on the microstructure and mechanical properties of SAC solders they have been widely studied as possible material reinforcements in solders.

The presented research was performed in order to establish changes in the microstructure of Cu/solder/Cu joints during thermal treatment. For this reason, as-cast solder joints were aged at a temperature of 150^0C for 10 and 20 days. The solders with 0.5, 1.0 and 2.0 wt.% of metal nanoparticles were prepared by mixing of self-synthesized Ni, Ni_3Sn and Ni_3Sn_2 nanoparticles (NPs) into the commercial Sn-3.0Ag-0.5Cu (SAC 305) solder paste, while the solder joints were prepared by placing the solder paste between two Cu pads. The microstructure was investigated based on scanning electron microscopy (SEM-EDX). The results of as-solidified solder joints showed that additions of Ni and Ni-Sn NPs lead initially to a decrease in the average thickness of the intermetallic compound (IMC) layer at the interface between solder and substrate, while further additions up to 2.0 wt.% did not induce any significant changes. It should also be noted a more significant impact of nano Ni additions on the average thickness of the interfacial IMC layer compared to Ni-Sn NPs. Based on the average thickness values estimated for solder joints with different aging times, the growth kinetics of the interfacial IMC layer was examined. The obtained values of the diffusion coefficient for the investigated solder joints were compared with literature values.

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Reassessment of the Oxidation State of Iron in MORB Glasses (Based on an Alternative Interpretation of Reference Mössbauer Spectra)

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Mid-ocean ridge basalt (MORB) glasses are the most common rock on the surface of the Earth. One might therefore expect that the degree of oxidation of its Fe component, $Fe^{3+}/\Sigma Fe$ (where $\Sigma Fe = Fe^{3+} + Fe^{2+}$), is accurately known. However, the most recent evaluations were 0.11(2) based on redox titrations over n = 104 representative samples [1, 2] and a substantially higher value of 0.16(1), n = 103, based on Fe K-edge x-ray absorption near edge structure (XANES) spectroscopy [3]. In this new work, an XANES investigation of MORB glasses from global sources yielded $Fe^{3+}/\Sigma Fe$ = 0.10(2), n = 42, in excellent agreement with the redox titration result.

XANES measurements are typically calibrated against standard specimens of known oxygen fugacity for which $Fe^{3+}/\Sigma Fe$ is determined using ^{57}Fe-Mössbauer spectroscopy. A key element of this new work was the availability of standard specimens ranging from full oxidation through to full reduction. The Mössbauer spectra for standard specimens of intermediate fugacity could then be fitted unambiguously as a linear combination of the end spectra, regardless of their form.

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Effect of Na excess and cation disorder on voltage and capacity of Na_xRuO_3 as Na ion battery cathode

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The applications of rechargeable batteries are ever expanding [1]. The conventional Li ions technology, however, faces severe limitations as Li resources are scarce and unevenly distributed throughout the globe [2]. Alternatively, utilizing Na ions instead of Li is promising but not without challenges. Na has larger ionic radius and smaller ionization potential compared to Li, all resulting in lower energy density [3]. Therefore, all performance enhancing auxiliary mechanisms must be carefully fine-tuned to make Na ion batteries competitive. These mechanisms include reversible oxygen redox that increases the capacity [4] and cation disorder that improves the ionic mobility [5].

Using density functional calculations, we examine oxygen's participation in redox reaction in two polymorphs of Na_xRuO_3. In both hexagonal ($R\overline{3}m$) and monoclinic (C2/m) Na_xRuO_3, the availability of O electrons for redox reaction originates from the local coordination environment. When O ions are coordinated by four or five Na ions, their 2p electrons are lifted closer to the Fermi level. This orbital rearrangement increases the capacity beyond that of single electron of the transition metal redox and facilitates extra Na extraction. Furthermore, no Ru migration was detected during the desodiation process in both polymorphs. This indicates structural integrity and good cyclability for both polymorphs. The calculated voltage for cation disordered hexagonal ($R\overline{3}m$) phase was 2.35 V which higher than that of cation ordered monoclinic phase (C2/m) which was 2.21 V.

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Unravelling the Iron Coordination in the Mössbauer Spectra of SFCA

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Much of current mineral processing relies on the use of appropriate sinters to hold the crushed ore in an open structure. The key bonding phases in iron ore sinter are frequently known by the terms SFCA and SFCA-I, which is shorthand for silico-ferrite of calcium and aluminium, with the latter being a higher iron composition. A typical SFCA iron ore may contain 60-76 wt% Fe_2O_3, 13-16 wt% CaO, 3-10 wt% SiO_2 and 4-10 wt% Al_2O_3. SFCA-I is a higher grade material with approximately 84 wt% of Fe_2O_3 at the expense of the silica and alumina.

The structure of these sinters is, not surprisingly, very complex [1,2]. For example, there are three different iron-calcium oxide phases as well as the brownmillerite phase which includes aluminium. In order to try and shed some light on the iron bonding we have taken room temperature Mössbauer spectra of 12 samples with differing compositions. However, the structure contains 11 distinct Fe or (Fe,Al) sites, and one may expect that many of them will be similar. Since the subspectra of each of the phases will be doublets, one is looking for up to 22 separate lines in spectra with very little resolution. Even when one can distinguish lines in the spectral envelope, it is not clear how to match them into doublets.

We will describe the various approaches, mainly involving spectral subtraction techniques, which we have attempted in trying to analyze these spectra and get an interpretation in terms of the different iron coordinations and how they vary with change in composition.

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Strain mechanisms in lead-free piezoelectric BNT-BT under the influence of an applied electric field

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Due to the rapidly increasing amount of electrical and electronic waste, the EU parliament adopted several legislations in order to protect human health and the environment from toxic substances. Lead containing substances used in piezoelectrics are solely allowed in the EU, because there is not yet a broadly appropriate substitute available. One of the most promising material for piezoelectric actuator applications is the solid solution $Bi_{0.5}Na_{0.5}TiO_3$-$BaTiO_3$ (BNT-BT) [1]. Beside the composition with 6–7 % BT, the BT-rich side also shows a remarkably high piezoelectric coefficient and large electric field induced strain response [2]. The high electric field induced strain mechanisms of piezoceramics were considered as follows: lattice strain (intrinsic effect), switching of ferroelectric domains (extrinsic effect) and phase transitions [3]. To analyze and quantify all these effects in strain mechanisms in 12 % BT, we developed a method with Strain, Texture, and Rietveld Analysis for Piezoceramics *(STRAP)* acquired from data using *in situ* X-ray powder diffraction. That allows a precise insight into the structural process of switching between the poled and the remanent state. Additionally, the experiments were carried out with several frequencies of the applied field using different setups. In order to correlate the results based on atomic scale with the macroscopic observations, electromechanical measurements were performed. The results jointly substantially contribute to the development of novel promising lead-free piezoceramics.

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Structure and dynamics in photovoltaic metal hydrides

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Solar cell technology is an active area of research with the quest to improve the efficiency of solar cells to above the current value of 44% [1]. Hot carrier solar cells are particular types of cells which may enable higher efficiencies to be obtained. However, these are only feasible where there is a sufficiently large band gap in the phonon dispersion of the bulk material to minimise energy loss to thermalisation, thus keeping the electrons 'hot'. Binary compounds with a large mass difference between the two constituent atoms, and high level of crystal symmetry such as titanium hydride, can have such a gap in their phonon dispersion.

Titanium hydride is an interesting photovoltaic material with a broad range of properties, which vary depending on the proportion of hydride present. Theoretical studies show TiH_2 has a phonon band gap of 95 meV in the bulk phase, however, experimentally this compound exists as a powder because the hydrogenation process causes large stresses in the lattice which are strong enough to crack the bulk sample. For solar cell absorber materials, a bulk sample is preferred and these can be manufactured by hydrogenating very pure Ti metal. We have previously studied $TiH_{1.65}$ using X-ray powder diffraction and inelastic neutron scattering and found that while the width of the acoustic and optical phonon bands is different from those of TiH_2, it did have a phonon band gap of 65 meV i.e. large enough to block Klemens' decay [2].

We present here an extension of this work with Fourier Transform Infra-red (FTIR) and Raman spectroscopy, along with X-Ray Diffraction (XRD) data from the photovoltaic materials, TiH_2 and ZrH_2.

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Investigating and tuning the pore structure of graphitic supercapacitor electrodes.

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In order to improve the energy density of supercapacitor (SC) devices, researchers are looking at increasing the surface area of electrode materials. However, some reports also show an increase in capacitance as the pore size of electrode materials approaches that of the electrolyte ion being employed.[1] Theoretical considerations support this idea in various pore geometries, explaining it by desolvation effects, and by constructively interfering electric double layers.[2] Much of the data comes from activated carbon derived electrodes, the basis of existing commercial SCs.

Graphene-based materials offer potential improvements over activated carbons, such as improved conductivity, and mechanical versatility. [3] Methods such as metallic reduction and acid refluxing have been demonstrated to enable tuneable pore structures in reduced graphene oxide based thin films. In this work, the ability to precisely target particular pore sizes is explored, with the aim to test and exploit the aforementioned proposed hypothesis of improved capacitance by pore-ion-size harmonisation.

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Quasi Free-Standing Graphene Growth on FIB-Patterned 3C-SiC Nanostructures

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There is a growing body of literature that recognizes the potential of graphene for use in electronics [1]. However, graphene's lack of bandgap challenges its remarkable range of applications [2]. Theoretical work suggests that a bandgap might be opened in graphene through quantum confinement, for example in graphene nanoribbons. Thermal decomposition of SiC has proven to be an excellent method to grow transfer-free wafer-scale graphene [3]. Growing graphene on SiC thin films on Si is a cheaper alternative to the growth on bulk SiC. In this research we attempt to manipulate the SiC substrate dimension to grow graphene over nanostructures and use hydrogen intercalation to produce quasi free-standing graphene.

SiC mesas have been fabricated by patterning SiC/Si substrates using Focused Ion Beam (FIB) milling [4]. Hydrogen intercalation procedure has been employed at 600 °C to fabricate free-standing graphene on the structures. Synchrotron radiation near-edge X-ray absorption fine structure (NEXAFS) with core-level photoelectron spectroscopy (PES), scanning tunnelling microscopy (STM), scanning electron microscopy (SEM), and Raman spectroscopy were used to investigate the process. Our result indicates the possibility of growing free-standing epitaxy graphene over SiC nanostructures. However, more research is needed to better understand the impact of patterning procedure on the graphene growth and decrease the damage caused by milling process.

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Synthesis and Characterization of Covalent Organic Frameworks as Thin Films

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Covalent organic frameworks (COFs) are polymer assemblies with high crystallinity, high porosity and configurable skeletal structure. They have potential applications in filtration, gas storage, and electronic devices among others. However, the realization of these applications requires a high degree of morphological control in their preparation, and permanent high crystallinity – bonds in these frameworks are easily reversed in humid atmospheres.[1] The construction of substrate-confined COF materials that are simultaneously highly crystalline, well-oriented and functional remains a challenge due to insufficient understanding of the basic mechanisms controlling the nucleation and growth of covalent organic frameworks, particularly on a substrate. This knowledge is crucial to further progress the development of more concrete techniques that will ultimately lead to covalent organic frameworks that are crystallographically and structurally well-defined in film form. In this poster, I will describe some of our recent progress towards synthesizing dense, crystalline COF layers.

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^{209}Bi NMR Study of Topological Insulator Bi_2Se_3 Single Crystals

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Three-dimensional topological insulators are still under intense investigation in laboratories all over the world. Due to its simple surface states described by a single Dirac-cone, Bi_2Se_3 fertilizes theoretical considerations and the desire for their experimental confirmation. ^{77}Se nuclear magnetic resonance (NMR) of Bi_2Se_3 has taught us that a unique electronic spin susceptibility yields an unusual strong indirect internuclear coupling among Selenium and Bismuth nuclei, producing significant field independent linewidths [1]. For ^{209}Bi NMR in Bi_2Se_3, we see a rapid transversal decay (T_2) that is in good agreement with a strong indirect coupling among ^{209}Bi nuclei that have a high natural abundance of 100%. Careful investigation of the orientation dependent ^{209}Bi resonances in various single crystals revealed a second, highly anisotropic ^{209}Bi NMR signal beneath the well-defined first order quadrupole pattern that proves a surprisingly big number of highly disordered Bismuth sites. Finally, T_2 effects together with the second signal might solve the difficulties reported in the literature about ^{209}Bi NMR of Bi_2Se_3 [2].

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Mechanical Characterisation of Soft Tissue: Investigation of Tear Resistance of Multi-fibrous Soft Tissue

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ABSTRACT

Tear resistance is one important mechanical property of multi-fibrous soft tissue indicating its ability to resist the effects of tearing. Multi-fibrous soft tissue such as skin consists of collagen fibres and soft matrix compositions which plays a critical role in tear resistance during tear extension. Due to the nonlinear elastic behaviour of the tissue, the evaluation of tear resistance remains a technical challenge. In this work, tear resistance of stationary cracks and growing cracks were investigated using Single Edge Notched (SEN) tensile testing. The stress intensity factor K (elastic energy relate G) and energy approach based on energy dissipated during tear extension was applied for stationary and growing cracks respectively. The tear resistance of stationary cracks with different ratio of notched length, a, to skin width, w, (a/w) were calculated by dividing the total strain energy U that stores in the samples with crack area A and the average values of tear resistance for a/w =0.1, 0.2, 0.3, and 0.4 are ~12.40, ~12.17, 11.88, and ~11.47 kJ/m^2 respectively. Finite element analysis (FEA) was used based on soft tissue properties to valid the tear resistance value from the experiments.

The tear resistance of a growing cracks were also calculated and the values vary from ~8.85 to ~19.95 kJ/m^2 with an average ~12.59 $\pm$ 2.91 kJ/m^2. We believe the approach and methods used in this work can be applicable to evaluation of other multi-fibrous biological soft tissues with similarity structure to skin. Tear resistance is considered to be a tissue parameter that can be used to identify the state of the tissue normal from defects.

Key Words: Tear resistance, Mechanical properties, Crack Extension, Skin, Nonlinear elastic, Biological soft tissue.