

# WAGGA

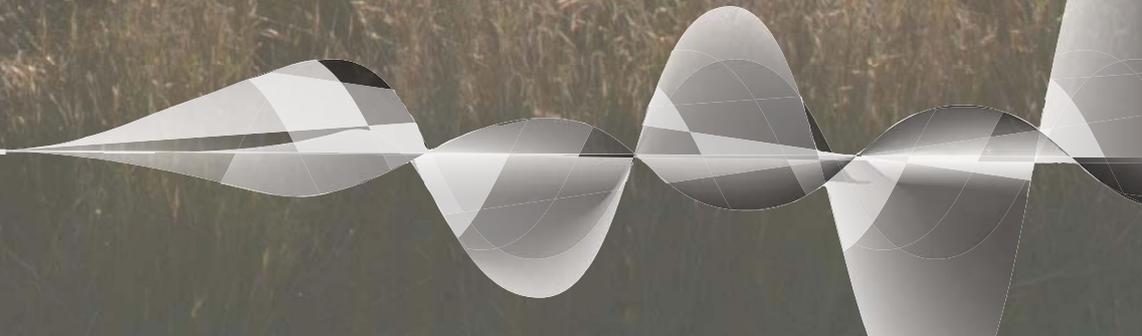


# 2017

## The 41<sup>st</sup> Annual Condensed Matter and Materials Meeting

31<sup>st</sup> January - 3<sup>rd</sup> February 2017  
Charles Sturt University  
Wagga Wagga, NSW, Australia

[www.wagga2017.unsw.edu.au](http://www.wagga2017.unsw.edu.au)





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School of Materials Science and Engineering  
School of Physics

Australian and New Zealand Institutes of Physics

# **41<sup>st</sup> Annual Condensed Matter and Materials Meeting**

Charles Sturt University, Wagga Wagga, NSW  
31<sup>st</sup> January 2017 – 3<sup>rd</sup> February 2017

## **CONFERENCE HANDBOOK**

 **2017 Organising Committee**

John Daniels • Clemens Ulrich  
Oleg Sushkov • Claudio Cazorla

The University of New South Wales, Kensington, NSW 2052,  
Australia

School of Material Science and Engineering @ UNSW  
School of Physics @ UNSW

**[www.wagga2017.unsw.edu.au](http://www.wagga2017.unsw.edu.au)**

## WWW 2017 Sponsor Details

**Australian Nuclear Science and Technology Organisation**  
**Australian Centre for Neutron Scattering**  
Locked Bag 2001  
Kirrawee DC NSW 2232



Australian Government

e-mail: [enquiries@ansto.gov.au](mailto:enquiries@ansto.gov.au)  
phone: +61 2 9717 3111  
<http://www.ansto.gov.au>



**Vacuum Society of Australia**



e-mail: [support@vacuumsociety.org.au](mailto:support@vacuumsociety.org.au)

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## WWW 2017 Sponsor Details

### **John Morris Scientific**

PO Box 447,  
Willoughby, NSW 2068



e-mail: [info@johnmorris.com.au](mailto:info@johnmorris.com.au)  
Phone: 1800 251 799  
Fax: 1800 446 926

[www.johnmorris.com.au](http://www.johnmorris.com.au)

### **Scitek**

Unit 1, 12 Chaplin Drive  
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e-mail: [contact@scitek.com.au](mailto:contact@scitek.com.au)  
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## WWW 2017 The CMM Group

The Annual Condensed Matter and Materials Meeting (CMM Meeting) is one of the oldest conference series in Australia and New Zealand and has gained great international reputation since its first iteration in 1977. It is a joint conference series between Australia and New Zealand, i.e. three years in a row it is held at the Charles Sturt University in Wagga Wagga NSW and the fourth year in New Zealand. Typically, around 100 scientists and research students attend the conference from the leading research organizations (ANSTO, CSIRO) and leading universities (UNSW, ANU, University of Sydney, UTS, UoW, etc.) throughout Australia, as well as from overseas countries (NZ, USA, Japan, China, Germany, France, Brasil, etc.).

The conference topics cover a broad range of specialty areas in condensed matter physics and materials science. Particular emphasis is focused on novel multifunctional properties, solid-state magnetism and superconductivity, 2D quantum materials, advanced characterisation methods, and other recent developments in condensed matter research.

Conference home page: <http://www.wagga2017.unsw.edu.au/>

The conference covers:

- Experimental Approaches + Theory and Modelling in Condensed Matter Physics, Material Sciences and Chemistry.
- State of the art Lab based techniques such as Optical Spectroscopy, AFM, electron microscopy or real space techniques with atomic resolution.
- Research performed at national as well as international large scale research facilities such as Neutron research and Synchrotron facilities.

The presented results allow researchers to obtain a fundamental understanding of the microscopic phenomena involved in modern materials and will as such enable a systematic search for novel materials with new functionalities in areas such as:

- rechargeable batteries
- solar cells
- novel multifunctional materials, application as sensor materials
- magnetic, electronic and photonic materials
- nanoscience and nanotechnology, in particular information technology
- surface and interface science – catalytic reactions

Therefore, the conference supports new innovations which will lead to industrial applications, i.e. in energy storage and solar cells, sensor applications, or in information technology. The invaluable exchange of ideas between scientists during this conference will enable new collaborations between research institutes and with industry.

The conference gives students and young scientists the opportunity to present their results in order to get critical and fruitful feedback and allow them to establish future collaborations.

**Conference organizers of the previous years:**

- 41<sup>st</sup> CMMM in 2017 The University of New South Wales (J. Daniels, C. Ulrich)
- 40<sup>th</sup> CMMM in 2016 The Australian Synchrotron (Anton Tadich)
- 39<sup>th</sup> CMMM in 2015 University of Wollongong (Roger Lewis)
- 38<sup>th</sup> CMMM in 2014 University of Auckland, (Tilo Soehnel) Waiheke Island NZ
- 37<sup>th</sup> CMMM in 2013 Bragg Institute, ANSTO (G. McIntyre)
- 36<sup>th</sup> CMMM in 2012 UNSW@ADFA (Wayne Hutchison)
- 35<sup>th</sup> CMMM in 2011 UNSW (Jaan Oitmaa)
- 34<sup>th</sup> CMMM in 2010 University of Auckland, (Tilo Soehnel) Waiheke Island NZ
- 33<sup>rd</sup> CMMM in 2009 CSIRO and Monash University (Tim Bastow)
- 32<sup>nd</sup> CMMM in 2008 UTS and Uni. Sydney (M.B. Cortie, Chris Ling)

An extended list is available on the website of the Australian Institute of Physics:

**<http://aip.org.au/annual-cmm-meetings/>**

**Take a look at the CMM Group website**

It can be accessed from the AIP national web site ([www.aip.org.au](http://www.aip.org.au)) by clicking on **AIP Groups** listed under “Related Groups” in the column at the left of the home page and then selecting **Condensed Matter and Materials Group (CMM)**. Alternatively, you can go directly to [pems.unsw.adfa.edu.au/cmm](http://pems.unsw.adfa.edu.au/cmm).

**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 to Glen Stewart ([g.stewart@adfa.edu.au](mailto:g.stewart@adfa.edu.au)) who will have them incorporated into the history section of the CMM Group website. 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.

**Organising committee**

John Daniels and Clemens Ulrich

**Program committee**

Clemens Ulrich, John Daniels, Oleg Sushkov and Claudio Cazorla

# 2017 Information for Participants

## 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 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 Shiralee Hillam at 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 10:00.

## Meals, Refreshments and Recreational Facilities

All meals will be served in the dining room, except the Conference Dinner on Wednesday, which will be held in the Convention Centre. You will receive a dining room pass on registration and a ticket to the Conference Dinner. The dining room pass must be presented at every meal. It may also be required as identification for use of all other campus facilities, which are at your disposal.

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 is open on weekdays from 12:00 until 18:00, as are the adjacent gymnasium (6:00-21:00) and squash courts. Tennis courts opposite the oval are also available. A wide range of facilities such as exercise bikes, weight training, table tennis, and basketball are available in the gymnasium. Access to these facilities is covered by your registration fee.

## Convention Centre Contact Numbers:

[wagga@unsw.edu.au](mailto:wagga@unsw.edu.au)

Registration Desk Phone (02) 6933 4989

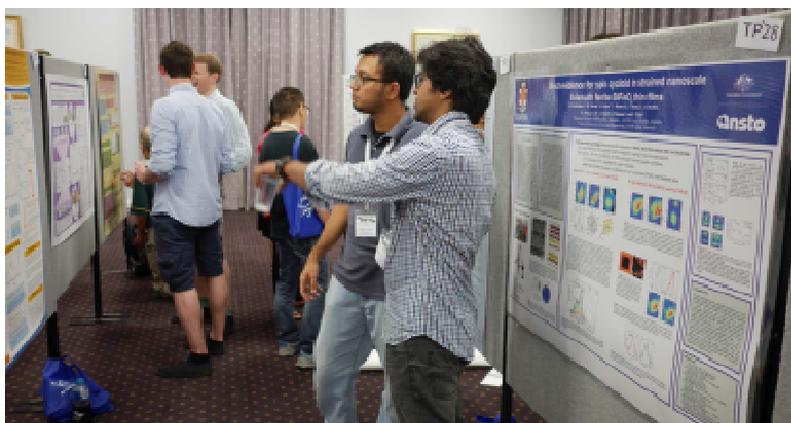
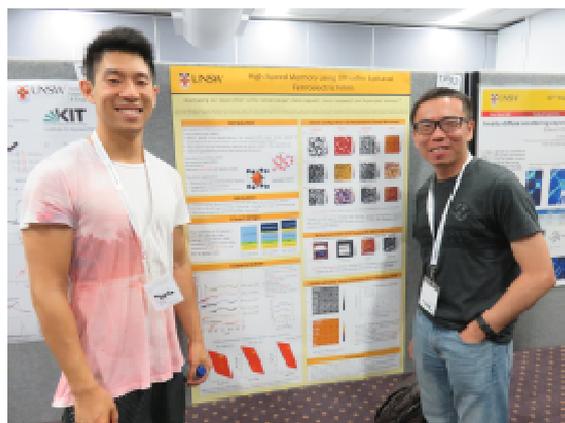
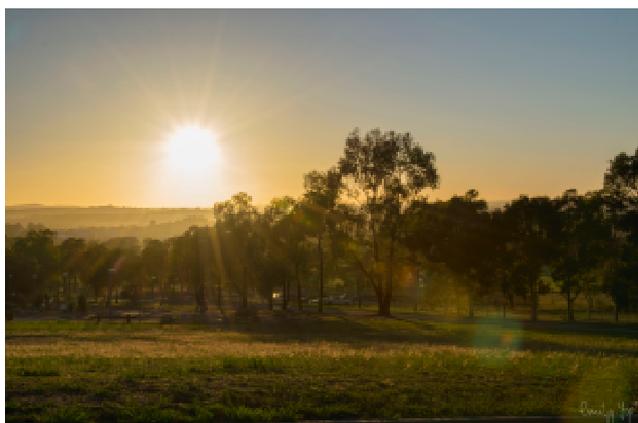
Convention Centre Office Phone (02) 6933 2606 Fax (02) 6933 2643

Events Office Phone (02) 6933 4974

After-hours Emergencies, Accommodation and Security Phone (02) 6933 2288

Internet access: **eduroam** internet access is available within the Convention Centre

# Impressions from Wagga Wagga 2016



## 2017 Conference Site – MAPS

### **Venue**

The venue for the Wagga meeting is at the Conference Centre of Charles Sturt University, Wagga Wagga campus. Wagga Wagga, NSW, is roughly equally distant, and within driving distance (just under 500 km), from Sydney and Melbourne.

### **Accommodation**

Comfortable student style accommodation is available within the University grounds. The air-conditioned rooms are constructed as single bed/study style accommodation, with access to shared bathroom and kitchen facilities. All cottages are a short walk from the Conference Centre. While staying on the grounds at Charles Sturt University, you are welcome to use the sporting facilities at the Wagga Wagga Campus, if available. These include outdoor swimming pool, gymnasium, tennis and squash courts.

### **About Charles Sturt University, Wagga Wagga Campus**

The Charles Sturt University Winery is an integral part of Australia's leading wine and food science school and, as such, is at the forefront of viticultural practices and wine making techniques. The Winery is located within the University grounds at Wagga Wagga. It was built in 1977 to support the Charles Sturt University teaching program. In 1990 the winery was restructured to become a commercial enterprise. The winery produces its own range of premium table, fortified and sparkling wines and has been awarded 22 trophies, 84 gold, 164 silver and 379 bronze medals in national wine shows.

The Charles Sturt University Cheese Factory was completed in 1998 with the Cheesemaker commencing in August of that year. Sales of cheese commenced in April 1999 from the Winery Cellar Door. As sales and reputation grew the distribution widened to stores throughout New South Wales and Victoria.

### **Address:**

Charles Sturt University  
Boorooma Street  
North Wagga NSW

### **About Wagga Wagga**

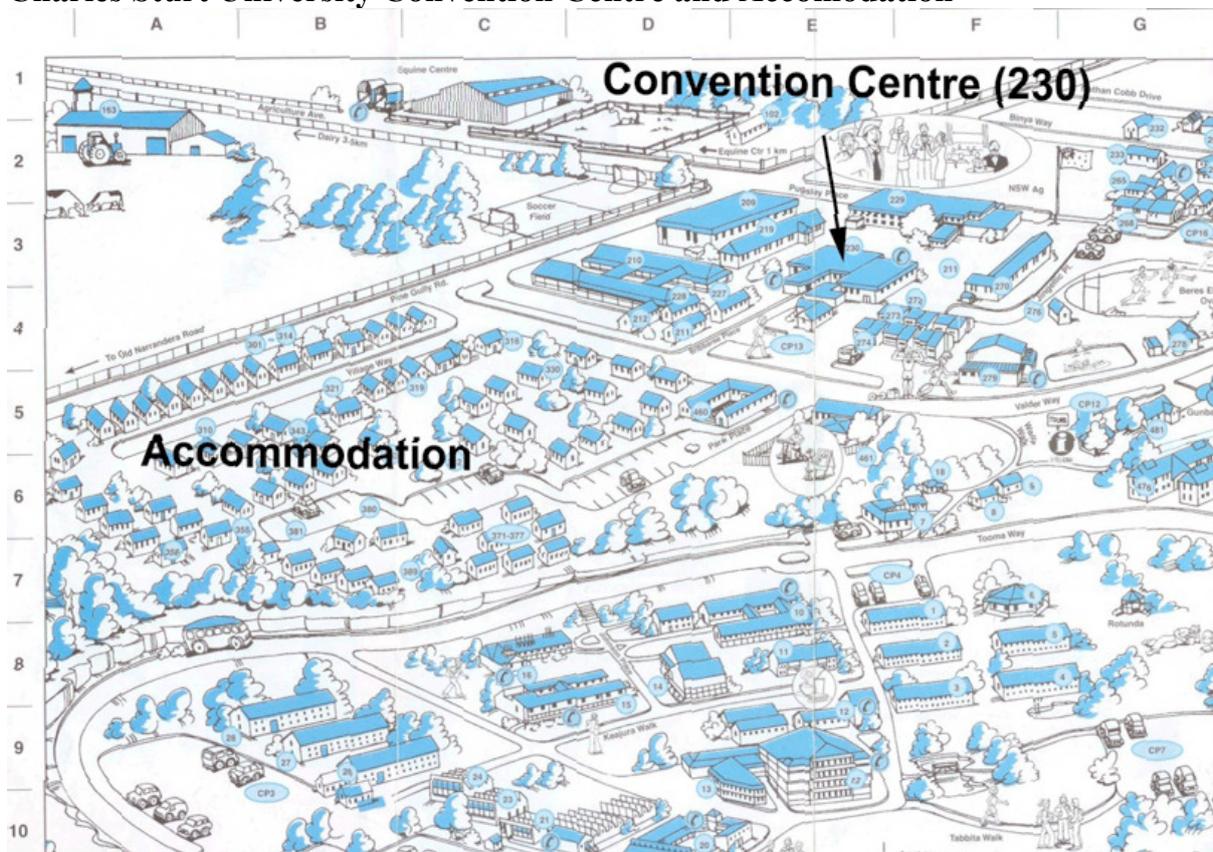
Wagga Wagga is in the centre of Australia's population triangle between Sydney, Canberra, Melbourne and Adelaide. It is accessible by air and rail services from both major cities. A region of sweeping contrasts and natural beauty where there is time to enjoy and reflect. Wagga Wagga is an 'events' City with major festivals occurring throughout the year. We have one of the longest main streets in Australia, which is lined with major national retailers, boutique stores, antique shops, commercial galleries and modern malls. The region also boasts an inland cultural oasis of live music, performing arts, galleries and arts & crafts.

For further information, visit [www.waggawaggaaustralia.com.au](http://www.waggawaggaaustralia.com.au)

### Wagga Wagga and the location of the Charles Sturt University campus

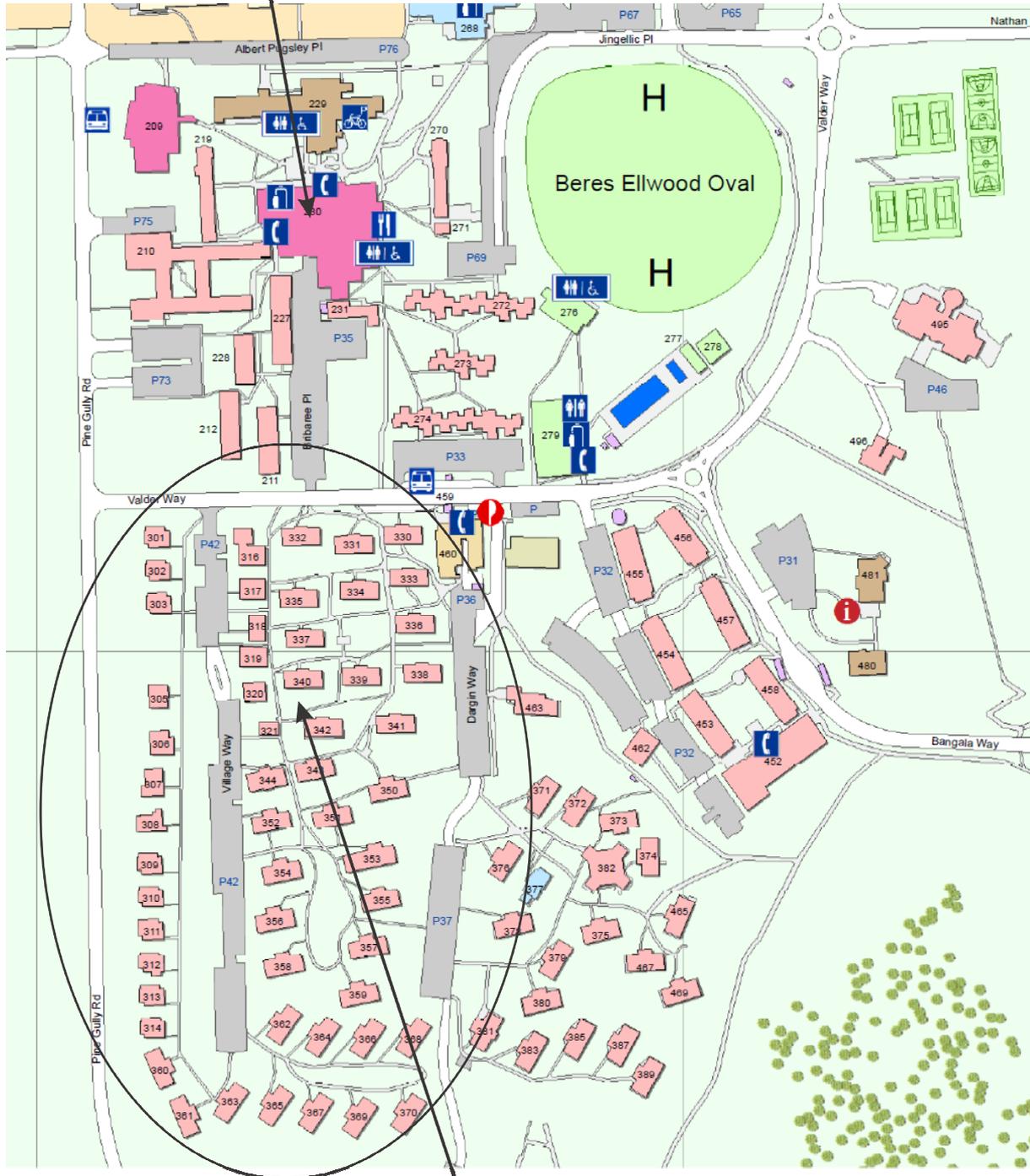


### Charles Sturt University Convention Centre and Accommodation



Charles Sturt University – Wagga Wagga Campus Directory

Conference Centre



Accommodation Area

## WWW 2017 Sponsor Details

**Lastek**  
10 Reid St  
Thebarton SA 5031  
Australia



e-mail: [sales@lastek.com.au](mailto:sales@lastek.com.au)  
Phone: 08 8443 8668  
Fax: 08 8443 8427

[www.lastek.com.au](http://www.lastek.com.au)

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Michael Anderson  
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Fax: +61 2 9748 7855

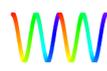
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Chirnside Park VIC 3116, Australia  
e-mail: [vic@ezzivision.com.au](mailto:vic@ezzivision.com.au)



Sydney Office  
B1/101 Rookwood Road,  
Yagoona NSW 2199, Australia  
e-mail: [nsw@ezzivision.com.au](mailto:nsw@ezzivision.com.au)  
phone: 1-800-46 3994 (1 800 GO EZZI)

[www.ezzivision.com.au](http://www.ezzivision.com.au)


**2017 List of Participants**

Last Name	First Name	Institution/Company	Email
Allison	Morgan	University of Sydney	mall6357@uni.sydney.edu.au
Alruwaili	Amani	RMIT	hhhhhh11@windowlive.com
Amjadipour	Mojtaba	Queensland Uni. Tech.	mojtaba.amjadipour@qut.edu.au
Bladwell	Samuel	UNSW	s.bladwell@unsw.edu.au
Bowden	Graham	University of Southampton	gjb@phys.soton.ac.uk
Burns	Stuart	UNSW	s.r.burns@student.unsw.edu.au
Cadogan	Sean	UNSW	s.cadogan@adfa.edu.au
Campbell	Stewart	UNSW Canberra	stewart.campbell@adfa.edu.au
Carter	James	John Morris Group	jamesc@johnmorris.com.au
Cashion	John	Monash University	john.cashion@monash.edu
Causar	Grace	ANSTO	glc052@uowmail.edu.au
Cedergren	Karin	UNSW	k.cedergren@unsw.edu.au
Chen	Ying	Deakin University	ian.chen@deakin.edu.au
Cortie	David	University of Wollongong	d.l.cortie@gmail.com
D'Adam	Tim	ANSTO/UNSW	timd@ansto.gov.au
Daniels	John	UNSW	j.daniels@unsw.edu.au
Deng	Guochu	ANSTO	guochu.deng@ansto.gov.au
Elewa	Nancy	UNSW Canberra	nancy.elewa@student.adfa.edu.au
Esan	Olajide Olakunle	Ekwusigo Local Government	ekwusigo@yahoo.com
Escobedo-Diaz	Juan Pablo	UNSW Australia	j.escobedo-diaz@adfa.edu.au
Etheridge	Joanne	Monash University	joanne.etheridge@monash.edu
Fiedler	Andrea	John Morris Group	andrea@johnmorris.com.au
Fuhrer	Michael	Monash University	michael.fuhrer@monash.edu
Hirai	Tadahiko	CSIRO	tadahiko.hirai@csiro.au
Hutchison	Wayne	UNSW Canberra	w.hutchison@adfa.edu.au
Iles	Gail	ANSTO	gail.iles@ansto.gov.au
Jahangir	Solmaz	UNSW	s.jahangir@student.unsw.edu.au
Kaneko	Taka	Ezzi Vision Pty Ltd	taka@ezzivacuum.com.au
Kareri	Yousef	UNSW	z3391688@unsw.edu.au
Kharkov	Yaroslav	UNSW	y.kharkov@gmail.com
Kim	Dohyung	UNSW	dohyung.kim@student.unsw.edu.au
Kong	Scarlet	UNSW Australia	scarlet.kong@student.unsw.edu.au
Lee	Wai Tung	ANSTO	wtl@ansto.gov.au
Lee	Stanley	ANSTO/ Vacuum Soc. Aus.	stanley.lee@ansto.gov.au
Lewis	Roger	University of Wollongong	roger@uow.edu.au
Li	Xi	ANSTO	cissy346@gmail.com
Ling	Chris	University of Sydney	chris.ling@sydney.edu.au
Liss	Klaus-Dieter	ANSTO	kdl@ansto.gov.au
Liu	Lisha	UNSW	lisha.liu@student.unsw.edu.au
MacLeod	Jennifer	Queensland Uni. Tech.	jennifer.macleod@qut.edu.au

41<sup>st</sup> Annual Condensed Matter and Materials Meeting

Makmor	Nazrul Fariq	UNSW	n.makmor@student.adfa.edu.au
Mantri	Sukriti	UNSW	s.mantri@unsw.edu.au
Marlton	Frederick	UNSW	f.marlton@unsw.edu.au
Martin	Andy	University of Melbourne	martinam@unimelb.edu.au
McIntyre	Garry	ANSTO	garry.mcintyre@ansto.gov.au
Miserev	Dmitry	UNSW	d.miserev@unsw.edu.au
Musavi Gharavi	Paria Sadat	UNSW	p.musavigharavi@student.unsw.edu.au
O'Brien	Joel	UNSW	j.obrien@student.unsw.edu.au
Oitmaa	Jaan	UNSW	j.oitmaa@unsw.edu.au
Ostrovskaya	Elena	Australian National University	elena.ostrovskaya@anu.edu.au
Paull	Oliver	ANSTO / U. Wollongong	ohcp627@uowmail.edu.au
Pereira	Jose	University of Copenhagen, DK	jose.enedilton@nbi.ku.dk
Polt	Julia	University of Sydney	jpol6668@uni.sydney.edu.au
Reilly	David	University of Sydney	david.reilly@sydney.edu.au
Ruck	Ben	Victoria Uni. Wellington, NZ	Ben.Ruck@vuw.ac.nz
Rybachuk	Maksym	Griffith University	m.rybachuk@griffith.edu.au
Saad	Hatem	UNSW Canberra	Hatem.Saad@student.adfa.edu.au
Sando	Daniel	UNSW	daniel.sando@unsw.edu.au
Saunders	Philip	Radiation Saunders	Phil@radsaunders.com
Saunders	Robert	Radiation Saunders	Rob@radsaunders.com
Schappeler	Tobias	Scitek	tobias@scitek.com.au
Sellar	Jeffrey	Monash University	jeff.sellar@monash.edu
Simmons	Michelle	CQCT/UNSW	michelle.simmons@unsw.edu.au
Smith	Andrew	Monash University	andrew.e.smith@monash.edu
Söhnél	Tilo	University of Auckland, NZ	t.soehnel@auckland.ac.nz
Stampfl	Anton	ANSTO	aps@ansto.gov.au
Stampfl	Catherine	University of Sydney	catherine.stampfl@sydney.edu.au
Stewart	Glen	UNSW Canberra	g.stewart@adfa.edu.au
Sushkov	Oleg	UNSW	sushkov@unsw.edu.au
Tadich	Anton	Australian Synchrotron	anton.tadich@synchrotron.org.au
Tian	Ruoming	Toyota Research Institute JPN	r.tian@toyotariken.jp
Tung	Patrick	UNSW	tungpatrick@gmail.com
Ulrich	Clemens	UNSW	c.ulrich@unsw.edu.au
Valanoor	Nagarajan	UNSW	nagarajan@unsw.edu.au
Wang	Lijun	UNSW	lijun.wang1@unsw.edu.au
White	Reyner	UNSW Canberra	Reyner.White@student.adfa.edu.au
Winkler	Richard	UNSW	r.winkler@student.unsw.edu.au
Wolba	Benjamin	UNSW/TU Dresden	benjamin.wolba@student.unsw.edu.au
Yan	Lianghong	China Academy of Physics	yanlianghong@126.com
Yang	Jianliang	University of Southampton UK	j.yang@soton.ac.uk
Yap	Emily Wern Jien	UNSW/CSIRO	emily.yap@student.unsw.edu.au
Zhang	Hao	University of Wollongong	hz968@uowmail.edu.au
Zhang	Qi	UNSW	peggy.zhang@unsw.edu.au
Zhou	Yanyu	UNSW	yanyu.zhou@student.unsw.edu.au

## WWM 2017 Program Overview

### Tuesday 31 January

14:00 –	Registration desk open
16:00 – 18:00	<i>Conference bar open</i>
18:00 – 19:30	<i>Dinner</i>
19:00 –	Posters WP can be mounted

### Wednesday 1 February

07:30 – 08:30	<i>Breakfast</i>
08:40 – 08:50	Conference Opening
<b>08:50 – 10:30</b>	<b>Oral Session: WM</b>
10:30 – 11:00	<i>Morning tea</i>
<b>11:00 – 12:30</b>	<b>Oral Session: WN</b>
12:30 – 14:00	<i>Lunch</i>
<b>14:00 – 15:40</b>	<b>Oral Session: WA</b>
<b>15:40 – 16:00</b>	<b>Poster Slam: WP</b>
16:00 – 16:30	<i>Afternoon Tea</i>
<b>16:00 – 18:00</b>	<b>Poster Session: WP</b>
18:00 –	Posters TP can be mounted
18:30 – 22:00	Conference Dinner (After Dinner Talk)

### Thursday 2 February

07:30 – 08:30	<i>Breakfast</i>
<b>08:50 – 10:30</b>	<b>Oral Session: TM</b>
10:30 – 11:00	<i>Morning tea</i>
<b>11:00 – 12:30</b>	<b>Oral Session: TN</b>
12:30 – 14:00	<i>Lunch</i>
<b>14:00 – 15:30</b>	<b>Oral Session: TA</b>
<b>15:30 – 16:00</b>	<b>Poster Slam: TP</b>
16:00 – 16:30	<i>Afternoon Tea</i>
<b>16:00 – 18:00</b>	<b>Poster Session: TP</b>
16:30 – 18:00	<i>Conference bar open</i>
18:00 – 19:30	<i>Dinner</i>
19:30 – 22:00	Trivia Night (Lindsay Davis Cup)

### Friday 3 February

07:30 – 08:30	<i>Breakfast</i>
<b>08:50 – 10:30</b>	<b>Oral Session: FM</b>
10:30 – 11:00	<i>Morning tea</i>
<b>11:00 – 12:20</b>	<b>Oral Session: FN</b>
12:20 – 12:40	Presentations and Closing
12:30 – 14:00	<i>Lunch</i>



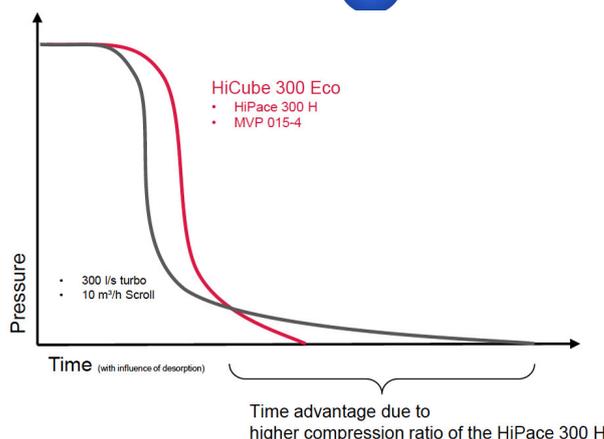
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## 2017 Invited Speakers

### *Invited After Dinner Talk*

**Prof. Michelle Simmons**, Director, Centre for Quantum Computation & Communication Technology, School of Physics, UNSW Australia

### *Invited Speakers*

**Dr David Cortie**, ANU College of Physical and Mathematical Sciences, ANU  
*Resolving spin dynamics at the nanometer-scale with radioactive ion-beams*

**Prof. Joanne Etheridge**, Department of Materials Science and Engineering - Monash Centre for Electron Microscopy, Monash University  
*Probing condensed matter with the modern fast electron*

**Prof. Michael Fuhrer**, School of Physics & Astronomy - Monash Centre for Atomically Thin Materials, Monash University  
*Electronic Properties of High-Quality Epitaxial Topological Dirac Semimetal Thin Films*

**Prof. Roger Lewis**, School of Physics - Institute for Superconducting and Electronic Materials, University of Wollongong  
*Terahertz Condensed Matter Physics*

**A/Prof. Andy Martin**, School of Physics, The University of Melbourne  
*Vortices, Vortex Lattices and the possibility of exotic superfluidity in dipolar quantum gases*

**A/Prof. Elena Ostrovskaya**, Research School of Physics & Engineering, ANU College of Physical & Mathematical Sciences, Australian National University  
*Condensation of exciton-polariton in structured microcavities*

**Prof. David Reilly**, Microsoft Corporation - Centre for Engineered Quantum Systems, The University of Sydney  
*Quantum Information Machines*

**A/Prof. Ben Ruck**, School of Chemical and Physical Sciences, Victoria University of Wellington  
*Novel magnetism, superconductivity, and spintronics potential in rare earth nitrides*

**Prof. Cathy Stampfl**, School of Physics - Condensed Matter Theory Group, The University of Sydney  
*Exploring New Materials for Nanoelectronics from ab initio Theory*

A photograph of a laboratory setting at ANSTO. In the foreground, a man in a grey polo shirt is adjusting a large, green cylindrical instrument mounted on a metal cart. A woman in a dark blue polo shirt stands behind the cart, smiling. The background shows a large industrial facility with a curved structure and various equipment. The top of the image features a blue gradient with light streaks.

  
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# WVW 2017 Program Details

## Tuesday 31 January

14:00 –	Registration desk open
16:00 – 18:00	<i>Conference bar open</i>
18:00 – 19:30	<i>Dinner</i>
19:00 –	Posters WP can be mounted

## Wednesday 1 February

<b>08:40 – 08:50</b>		<b>Opening: John Daniels and Clemens Ulrich (UNSW)</b>	
<b>08:50 – 10:30</b>	<b>WM</b>	<b>Low Dimensional Electronic Systems</b> Chairperson: Clemens Ulrich (UNSW)	
08:50 – 09:20	WM1	Electronic Properties of High-Quality Epitaxial Topological Dirac Semimetal Thin Films <i>Michael S. Fuhrer, Monash University</i>	INVITED
09:20 – 09:50	WM2	Exploring New Materials for Nanoelectronics from ab initio Theory <i>Catherine Stampfl, University of Sydney</i>	INVITED
09:50 – 10:10	WM3	Graphene heterostructures: towards a material for 2D electronics <i>Mojtaba Amjadipour, Queensland University of Technology</i>	
10:10 – 10:30	WM4	Hybrid graphite-like/polymer-like amorphous carbon materials by plasma synthesis <i>M. Rybachuk, Griffith University</i>	
<b>10:30 – 11:00</b>		<b>Morning Tea</b>	
<b>11:00 – 12:30</b>	<b>WN</b>	<b>Magnetism</b> Chairperson: Garry McIntyre (ANSTO)	
11:00 – 11:30	WN1	Resolving spin dynamics at the nanometer-scale with radioactive ion-beams <i>David Cortie, University of British Columbia, Canada, ANU</i>	INVITED
11:30 – 11:50	WN2	It has it all: Cu <sub>5</sub> Sb <sub>2</sub> SiO <sub>12</sub> - Seven crystallographic independent positions for Cu <sup>2+</sup> in one compound <i>Tilo Söhnel, University of Auckland, NZ</i>	
11:50 – 12:10	WN3	Magnetic Structure and Spin Dynamics of Multiferroic System Co <sub>4</sub> Nb <sub>2</sub> O <sub>9</sub> <i>Guochu Deng, Australia Center for Neutron Scattering</i>	
12:10 – 12:30	WN4	Exotic oxide species and oxygen dynamics in the double perovskites Sr <sub>3-x</sub> Y <sub>x</sub> NbO <sub>5.5+1/2x</sub> <i>J. Polt, University of Syd0065y</i>	
<b>12:30 – 14.00</b>		<b>Lunch</b>	

<b>14:00 – 15:40</b>	<b>WA</b>	<b>Material Science: Ferroelectrics and Thermoelectrics</b> Chairperson: Daniel Sando (UNSW)
14:00 – 14:20	WA1	Magnetic and structural transitions in magnetocaloric Mn(Co <sub>1-x</sub> Ni <sub>x</sub> )Ge alloys <i>Wayne D. Hutchison, UNSW Canberra</i>
14:20 – 14:40	WA2	Inorganic-organic hybridization: new strategy for flexible thermoelectric devices <i>Ruoming Tian, Toyota Research Institute, Nagakute</i>
14:40 – 15:00	WA3	Five dimensional analysis of ferroelectric domain continuity over grain boundaries <i>Sukriti Mantri, UNSW</i>
15:00 – 15:20	WA4	Magnetic switching along hard-axes in Er-doped DyFe <sub>2</sub> /YFe <sub>2</sub> thin films <i>G. J. Bowden, University of Southampton, UK</i>
15:20 – 15:40	WA5	Magneto-Electronic Hydrogen Gas Sensing <i>G. L. Causer, ANSTO</i>
<b>15:40 – 16:00</b>	<b>WP</b>	<b>Poster Slam: WP</b>
<b>16:00 – 16:30</b>		<b>Afternoon Tea</b>
<b>16:30 – 18:00</b>	<b>WP</b>	<b>Poster Session</b>
19:00 -		Posters TP can be mounted
<b>18:30 – 22:00</b>		<b>Conference Dinner</b> <b>After Dinner Talk: Michelle Simmons, UNSW</b>

**Thursday 2 February**

<b>08:50 – 10:30</b>	<b>TM</b>	<b>Low Dimensional Electronic Systems</b> Chairperson: John Daniels (UNSW)	
08:50 – 09:20	TM1	Quantum Information Machines <i>David Reilly, Microsoft Corp., University of Sydney</i>	INVITED
09:20 – 09:50	TM2	Condensation of exciton-polariton in structures microcavities <i>Elena Ostrovskaya, Australian National University</i>	INVITED
09:50 – 10:10	TM3	A two-dimensional hydrogen-bonded molecular substitutional solid solution <i>Jennifer M. MacLeod, Queensland University of Technology</i>	
10:10 – 10:30	TM4	Modeling Conductive Domain Walls by means of Random Resistor Networks <i>Benjamin Wolba, Technical University Dresden Germany</i>	
<b>10:30 – 11:00</b>		<b>Morning Tea</b>	
<b>11:00 – 12:30</b>	<b>TN</b>	<b>Optics and Spectroscopy</b> Chairperson: Tilo Söhnle (University of Auckland)	
11:00 – 11:30	TN1	Terahertz Condensed Matter Physics <i>Roger A. Lewis, University of Wollongong</i>	INVITED
11:30 – 11:50	TN2	Molecule-Induced Conformational Change in 2D Nanomaterials with Enhanced Surface Adsorption <i>Ying Chen, Deakin University</i>	
11:50 – 12:10	TN3	A Novel Vertical-type Light-Emitting Transistor and Approach to Normally-OFF Operation <i>Tadahiko Hirai, CSIRO, Clayton</i>	
12:10 – 12:30	TN4	Towards ARPES at the Australian Synchrotron: 4th Generation Toroidal Angle Resolving Electron Energy Spectrometer <i>Anton Tadich, Australian Synchrotron, Clayton</i>	
<b>12:30 – 14:00</b>		<b>Lunch</b>	
<b>14:00 – 15:30</b>	<b>TA</b>	<b>Condensed Matter: Structures</b> Chairperson: Jeffrey Sellar (Monash University)	
14:00 – 14:30	TA1	Probing condensed matter with the modern fast electron <i>J. Etheridge, Monash University</i>	INVITED
14:30 – 14:50	TA2	Phase transformations and associated microstructural evolution during shock compression of materials <i>J.P. Escobedo-Diaz, UNSW Canberra</i>	
14:50 – 15:10	TA3	Towards Generic Mathematical Descriptors for Structural Analysis and Their Applications in the Property Predictions for Molecular Crystals <i>Jack Yang, University of Southampton, UK</i>	
15:10 – 15:30	TA4	Laser-induced Ignition of RDX Explosive Crystals <i>X.T. Zu, University of Electronic Science and Technology of China, Chengdu, China</i>	
<b>15:30 – 16:00</b>	<b>TP</b>	<b>Poster Slam: TP</b>	
<b>16:00 – 18:00</b>	<b>TP</b>	<b>Poster Session and Afternoon Tea</b>	
<b>19:30 – 22:00</b>		<b>Trivia Night (Lindsay Davis Cup)</b>	

**Friday 3 February**

<b>08:50 – 10:30</b>	<b>FM</b>	<b>Superconductivity and Bose-Einstein Condensates</b> Chairperson: Sean Cadogan (UNSW Canberra)
08:50 – 09:20	FM1	Vortices, Vortex Lattices and the possibility of exotic superfluidity in dipolar quantum gases <i>Andy Martin, University of Melbourne</i> INVITED
09:20 – 09:50	FM2	Novel magnetism, superconductivity, and spintronics potential in rare earth nitrides <i>B.J. Ruck, Victoria University of Wellington, NZ</i> INVITED
09:50 – 10:10	FM3	Approaching the Bose glass-superfluid quantum phase transition using nano-structured chains of Josephson junctions <i>K. Cedergren, UNSW</i>
10:10 – 10:30	FM3	Mechanisms of the in-plane g-factor anisotropy in p-type quantum point contacts <i>D.S. Miserev, UNSW</i>
<b>10:30 – 11:00</b>		<b>Morning Tea</b>
<b>11:00 – 12:20</b>	<b>FN</b>	<b>Material Science: Complementary Techniques</b> Chairperson: Oleg Sushkov
11:00 – 11:20	FN1	Structural Evolution of Metals at High Temperature: Complementary Investigations with Neutron and Synchrotron Quantum Beams <i>Klaus-Dieter Liss, ANSTO</i>
11:20 – 11:40	FN2	Spectroscopic Studies of Glycine/Alumina Surfaces <i>Anton Stampfl, ANSTO</i>
11:40 – 12:00	FN3	Pressure-induced valence transitions: squeezing electrons from big orbitals to smaller ones <i>C.D. Ling, The University of Sydney</i>
12:00 – 12:20	FN4	Hydrogen bond dynamics, conformational flexibility and polymorphism in antipsychotics <i>José E.M. Pereira, Niels Bohr Institute, University of Copenhagen, Denmark</i>
<b>12:20 – 12:40</b>		<b>Awards and Closing</b> John Daniels, Oleg Sushkov and Clemens Ulrich (UNSW)
<b>12:40 – 14.00</b>		<b>Lunch</b>

## 2017 Poster Session

### POSTER WEDNESDAY: WP1 – WP21

- WP1** Application of Linear Spin Wave Theory to the Cr<sub>8</sub> Antiferromagnetic Heisenberg Ring  
*T. D'Adam, R. Mole and J. Stride*
- WP2** Structure and magnetic properties of the AB<sub>3</sub>Si<sub>2</sub>Sn<sub>7</sub>O<sub>16</sub> layered oxides  
*M. Allison, C. Ling, S. Schmid, M. Avdeev, G. Stuart and T. Söhnle*
- WP3** Mössbauer Study of the Coolidge carbonaceous chondrite meteorite  
*Nancy N. Elewa and J. M. Cadogan*
- WP4** Investigation on the Nature of the Verwey Transition in Cu-doped Fe<sub>3</sub>O<sub>4</sub>  
*Yousef Kareri, F. Chang, J. Hester and C. Ulrich*
- WP5** Investigations of the Magnetic and Crystal Field Excitations in Orthorhombically Distorted Perovskites RVO<sub>3</sub> (R = Dy, Tb, Pr, Ce)  
*Joel O'Brien, N. Reynolds, R. Mole, P. Rovillain, S. Danilkin, K. Schmalzl, M. Reehuis, S. Miyasaka, F. Fujioka, Y. Tokura, B. Keimer, G. McIntyre, and C. Ulrich*
- WP6** Crystal field excitations for Ho<sup>3+</sup> in HoFeO<sub>3</sub>  
*G.A. Stewart, G.N. Iles, R.A. Mole, Z. Yamani and D.H. Ryan*
- WP7** Magnetic Transitions and Magnetocaloric Effect in MnCoGe<sub>1-x</sub>Al<sub>x</sub>  
*N. F. Makmor, W. D. Hutchison, Q. Y. Ren and J. L. Wang*
- WP8** Investigation of the magnetism of RTi<sub>2</sub>Ga<sub>4</sub> (R = Er, Ho, Dy) intermetallic compounds  
*Hatem Saad, W.D. Hutchison and J.M. Cadogan*
- WP9** Determination of the Crystal Field Levels in TmV<sub>2</sub>Al<sub>20</sub>  
*R. White, W.D. Hutchison, G.N. Iles, R.A. Mole, J.M. Cadogan, T. Namiki and K. Nishimura*
- WP10** Multiple Magnetic Phases in DyNiAl<sub>4</sub>  
*R. White, W.D. Hutchison and M. Avdeev*
- WP11** Analysis of interfacial structure and chemistry in FeV<sub>2</sub>O<sub>4</sub>-based heterostructures on (001)-oriented SrTiO<sub>3</sub>  
*Y. Zhou, D. Zhou, D. R. M. Mitchel, N. Valanoor and P. R. Munroe*

- WP12** Magnetic Proximity Effect in YBCO/STO/LCMO Multilayers  
*O. Paull, G. Causer, A. V. Pan and F. Klose*
- WP13** Spatial modulation of a superconducting order in cuprates  
*Y. Kharkov and O. Sushkov*
- WP14** Interference effects in magnetic focusing with strong spin orbit interactions  
*S. Bladwell and O. P. Sushkov*
- WP15** Growth of Graphene on 3C-SiC Nanostructures by UHV Annealing  
*Mojtaba Amjadi Pour, Jennifer MacLeod, Josh Lipton-Duffin, Francesca Iacopi, Jose Alarco, and Nunzio Motta*
- WP16** CVD Synthesis of Transition Metal Dichalcogenides on Epitaxial Graphene/SiC  
*J. Bradford, J. Lipton-Duffin, M. Shafiei, J. MacLeod and N. Motta*
- WP17** Terahertz Spectroscopic Characterization for Carbon-based Materials  
*H. Zhang, J. Horvat and R. A. Lewis*
- WP18** PELICAN: cold-neutron time-of-flight spectrometer at the Australian Centre for Neutron Scattering  
*G.N. Iles, R.A. Mole and D.H. Yu*
- WP19** First users on EMU, the cold-neutron backscattering spectrometer at the Australian Centre for Neutron Scattering  
*G.N. Iles, N.R. de Souza and A. Klapproth*
- WP20** Design of a low-energy electron source for inverse photoelectron spectroscopy  
*Joshua A. Lipton-Duffin and Jennifer M. MacLeod*
- WP21** Investigation of the Emission of X-Rays in a Pyroelectric Micro X-Ray Generator  
*Emily W.J. Yap, Rhys M. Preston, James R. Tickner, John E. Daniels*

## WWW 2017 Poster Session

### POSTER THURSDAY: TP1 – TP21

- TP1** Integration of Polarised  $^3\text{He}$  Infrastructure with Sample Environment Equipment  
*T. D'Adam, N. Booth, G. Davidson, S. Lee, A. Manning, N. Timperon and P. Imperia*
- TP2** Polarised neutron diffraction study of the spin cycloid in strained nanoscale bismuth ferrite thin films  
*Wai Tung Lee, J. Bertinshaw, R. Maran, S. J. Callori, V. Ramesh, J. Cheung, S. A. Danilkin, S. Hu, J. Seidel, N. Valanoor, and C. Ulrich*
- TP3** Direct evidence for the spin cycloid in strained nanoscale bismuth ferrite  $\text{BiFeO}_3$  thin films  
*J. Bertinshaw, R. Maran, S. J. Callori, V. Ramesh, J. Cheung, S. A. Danilkin, W.T. Lee, S. Hu, J. Seidel, N. Valanoor, and C. Ulrich*
- TP4** Strain and Magnetic Field-Induced Spin Structure Transitions in Multiferroic  $\text{BiFeO}_3$   
*A. Agbelele, D. Sando, C. Toulouse, R. D. Johnson, R. Rüffer, A.F. Popkov, C. Carrétéro, J.-M. Le Breton, B. Dkhil, M. Cazayous, A. K. Zvezdin, A. Barthélémy, J. Juraszek, and M. Bibes*
- TP5** Tuning domain structure and domain conductivity in  $\text{BiFeO}_3$  thin films  
*V. Ramesh, D. Sando, Q. Zhang and N. Valanoor*
- TP6** In situ Poling and the Strong Post-poling Relaxation of non- $180^\circ$  Domain Texture in Bismuth Ferrite Ceramics  
*Lisha Liu and John Daniels*
- TP7** The Wonderful World of Oxide Interfaces through the Lens of A Transmission Electron Microscopy  
*P. S. Musavi Gharavi and Nagarajan Valanoor*
- TP8** Conduction Behaviour of Domains, Domain Walls, and Grain Boundaries in Pure and La-doped  $\text{BaTiO}_3$  Ceramics  
*Dohyung Kim, Marty Gregg and Jan Seidel*
- TP9** Reversible Polarization in  $\text{PbZrTiO}_3$  Bilayers Grown Upon Silicon Substrates  
*R.S. Winkler and N. Valanoor*

- TP10** Focused Ion Beam Methodologies pave the way for “Ferroelectronics”:  
Release the Kraken  
*S.R. Burns, J.M. Gregg and N. Valanoor*
- TP11** Epitaxial PbZr<sub>x</sub>Ti<sub>1-x</sub>O<sub>3</sub> ferroelectric bilayers with giant electromechanical  
properties  
*Guangqing Liu, Hsin-Hui Huang, Qi Zhang, Esther Huang, Ronald Maran,  
Hugh Simons, Zijian Hong, Osami Sakata, Yoshitaka Ehara, Takahisa,  
Shiraishi, Hiroshi Funakubo, Long-Qing Chen, Paul Munroe and  
Valanoor Nagarajan*
- TP12** Combinatorial high resolution scanning X-ray diffraction in lead-free  
piezoelectrics  
*F. Marlton, O. Standard and J. Daniels*
- TP13** Disordered structures in lead-free piezoelectrics from diffuse x-ray and neutron  
scattering  
*P. Tung, M. Major, J. Hudspeth, J. Daniels*
- TP14** Electron Diffraction from Micro- and Nano-structured cubic zirconia  
*Chris Yu Chen and J.R. Sellar*
- TP15** In-situ studies of β-based Ti-Al alloys using synchrotron X-ray and neutron  
diffraction  
*Xi Li, Klaus-Dieter Liss and Rian Dippenaar*
- TP16** High-Pressure Single-Crystal Neutron Diffraction  
*G.J. McIntyre, J. Binns and S. Parsons*
- TP17** Use of the Isolated Atom Model in Quantitative Convergent Beam Electron  
Diffraction  
*A.E. Smith, T. Liu, D. Peng, L. Bourgeois and P.N.H. Nakashima*
- TP18** In-situ study of solid state dewetting in single crystal Ni films  
*S. Jahangir, C. V. Thompson and N. Valanoor*
- TP19** Arsenic Removal from Groundwater by a Goethite-Coated Mineral Sand  
*S. Kahn, J.D. Cashion, A.F. Patti, W.P. Gates\* and S. Adeloju*
- TP20** Boron Nitride Nanosheets Improve Sensitivity and Reusability of  
Surface-Enhanced Raman Spectroscopy  
*Ying Chen, Qiran Cai, Srikanth Mateti, Aijun Du, and Lu Hua Li*
- TP21** Surface Modification of Fused Silica Optics with CO<sub>2</sub> Laser for Improving  
Optical Performance  
*W. Liao, C.C. Zhang, X. Xiang, X.D. Yuan and X.T. Zu*

**WWW 2017 Conference Abstracts**

**ABSTRACTS  
WEDNESDAY**

## Electronic Properties of High-Quality Epitaxial Topological Dirac Semimetal Thin Films

Michael S. Fuhrer<sup>a</sup>

<sup>a</sup> *Monash Centre for Atomically Thin Materials, and School of Physics & Astronomy, Monash University, Victoria 3800, Australia.*

Topological Dirac semimetals (TDS) are three-dimensional analogues of graphene, with linear electronic dispersions in three dimensions. Electrical measurements on bulk TDS crystals reveal unusual magnetoresistance related to the chiral anomaly. Here we demonstrate TDS thin films, with electronic transport and scanning tunnelling microscopy (STM) performed in ultra-high vacuum (UHV). Such films open numerous new possibilities, including studying the conventional-to-topological quantum phase transition (QPT) as a function of layer thickness or incorporating gate electrodes to enable an electric field-tuned QPT, realizing a topological transistor. Na<sub>3</sub>Bi thin films are grown by molecular beam epitaxial and transferred in UHV a low-temperature STM capable of magnetotransport at 5 K. Thin films (20 nm) of Na<sub>3</sub>Bi on  $\alpha$ -Al<sub>2</sub>O<sub>3</sub>(0001) substrates are found to possess low temperature charge carrier mobilities exceeding 6000 cm<sup>2</sup>V<sup>-1</sup>s<sup>-1</sup> with *n*-type carrier densities below 1 x 10<sup>18</sup> cm<sup>-3</sup>[1], comparable to the best single crystal values. Mapping the local Dirac point via scanning tunneling spectroscopy reveals a high degree of spatial uniformity, with *rms* variations in Dirac point energy less than 5 meV[2], comparable to the best graphene samples on hexagonal boron nitride. Chemical doping[3] and electrostatic gating[4] (using SiO<sub>2</sub>/Si substrates) can be used to tune the carrier density and allow a closer approach to the Dirac point.

[1] J. Hellerstedt, M. T. Edmonds, N. Ramakrishnan, C. Liu, B. Weber, A. Tadich, K. M. O'Donnell, S. Adam, M. S. Fuhrer *Nano Letters* **16**, 3210 (2016).

[2] M.T. Edmonds, J.L. Collins, J. Hellerstedt, I. Yudhistira, S. Adam, M.S. Fuhrer, *in preparation*.

[3] M.T. Edmonds, J. Hellerstedt, K.M. O'Donnell, A. Tadich, and M.S. Fuhrer, *ACS Appl. Mater. Interfaces* **8**, 16412 (2016).

[4] J. Hellerstedt, I. Yudhistira, M.T. Edmonds, C. Liu, J. Collins, S. Adam, and M.S. Fuhrer, *in preparation*.

## Exploring New Materials for Nanoelectronics from *ab initio* Theory

Catherine Stampfl<sup>a</sup>

<sup>a</sup> *School of Physics, The University of Sydney, NSW 2006, Australia.*

The development of new sophisticated electronic device technology requires deep understanding of the fundamental physical phenomena taking place in the materials, which underlie device operation and function. Structures are progressively becoming smaller and the number of components on a chip increasing, but there is a limit. Even before this limitation is reached there is the problem of energy loss or dissipation as signals pass to the next component. A new generation of nanomaterials is required to progress beyond this threshold. Materials design and modelling through computer simulation represents a powerful approach to investigate, understand and predict new structures, which due to their small scale, quantum effects become important and key to their function (e.g. spintronics and topological insulators, molecular electronics). In the present talk we present recent results of *ab initio* investigations into various systems to explore the electronic and magnetic structure and associated electron transport properties. For example, hybrid inorganic-organic structures [1], diamondoids [2], ultrathin polymorphic  $V_2VI_3$  topological insulator nanofilms [3], and dilute magnetic ferroelectrics (DMF) [4]. We find interesting phenomena such as near-perfect spin filtering, high on/off conductance switching, and bistable magnetism in the doped DMF suggesting potential for voltage-induced spin cross over. The prediction of these phenomena suggest potential applications of such structures in nanoelectronic and nanospinronic applications.

[1] S. A. Tawfik *et al.* J. Chem. Theory and Comp. 11, 4154 (2015)

[2] S. A. Tawfik *et al.* Nanoscale 8, 3461 (2016)

[3] C. Li *et al.* Phys. Rev B 90, 075438 (2014)

[4] L. Weston *et al.* Phys Rev. Lett. 114, 247601 (2015)

**Graphene heterostructures: towards a material for 2D electronics**

Mojtaba Amjadipour<sup>a</sup>, Jonathan Bradford<sup>a</sup>, Bharati Gupta<sup>a</sup>, Mahnaz Shafiei<sup>a</sup>, Francesca Iacopi<sup>b</sup>, Jennifer MacLeod<sup>a</sup>, Josh Lipton Duffin<sup>a</sup> and Nunzio Motta<sup>a</sup>

<sup>a</sup>School of Chemistry, Physics and Mechanical Engineering and Institute for Future Environments, Queensland University of Technology, 2 George Street, Brisbane 4001, QLD, Australia

<sup>b</sup>School of Computing and Communications, Faculty of Engineering and Information Technology, University of Technology Sydney, Broadway 2007, NSW, Australia

Many of the expectations about the great potential of graphene for future 2D electronics, due to the conduction properties of its Dirac massless electrons, have not yet been fulfilled. Graphene is a semimetal with zero bandgap, a key issue that still challenges its use as controlled resistor or switch. Scientists are now actively looking at producing a bandgap in graphene or at searching alternative materials. Amongst the plethora of recently discovered 2D materials (more than 2000!) there is a group displaying a band gap which makes them semiconducting, opening the way, in combination with graphene, to real applications in 2D electronics.

In this talk I will discuss recent results obtained at QUT on the growth of graphene nanoribbons and heterostructures. I will briefly review our studies on the formation of epitaxial graphene on patterned SiC to form nanoribbons by high temperature annealing in ultra-high vacuum and the development of hybrid 2D materials (hBN/Gr; MoS<sub>2</sub>/Gr) by CVD deposition on Graphene/SiC(0001) substrates. I will also discuss the results obtained in applying lower quality graphene and graphene oxide to supercapacitors and sensors.

**References**

- [1] Mishra, N., J. Boeckl, N. Motta, and F. Iacopi, *Graphene growth on silicon carbide: A review*. *physica status solidi (a)*, 2016(1-13). DOI: 10.1002/pssa.201600091
- [2] Zarotti, F., B. Gupta, F. Iacopi, A. Sgarlata, M. Tomellini, and N. Motta, *Time evolution of graphene growth on SiC as a function of annealing temperature*. *Carbon*, 2016. **98**: p. 307-312.
- [3] Wang, B., J. Liu, Y. Zhao, Y. Li, W. Xian, M. Amjadipour, J. MacLeod, and N. Motta, *Role of Graphene Oxide Liquid Crystals in Hydrothermal Reduction and Supercapacitor Performance*. *ACS Applied Materials & Interfaces*, 2016. **8**(34): p. 22316-22323.

## Hybrid graphite-like/polymer-like amorphous carbon materials by plasma synthesis

M. Rybachuk<sup>a,b</sup>

<sup>a</sup>*School of Engineering, Griffith University, Engineering Drive, Southport QLD 4222, AUSTRALIA*

<sup>b</sup>*Queensland Micro- and Nanotechnology Centre, Griffith University, Nathan QLD 4111, AUSTRALIA*

The presentation will address the means for controlled growth of polymeric and graphitic nano-inclusions in amorphous carbon (*a*-C) materials by microwave (MW) and radio frequency (RF) plasma fabrication processes. Polymer-like and graphite-like nano-inclusions are known as undesirable by-products occurring in carbon materials such as CVD diamond, diamond-like carbon and other materials synthesized using hydrocarbon gases as precursors. These are basic  $\pi$ -conjugated polymers (*e.g.* *trans*-polyacetylene, polyphenylene and polyphenylene vinylene), graphite nanoparticles and an  $sp^1$ -hybridised nanowire inclusions. These by-products can be produced in abundance under a non-equilibrium plasma conditions and, remarkably, the inclusions award unusual and highly desirable opto-electronic properties to *a*-C materials. That is, properties of *a*-C containing polymeric and/or graphitic nano-inclusions could be modified for paramagnetic behaviour and, *a*-C materials fabricated under the MW excited plasma can, in addition, become absorption-free in visible (red) - near infrared (N-IR) wavelength range (600 - 1200 nm) with their refractive index tailored (*e.g.* with a maximum value of 1.9 at 400 nm). The *a*-C materials produced under the RF plasma exhibit non-stoichiometric properties of graphite-like materials with an ultra-low hydrogen content (~15 at.%), high refractive index (~2.4 in red – N-IR) and unpaired electron concentration (~ $10^{21}$  cm<sup>-3</sup>) and a narrow band gap (0.4 – 0.6 eV) mimicking the properties of phenyl polymers [1]. These findings suggest that these nano-inclusions in *a*-C materials could be promising in the development of bulk nanostructured ‘all-carbon’ opto-electronic systems [2,3].

[1] M. Rybachuk et al. Applied Physics Letters **under review** (2016)

[2] M. Rybachuk et al. Applied Physics Letters **93**, 051904 (2008)

[3] M. Rybachuk et al. Applied Physics Letters **96**, 211909 (2010)

**Resolving spin dynamics at the nanometer-scale with radioactive ion-beams**

D. L. Cortie<sup>a,b,c\*</sup>, R. L. McFadden<sup>a</sup>, M. Dehn<sup>a</sup>, G.D Morris<sup>c</sup>, I. McKenzie<sup>c</sup>, X. L. Wang<sup>d</sup>,  
R. Kiefl<sup>a,c</sup> and W. A. MacFarlane<sup>a</sup>

<sup>a</sup> *Quantum Matter Institute, The University of British Columbia, BC, Canada V6T 1Z4*

<sup>b</sup> *Research School of Chemistry, Australian National University V6T 1Z4*

<sup>c</sup> *TRIUMF, 4004 Wesbrook Mall, Vancouver, British Columbia, Canada V6T 2A3*

<sup>d</sup> *Institute for Superconducting and Electronic Materials, University of Wollongong, Australia*

Interfaces can drastically affect local spin dynamics by introducing new states that manifest as additional degrees of freedom in the local electronic environment. For this reason, low energy spin dynamics can have an important influence on the resulting states of quantum matter in thin films and surface regions. Historically, the spin relaxation rate (SLR) measured in nuclear magnetic resonance (NMR) has been a useful technique for detecting sub-THz dynamics via hyperfine coupling; however, nanointerfaces typically produce a very weak NMR signal that is conflated with the dominant signal of the bulk surroundings. These challenges have motivated a variety of ingenious new NMR schemes specifically designed to study thin films and surfaces<sup>1</sup>. In this talk, I will present a radioactive ion-beam-based version of NMR<sup>2</sup> which performs sensitive read-out of implanted nuclear spins using the anisotropic beta-decay process, resulting in a billion-fold enhancement of the signal from interfacial regions. This is illustrated using some recent data which studied the spin lattice relaxation rate of low-energy radioactive <sup>8</sup>Li ion beams in order to detect spin dynamics in correlated metal oxides<sup>3</sup> and antiferromagnetic surfaces<sup>4</sup>. There are now ongoing efforts to use this technique to detect the paramagnetic fluctuations from delocalized electrons near the surface of topological insulators.

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## It has it all: $\text{Cu}_5\text{Sb}_2\text{SiO}_{12}$ - Seven crystallographic independent positions for $\text{Cu}^{2+}$ in one compound

T. Olney<sup>a</sup>, D. Wilson<sup>a</sup>, M. Avdeev<sup>b</sup> and T. Söhnel<sup>b</sup>

<sup>a</sup> School of Chemical Sciences, University of Auckland, Auckland 1142, New Zealand.

<sup>b</sup> Australian Centre for Neutron Scattering, ANSTO, Lucas Heights, NSW, Australia.

$\text{Cu}_5\text{Sb}_2\text{SiO}_{12}$  is the only copper – antimony silicate known so far. We were also able to grow single crystals of  $\text{Cu}_5\text{Sb}_2\text{SiO}_{12}$  using chemical transport reactions and to solve the crystal structure completely. The crystal structure of the compound is truly remarkable as it contains seven structurally independent  $\text{Cu}^{2+}$ -positions, all of them showing different coordination spheres (typical distorted  $\text{CuO}_6$  octahedra, [2+2+2] coordination, 5-fold coordination and  $\text{CuO}_8$  with 4 medium and 4 long bonds [4+4]). This is a very unique and very promising situation, which could be used for partial oxidation and reduction of Cu analogous to Cu-containing high temperature superconductors, as well as replacing Cu with other  $\text{M}^{2+}$  transition metals. An anti-ferromagnetic long range ordering of  $\text{Cu}^{2+}$  could be shown for  $\text{Cu}_5\text{Sb}_2\text{SiO}_{12}$  below 27 K [1]. First NPD measurements without magnetic field at temperatures below the ordering temperature do not show any magnetic peaks, which should be observed for a long range antiferromagnetic ordering. Our own field-dependent measurements confirm the magnetic ordering, but the magnetic ordering is only clearly visible in susceptibility data with external fields of about 3 T and higher. Manganese and Cobalt doped versions of the copper-antimony silicate have been synthesised. Since there are *seven* crystallographic independent positions for  $\text{Cu}^{2+}$  with very different coordination spheres, there should be preferential sites for the Mn and Co to be incorporated into the structure. Lab X-ray and neutron powder diffraction data show that doping appears to work well up until  $\text{Cu}_2\text{Mn}_3\text{Sb}_2\text{SiO}_{12}$ . All materials have been synthesised at 900 C in air, a temperature where the stable ion should be  $\text{Mn}^{3+}$  rather than  $\text{Mn}^{2+}$ , which can be seen in studies of the  $\text{Cu}_{5-x}\text{Mn}_x\text{SbO}_6$  system [2]. Mn doping leads to much stronger magnetic ordering in the compounds and the antiferromagnetic ordering could finally be observed in neutron powder data.

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**Magnetic Structure and Spin Dynamics of Multiferroic System Co<sub>4</sub>Nb<sub>2</sub>O<sub>9</sub>**

Guochu Deng<sup>a</sup>, Yiming Cao<sup>b</sup>, Wei Ren<sup>b</sup>, Shixun Cao<sup>b</sup>, Nicolas Gauthier<sup>c</sup>, Michel Kenzelmann<sup>c</sup>, Andrew Studer<sup>a</sup>, Kirrily Rule<sup>a</sup>, Jason S. Gardner<sup>d</sup>, Gene Davison<sup>a</sup>, Paolo Imperia<sup>a</sup> and Garry J. McIntyre<sup>a</sup>

<sup>a</sup> *Australia Center for Neutron Scattering, Australian Nuclear Science and Technology Organisation, New Illawarra Road, Lucas Heights NSW 2234, Australia*

<sup>b</sup> *Department of Physics, International Center of Quantum and Molecular Structures, and Materials Genome Institute, Shanghai University, Shanghai 200444, China*

<sup>c</sup> *Laboratory for Scientific Developments & Novel Materials, Paul Scherrer Institute, CH-5232 Villigen-PSI, Switzerland.*

<sup>d</sup> *Neutron Group, National Synchrotron Radiation Research Center, Hsinchu 30076, Taiwan*

Co<sub>4</sub>Nb<sub>2</sub>O<sub>9</sub>, was recently reported to have large magneto-dielectric coupling effect under a certain magnetic field.<sup>[1,2]</sup> This compound has a corundum-type crystal structure of space group P-3c1 of ref. [3] and undergoes antiferromagnetic phase transition around 27 K. It was previously believed that the magnetic moments of Co<sup>2+</sup> order into a collinear antiferromagnetic structure in which Co<sup>2+</sup> spins order parallel to the c-direction and form ferromagnetic chains with antiparallel inter-chain coupling.<sup>[3]</sup> However, the recent study has shown that this magnetic structure model is incorrect.<sup>[4]</sup> In this study, we found that the Co<sup>2+</sup> magnetic moments align in the *ab* plane with a non-collinear configuration. Using inelastic neutron scattering, we measured the spin wave excitation from its magnetic phase along (*h*00) and (00*l*). A magnetic model was proposed to explain the observed spin dynamical behavior. There are two inequivalent Co sites, which form spin chains in an alternative way along *c* axis. Each Co<sup>2+</sup> moment couples with its two inequivalent neighbors on the same chain with ferromagnetic interactions. Co<sup>2+</sup> moments from each site form a zig-zag hexagonal ring perpendicular to the *c* axis, where antiferromagnetic interactions dominate. On the basis of this model, the observed spin wave spectra can be well simulated by SpinW. [5]

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**Exotic oxide species and oxygen dynamics in the double perovskites**

J. Polt<sup>a</sup>, B.J. Kennedy<sup>a</sup> and C.D. Ling<sup>a</sup>

<sup>a</sup> *School of Chemistry, University of Sydney, NSW 2006, Australia.*

There is a pressing need for new oxide ion conductors that show appreciable conductivity at moderate temperatures (500-700°C). Such materials would have diverse applications in solid-oxide fuel cells, oxygen separation membranes, oxygen storage materials and catalytic convertors. A thorough understanding of the fundamental aspects of oxygen diffusion in solids is a necessary step towards rationally optimising their local chemistry and structure, in order to improve their conduction properties.

To date, the majority of research has focused on materials with ionic conduction based on vacancies in an oxygen sub-lattice. Our approach focuses on the rarely investigated case of materials with oxygen-excess. This includes materials with oxide ions in the interstitial sites of a crystalline structure, and those containing superoxide species in normal lattice sites. Understanding these will provide insight into the structure-property relationship of O<sup>2-</sup> conduction and provide a systematic route to enhanced performance and new materials, with improved ionic conduction at moderate temperatures.

In this talk I will present results regarding the crystal structures and oxygen dynamics in the series Sr<sub>3-x</sub>Y<sub>x</sub>NbO<sub>5.5+1/2x</sub>. Based on the work of Li and Hong [1], we expected high oxygen disorder and possibly interstitial oxides in the compounds with low Y doping, both of which promise excellent ionic conduction properties. A variety of techniques including synchrotron x-ray and neutron powder diffraction as well as quasi-elastic neutron scattering and impedance spectroscopy experiments have been applied to characterize the structures and properties of these compounds.

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**Magnetic and structural transitions in magnetocaloric****Mn(Co<sub>1-x</sub>Ni<sub>x</sub>)Ge alloys**Q.Y. Ren,<sup>1</sup> W.D. Hutchison,<sup>1</sup> J.L. Wang,<sup>2</sup> A.J. Studer,<sup>3</sup> J.M. Cadogan<sup>1</sup> and S.J. Campbell<sup>1</sup><sup>1</sup>*School of Physical, Environmental and Mathematical Sciences, The University of New South Wales, Canberra, ACT 2600, Australia*<sup>2</sup>*Institute for Superconductivity and Electronic Materials, University of Wollongong, NSW 2522*<sup>3</sup>*Australian Nuclear Science and Technology Organisation, Lucas Heights, NSW 2234, Australia*

The magnetocaloric effect (MCE) - a significant temperature change due to the entropy change around magnetic transitions in materials driven by magnetisation or demagnetisation - has emerged as an increasingly important topic in condensed matter physics in the past two decades (*e.g.*[1]). A direct (positive) MCE occurs around a magnetic transition from ferromagnetism (FM) to paramagnetism (PM), while an inverse (negative) MCE is obtained around a magnetic transition from antiferromagnetism (AFM) to FM [2]. If such magnetic transitions couple with a structural transition, a first-order magneto-structural transition can form and hence strengthen the MCE (*e.g.* [3]).

In this work, the magnetic and structural transitions have been tuned by substitution of Ni for Co in MnCoGe. The Mn(Co<sub>1-x</sub>Ni<sub>x</sub>)Ge samples ( $x = 0.14 - 1.00$ ) were studied by magnetisation, x-ray and neutron powder diffraction measurements over the temperature range 5 - 450 K. Mn(Co<sub>1-x</sub>Ni<sub>x</sub>)Ge alloys have an orthorhombic (Orth) TiNiSi-type structure (*Pnma*) at low temperature with transformation to a hexagonal (Hex) Ni<sub>2</sub>In-type structure (*P6<sub>3</sub>/mmc*) at the martensitic transformation temperature  $T_M$ . The increase of the Ni content changes the orthorhombic phase from FM ( $x < 0.55$ ) to spiral-AFM ( $x \geq 0.55$ ). In addition, the transformation temperature  $T_M$  for the reverse martensitic transformation - from orthorhombic to hexagonal - decreases with Ni content  $x$  when  $x < 0.55$  and then increases when  $x \geq 0.55$ . The adjustment of  $T_M$  leads to the occurrences of first-order FM-Orth/PM-Hex magneto-structural transitions and large values of the direct MCE in the samples with  $\sim 0.20 < x < \sim 0.60$ . Moreover, the spiral-AFM/FM magnetic transitions in the orthorhombic phase for samples with  $\sim 0.55 < x < \sim 0.75$  result in an inverse MCE.

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**Inorganic-organic hybridization:  
new strategy for flexible thermoelectric devices**

Ruoming Tian<sup>1</sup>, Chunlei Wan<sup>2</sup>, Yifeng Wang<sup>3</sup>, Qingshuo Wei<sup>4</sup>, Takao Ishida<sup>4</sup>, Atsushi Yamamoto<sup>4</sup>, Akihiro Tsuruta<sup>5</sup>, Woosuck Shin<sup>5</sup>, Sean Li<sup>6</sup> and Kunihiro Koumoto<sup>1,\*</sup>

<sup>1</sup> Toyota Physical and Chemical Research Institute, Nagakute, 480-1192, Japan

<sup>2</sup> Tsinghua University, Beijing 100084, China

<sup>3</sup> Nanjing Tech University, Nanjing 210009, China

<sup>4</sup> National Institute of Advanced Industrial Science and Technology, Tsukuba, Japan

<sup>5</sup> National Institute of Advanced Industrial Science and Technology, Nagoya 463-8560, Japan

<sup>6</sup> School of Materials Science and Engineering, UNSW Australia, NSW 2052, Australia

The demand for flexible thermoelectric materials driven by the integration of wearable electronics has stimulated the development of various organic/inorganic hybrid composites from micro- to nano- scales. However, the organic/inorganic interfaces have to be carefully engineered to permit good adhesion and efficient charge transfer across the boundaries. On the other hand, liquid exfoliation has proven to be an effective approach to obtain large-scale 2D nanosheets in graphene, boron nitrides, layered perovskites and transition metal dichalcogenides. This also provides fresh insights into the hybridization of inorganics/organics at the sub-nanoscales.

Here, we present a liquid-exfoliation-and-self-assembly method to produce TiS<sub>2</sub>/organics superlattice film, which can be either free-standing or deposited onto substrates.<sup>[1][2]</sup> Charge transfer occurs when TiS<sub>2</sub> and organic molecules form intercalation complexes, which gives rise to a high electrical conductivity. Moreover, it is found that the presence of organic molecules in the matrix can greatly suppress the thermal conductivity and allow the material flexible. In addition, we have fabricated a prototype flexible thermoelectric module, and the performance of our module will also be presented.

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## Five dimensional analysis of ferroelectric domain continuity over grain boundaries

Sukriti Mantri<sup>a</sup>, Jette Oddershede<sup>b</sup>, Dragan Damjanovic<sup>c</sup> and John E. Daniels<sup>a</sup>

<sup>a</sup>*School of Materials Science and Engineering, UNSW Australia, Sydney, NSW 2052, Australia*

<sup>b</sup>*Department of Physics, Technical University of Denmark, Fysikvej, 2800, Kgs. Lyngby, Denmark*

<sup>c</sup>*Ceramics Laboratory, Swiss Federal Institute of Technology in Lausanne-EPFL, 1015 Lausanne, Switzerland*

Ferroelectrics materials are incorporated into many modern electronic devices. They play important roles in components including capacitors, ferroelectric RAM and acoustic transducers. However, cheaper to make bulk polycrystalline ferroelectrics contain grain boundaries responsible for limiting their properties. Grain boundaries limit the macroscopic ferroelectric properties by limiting the mobility of domain walls. Domain wall continuity across grain boundaries has been observed since 1950's and is speculated to change these grain boundary-domain wall interactions. The collective ferroelectric response of neighbouring grains been observed in thin films might also be due to correlated domains structures. However, detailed 5- dimensional study on such correlated domain structures across the grain boundaries has not been done. This paper pertains to the computational study on possibility of such correlated domain structures across grain boundaries. In this work, we have developed the mathematical requirements for domain wall plane matching at grain boundaries. We have also incorporated the grain boundary ferroelectric polarisation charge that is caused when any two domains meet at the grain boundary plane. By utilising 3D microstructural mapping methods like sectioned EBSD and 3D-XRD, and calculating the 5-dimensional grain boundary character, we can apply this knowledge to optimise processing techniques to result in desired interactions between grain boundaries and domain walls.

**Magnetic switching along hard-axes in Er-doped DyFe<sub>2</sub>/YFe<sub>2</sub> thin films**

G. J. Bowden<sup>a</sup>, G. B. G. Stenning<sup>b</sup>, G. van der Laan<sup>c</sup>, A. I. Figueroa<sup>c</sup>, P. Bencok<sup>d</sup>,  
P. Steadman<sup>d</sup> and T. Hesjedal<sup>e</sup>

<sup>a</sup> School of Physics and Astronomy, University of Southampton, SO17 1BJ, UK.

<sup>b</sup> ISIS Neutron and Muon Source, Rutherford Appleton Lab., Didcot OX11 0QX, UK.

<sup>c</sup> Magnetic Spectroscopy Group, Diamond Light Source, Didcot OX11 0DE, UK.

<sup>d</sup> Diamond Light Source, Didcot OX11 0DE, UK.

<sup>e</sup> Clarendon Laboratory, University of Oxford, OX1 3PU, UK.

Molecular-beam-epitaxial (MBE) grown [DyFe<sub>2</sub>/YFe<sub>2</sub>] multilayer films form an ideal model system for the study of magnetic exchange springs. Here the DyFe<sub>2</sub> (YFe<sub>2</sub>) layers are magnetically hard (soft), respectively. Thus, in the presence of a magnetic field exchange springs form in the YFe<sub>2</sub> layers. Recently, it has been shown that placing small amounts of Er into the centre of the YFe<sub>2</sub> springs generates substantial changes in magnetic behaviour<sup>1</sup>. In particular, (i) the number of exchange-spring states is increased dramatically, (ii) the resulting domain wall states are not simply describable either as Néel or Bloch walls, (iii) the Er and Dy magnetic loops differ strikingly, and (iv) the phenomenon of Er-induced magnetic exchange-spring collapse. Here we present results for Er-doped (110)-oriented [DyFe<sub>2</sub>(60 Å)/YFe<sub>2</sub>(240 Å)]<sub>15</sub> multilayer films, at 100 K in fields of up to ±14 T. In particular, results are contrasted for fields applied along seemingly equivalent hard-magnetic [110]-type axes. MBE grown cubic Laves thin films offer the unique feature of allowing the magnetic field to be applied along a hard out-of-plane [110]-axis (the growth axis), and a similar hard in-plane [ $\bar{1}$ 10]-axis. Differences are found and attributed to (i) the  $\epsilon_{xy}$  strain term induced during crystal growth, and (ii) the long-range dipole-dipole interaction, calculated using a model recently developed for thin films<sup>2</sup>. In particular, the out-of-plane [110] Er-results reveal the existence of a new magnetic exchange spring state, which could only be identified using element-selective x-ray magnetic circular dichroism (XMCD).

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**Magneto-Electronic Hydrogen Gas Sensing**

G. L. Causer<sup>a</sup>, C. Lueng<sup>b</sup>, S. J. Callori<sup>c</sup>, P. Metaxas<sup>b</sup>, F. Klose<sup>a</sup> and M. Kostylev<sup>b</sup>

<sup>a</sup> *Australian Nuclear Science and Technology Organisation, Lucas Heights 2234, Australia.*

<sup>b</sup> *School of Physics, University of Western Australia, Crawley 6009, Australia*

<sup>c</sup> *Department of Physics, California State University, San Bernardino 92407, USA*

Hydrogen (H<sub>2</sub>) as an energy carrier and associated H<sub>2</sub> technologies such as fuel cells are establishing themselves as key players in the current green energy revolution. To address safety issues associated with H<sub>2</sub>, robust hydrogen gas sensors are required. We report on a superior method of using magneto-electronics to detect the presence of H<sub>2</sub>.

Exploiting the strong affinity of Pd to reversibly absorb and chemically bind H<sub>2</sub>, resulting in the formation of PdH which expands the Pd lattice by up to 3% [1], our prototype device [2] is based on the modification of magnetic, structural and electronic properties that occur upon hydrogenation of a Pd layer in a Pd/Co bilayer film. As H<sub>2</sub> is absorbed by the Pd lattice, modifications to the perpendicular magnetic anisotropy (PMA) of interfacial Co moments result, leading to a variation of the ferromagnetic resonance (FMR) response of the Co layer. We report on data obtained from the first in-situ FMR polarised neutron reflectometry (PNR) measurement performed on the time-of-flight neutron reflectometer PLATYPUS at ANSTO. Here we simultaneously probed hydrogen depth profiles within Pd as a function of external H<sub>2</sub> partial pressure (HPP), and correlated these against hydrogen induced changes to the FMR signal in the ferromagnetic layer. Decreases in the FMR field in excess of 30 Oe were observed upon H<sub>2</sub> absorption, as a result of weakening PMA strength due to changes in interfacial electronic properties. In addition, we systematically investigated the relationship between Pd layer thickness and H<sub>2</sub> concentration in the Pd layer in the presence of 3.5% HPP, and found that the uptake of hydrogen is severely hindered by post-deposition annealing. Although the annealing process served to remove lattice dislocations which could otherwise be occupied by H<sub>2</sub>, it led to more repeatable magnetic behaviors of the materials when measured over several H<sub>2</sub> absorption/desorption cycles.

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**WWW 2017 Conference Abstracts**

**ABSTRACTS**

**POSTER**

**WEDNESDAY**

## Application of Linear Spin Wave Theory to the Cr<sub>8</sub> Antiferromagnetic Heisenberg Ring

T. D'Adam<sup>a</sup>, R. Mole<sup>a</sup> and J. Stride<sup>b</sup>

<sup>a</sup> ACNS, Australian Nuclear Science and Technology Organisation, Lucas Heights, Australia.

<sup>b</sup> School of Chemistry, University of NSW, Kensington, Australia.

The investigation of single molecule magnets (SMMs) has proven to be a focal point of magnetism research for over three decades, leading to the discovery of structures which may find applications in data storage, quantum information processing (QIP) and spintronics. Though molecular magnetism is not a new field, there are still many complexes to investigate and understand, including a range chains, rings, discs and cages. Amongst the considerable number of structures, particular interest has been shown to antiferromagnetic Heisenberg rings (AFHR) such as Cr<sub>8</sub>, CsFe<sub>8</sub> and Fe<sub>18</sub>. These structures have been investigated due to their interesting magnetic behaviours which include quantum tunnelling of the Neel vector (QTNV) and a long magnetic relaxation time below their blocking temperature T<sub>B</sub> [1].

The Cr<sub>8</sub> homometallic AFHR is one of the most well understood structures of its type having been extensively investigated since its initial synthesis using techniques including high-field EPR, cantilever torque magnetometry [2] and INS [3]. Through application of Linear Spin Wave Theory (LSWT) using the SpinW Matlab library [4] it has been possible to calculate the dynamic structure factor of the Cr<sub>8</sub> ring; this agrees well with both the INS data collected for this structure as well as models produced using alternate methods [3]. This demonstrates that LSWT is applicable to the Cr<sub>8</sub> ring and we plan to use this method to analyse more complex structures which also do not exhibit long range magnetic ordering.

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## Structure and magnetic properties of the $AB_3Si_2Sn_7O_{16}$ layered oxides

M. Allison<sup>a,b</sup>, C. Ling<sup>a</sup>, S. Schmid<sup>a</sup>, M. Avdeev<sup>c</sup>, G. Stuart<sup>d</sup> and T. Söhnel<sup>b</sup>

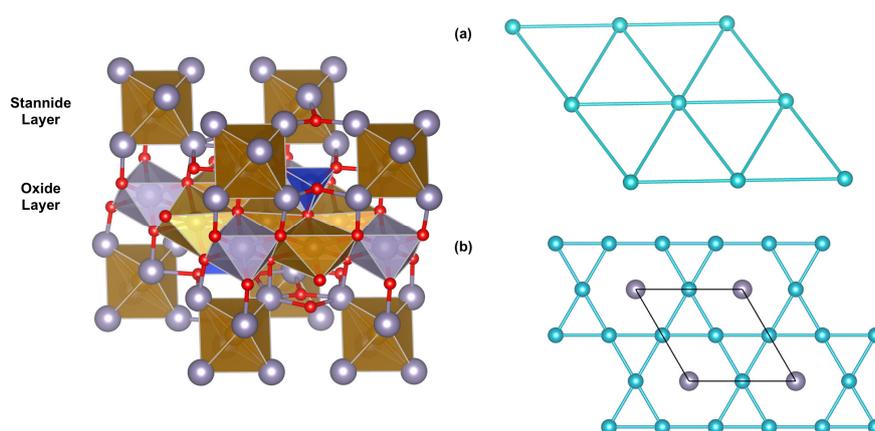
<sup>a</sup> School of Chemistry, University of Sydney, NSW, Australia.

<sup>b</sup> School of Chemical Sciences, University of Auckland, New Zealand.

<sup>c</sup> Australian Nuclear Science and Technology Organisation, Lucas Heights, NSW, Australia

<sup>d</sup> School of PEMS, UNSW@AFDA, Canberra, Australia.

Layered transition metal compounds with geometrically frustrated architectures are widely studied due to the novel effects that arise in a material where lattice geometry prevents the formation of a stable low temperature magnetic ground state in which all interactions between electron spins are satisfied. The parent compound for this study,  $Fe_4Si_2Sn_7O_{16}$  [1] (Fig. 1), provides a novel situation in oxide compounds. It can be described as a layered composite of oxygen linked ( $FeSn_6$ ) octahedra (the stannide layer) and  $(FeO_6)/(SnO_6)$  octahedra with a kagomé topology (the oxide layer). These layers are separated by  $SiO_4$  tetrahedra and the divalent iron in both layers appear to highly substitutionally liable, this combination of features therefore provides a rare opportunity to study a new series of materials with two discrete magnetically frustrated lattices (triangular and kagomé). To date, we have studied the changes in structure as iron is systematically replaced in the structure with iridium, ruthenium, cobalt and/or manganese. Refinements of the X-ray and neutron powder diffraction data show that each transition metal has strong preferences for either the stannide or oxide layer positions dependent upon ionic size and electronic configuration. In this presentation we will show the current results of our studies on the structure, electronic configuration and magnetic properties.



**Fig 1.** Crystal structure (left) and transition metal lattices (a) Stannide (triangular), (b) Oxide (kagomé) of the  $AB_3Si_2Sn_7O_{16}$  series.

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**Mössbauer Study of the Coolidge carbonaceous chondrite meteorite**

Nancy N. Elewa<sup>a</sup> and J. M. Cadogan<sup>a</sup>

<sup>a</sup> *School of Physical, Environmental and Mathematical Sciences, The University of New South Wales at the Australian Defence Force Academy, Canberra 2610, Australia*

The Coolidge meteorite is considered rare as it is one of only three equilibrated carbonaceous chondrite meteorites of petrologic type 4 that do not belong to the CK group. Furthermore, it is characterized by an abundance of chondrules and a homogenous olivine composition resulting from early metamorphism. Several attempts at classification of this meteorite have been made but it remains unclassified and may in fact represent a separate chondrite group along with Loongana 001, a meteorite recovered from Western Australia [1]. Coolidge was found in 1937 in Kansas, USA at coordinates 38° 2' N and 101° 59' W [2] [3]. Here, we report the characterization of the Fe-bearing phases in this important chondrite using <sup>57</sup>Fe Mössbauer spectroscopy carried out at 298 K and 10 K. Weathered ferric components dominate the room temperature spectrum, accounting for around 59% of the total spectral area. We also observed the presence of iron-nickel metal (most likely taenite) and paramagnetic components corresponding to olivine and pyroxene.

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**Investigation on the Nature of the Verwey Transition in Cu-doped Fe<sub>3</sub>O<sub>4</sub>**Y. Kareri<sup>a</sup>, F. Chang<sup>a</sup>, J. Hester<sup>b</sup> and C. Ulrich<sup>a</sup><sup>a</sup> *School of Physics, University of New South Wales, 2052 NSW, Australia.*<sup>b</sup> *Australian Centre for Neutron Scattering, Australian Nuclear Science and Technology Organization, Lucas Heights, NSW, Australia.*

Magnetite (Fe<sub>3</sub>O<sub>4</sub>), 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<sub>3</sub>O<sub>4</sub> is the occurrence of a metal-insulator transition at ~120 K (T<sub>V</sub>), the so-called Verwey transition, which was associated with charge ordering below T<sub>V</sub>, accompanied by a structural transition from the cubic phase to the monoclinic phase. However, due to the twinning of crystal domains, 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<sub>3</sub>O<sub>4</sub> to approach the problem through the determination of the phase diagram of Fe<sub>1-x</sub>Cu<sub>x</sub>Fe<sub>2</sub>O<sub>4</sub>.

Using neutron diffraction and high resolution X-ray synchrotron diffraction we have investigated both the crystallographic and magnetic structure of Cu-doped Fe<sub>3</sub>O<sub>4</sub> 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, remain unchanged up to high doping levels of 85% Cu-substitution. This is a surprising result at first glance and required a systematic investigation. The analysis of our high resolution X-ray synchrotron diffraction data allowed us to extract detailed information on the precise doping mechanism, including the distribution of Cu-ions between tetrahedral and octahedral sites in the spinel structure. The diffraction data therefore provide valuable information on the detailed mechanism behind the Verwey transition.

## Investigations of the Magnetic and Crystal Field Excitations in Orthorhombically Distorted Perovskites $RVO_3$ ( $R=Dy, Tb, Pr, Ce$ )

J. O'Brien<sup>a</sup>, N. Reynolds<sup>a</sup>, R. Mole<sup>b</sup>, P. Rovillain<sup>a,b</sup>, S. Danilkin<sup>b</sup>, K. Schmalzl<sup>c</sup>, M. Reehuis<sup>d</sup>, S. Miyasaka<sup>e</sup>, F. Fujioka<sup>e</sup>, Y. Tokura<sup>e</sup>, B. Keimer<sup>f</sup>, G. McIntyre<sup>b</sup> and C. Ulrich<sup>a,b</sup>

<sup>a</sup> School of Physics, University of New South Wales, Sydney NSW 2052, Australia.

<sup>b</sup> Australian Centre for Neutron Scattering, ANSTO, 2234 NSW, Australia.

<sup>c</sup> Institut Laue Langevin, BP 156, 38042 Grenoble Cedex 9, France.

<sup>d</sup> Helmholtz-Zentrum for Materials and Energy, 14109 Berlin, Germany.

<sup>e</sup> Department of Applied Physics, University of Tokyo, Tokyo 113-8656, Japan.

<sup>f</sup> Max-Planck-Institute for Solid State Research, Stuttgart, Germany.

Inelastic neutron scattering experiments have been performed on a series of vanadates, in particular  $DyVO_3$ ,  $TbVO_3$ ,  $PrVO_3$ , and  $CeVO_3$ , to categorise the crystal field and magnetic excitations. The vanadates are isostructural to the multiferroic manganites  $TbMnO_3$  and  $DyMnO_3$ , with corner sharing, Jahn-Teller distorted  $VO_6$  octahedra (orthorhombic space group  $Pbnm$ ). However, they possess a collinear C-type antiferromagnetic structure, instead of an incommensurate spin arrangement as in the manganites. In the vanadates, the antiferromagnetic order sets in below Neel temperatures of  $T_N = 110$  K to 124 K [1-5]. Using inelastic neutron scattering on single crystals we were able to determine the crystal field spectrum and spin wave dispersion relations independently. In order to determine the nature of the crystal field excitations of these materials and in order to understand how the magnetic and crystal field excitations influence one another, we have theoretically calculated the crystal field excitation spectrum. The results are compared to the crystal field and spin wave excitations in the multiferroic manganites [6], in order to obtain a deeper understanding of the coupling mechanism between the rare earth elements and the transition metals in  $RVO_3$  and  $RMnO_3$ , respectively.

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## Crystal field excitations for $\text{Ho}^{3+}$ in $\text{HoFeO}_3$

G.A. Stewart<sup>a</sup>, G.N. Iles<sup>b</sup>, R.A. Mole<sup>b</sup>, Z. Yamani<sup>c</sup> and D.H. Ryan<sup>d</sup>

<sup>a</sup> School of Physical, Environmental and Mathematical Sciences, University of New South Wales, ADFA, Canberra, ACT, Australia.

<sup>b</sup> Australian Neutron Beam Centre, ANSTO, Lucas Heights, NSW, Australia.

<sup>c</sup> Canadian Neutron Beam Centre, National Research Council, Chalk River, Ontario, Canada.

<sup>d</sup> Centre for the Physics of Materials and Physics Department, McGill University, Montreal, Quebec, Canada.

The orthoferrites,  $\text{RFeO}_3$  (R = rare earth), are promising candidates for innovative spintronic applications.  $\text{HoFeO}_3$  is of particular interest because optical measurements indicate that the magnetic splitting of the  $\text{Ho}^{3+}$  ion's crystal field (CF) ground state lies in the range of antiferromagnetic–resonance frequencies for the Fe subsystem [1]. Inelastic neutron scattering data recorded on the Australian Neutron Beam Centre's PELICAN time-of-flight spectrometer are consistent with  $\text{Ho}^{3+}$  CF levels at about 10.5, 15.4 and 22.0 meV. Additional low energy transitions ( $< 1$  meV) exhibit behaviour that groups into three distinct temperature ranges (Fig. 1). Given that the Fe sub-lattice undergoes magnetic reorientation over the temperature range of 35 K to 60 K, it is believed that these excitations are associated with magnetic splitting of the  $\text{Ho}^{3+}$  ground CF level due to an exchange field originating from the Fe sub-lattice.

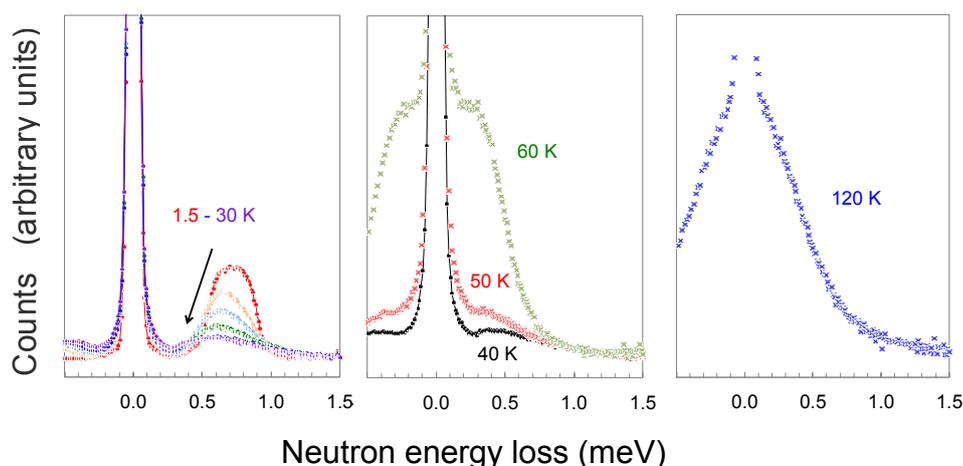


Fig. 1 Inelastic neutron spectra recorded for  $\text{HoFeO}_3$  on PELICAN with  $\lambda = 6 \text{ \AA}$ .

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**Magnetic Transitions and Magnetocaloric Effect in MnCoGe<sub>1-x</sub>Al<sub>x</sub>**N. F. Makmor<sup>a</sup>, W. D. Hutchison<sup>a</sup>, Q. Y. Ren<sup>a</sup> and J. L. Wang<sup>a,b</sup><sup>a</sup> *School of Physical, Environmental and Mathematical Sciences, The University of New South Wales, Canberra, ACT 2600*<sup>b</sup> *Institute for Superconductivity and Electronic Materials, University of Wollongong, Wollongong, NSW, 2522*

Recent interest in the exploration of suitable materials for refrigeration based on the magnetocaloric effect (MCE) has novel technical applications as well as potential for energy-savings and environmental advantages as motivating factors [1]. The ideal material for magnetic cooling often is one in which a structural transition is coupled to a magnetic phase change to form a first order magnetostructural transition. Compounds based on MnCoGe have potential in this regard. They also have the additional advantage of being rare earth free (eg. see [2] and references therein).

The structural properties in the series compounds of MnCoGe<sub>1-x</sub>Al<sub>x</sub> ( $x = 0.02 - 0.10$ ) have been investigated in detail using X-ray diffraction and magnetisation measurements from 5 K to 310 K. MnCoGe<sub>1-x</sub>Al<sub>x</sub> compounds exhibit two crystal structures, the hexagonal Ni<sub>2</sub>In-type structure (*P63/mmc*) and the orthorhombic TiNiSi-type structure (*Pnma*). In this report the effect of substitution of Al is observed and discussed terms of magnetic phase transitions, transition temperatures between the hexagonal and orthorhombic structures, and also the phase fraction and magnetocaloric effect (MCE).

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## Investigation of the magnetism of RTi<sub>2</sub>Ga<sub>4</sub> (R=Er, Ho, Dy) intermetallic compounds

Hatem Saad<sup>a</sup>, W.D. Hutchison<sup>a</sup> and J.M. Cadogan<sup>a</sup>

<sup>a</sup> School of Physical, Environmental and Mathematical Sciences,  
The University of New South Wales, Canberra, ACT 2600

The ternary intermetallic compounds RTi<sub>2</sub>Ga<sub>4</sub>, (R=Er, Ho, Dy) have been prepared by arc-melting under high-purity argon. The sample purities, as determined from refinements of powder x-ray diffraction (XRD) patterns, are at least 97 wt%. These compounds were first synthesised by Grin *et al.* in 1980 [1] and crystallise in the tetragonal YbMo<sub>2</sub>Al<sub>4</sub>-type tI14 structure [2] with the I4/mmm (#139) space group.

The first study of magnetism in the RTi<sub>2</sub>Ga<sub>4</sub> system was reported by Ghosh *et al.* in 1993 [3] who observed unusual magnetic behaviour in the RTi<sub>2</sub>Ga<sub>4</sub> compounds (R = Ho, Er and Dy) by susceptibility (AC and DC) and resistivity measurements. They concluded that these compounds exhibit the effects of mixed Ferro/Antiferromagnetic exchange interactions and they suggested that the magnetic structures might involve helical order of the R moments.

We have carried out XRD, DC and AC magnetisation measurements in order to determine the structural parameters and magnetic ordering temperatures of the RTi<sub>2</sub>Ga<sub>4</sub>, (R=Er, Ho, Dy) compounds as a precursor to neutron diffraction measurements. AC susceptibility was measured at different frequencies at a number of applied magnetic field strengths (2, 20, 60, 100 and 150 mT). The effective magnetic moments were calculated by Curie-Weiss analysis of the temperature dependence of the susceptibilities. The Curie temperatures are ~16 K (Dy), ~11 K (Ho) and ~10 K (Er) derived from our magnetometry data for DyTi<sub>2</sub>Ga<sub>4</sub>, HoTi<sub>2</sub>Ga<sub>4</sub> and ErTi<sub>2</sub>Ga<sub>4</sub>, respectively.

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**Determination of the Crystal Field Levels in TmV<sub>2</sub>Al<sub>20</sub>**

R. White<sup>a</sup>, W.D. Hutchison<sup>a</sup>, G.N. Iles<sup>b</sup>, R.A. Mole<sup>b</sup>, J.M. Cadogan<sup>a</sup>, T. Namiki<sup>c</sup> and  
K. Nishimura<sup>c</sup>

<sup>a</sup> *School of Physical, Environmental and Mathematical Sciences, The University of New South  
Wales, Canberra, ACT, 2600, Australia*

<sup>b</sup> *Australian Centre for Neutron Scattering, Australian Nuclear Science and Technology  
Organisation, Kirrawee DC, NSW, 2232, Australia*

<sup>c</sup> *Graduate School of Science and Engineering, University of Toyama, Toyama, Japan*

Recent interest in so called *caged rare earth* compounds of the RM<sub>2</sub>Al<sub>20</sub>-type (R = lanthanide, M = transition metal) follow from their fascinating physical and magnetic properties at low temperatures. Recent work on PrV<sub>2</sub>Al<sub>20</sub> and PrTi<sub>2</sub>Al<sub>20</sub> revealed unusual phenomena, including a quadrupolar Kondo effect [1, 2] and superconductivity [3, 4], brought about by the cubic symmetry of the Pr<sup>3+</sup> site inducing a non-magnetic ground state in the ion. As a hole analogue of the PrV<sub>2</sub>Al<sub>20</sub> compound, TmV<sub>2</sub>Al<sub>20</sub> has been investigated for equivalent heavy Fermion behaviour at low temperatures. In previous work [5], specific heat and magnetisation data were modelled with the crystal field parameters  $W = 0.5$  K and  $x = -0.6$  based on the Lea, Leask and Wolf formalism [6]. However, the experimental zero field specific heat near 0.5 K could only be matched in the modelled curves using an artificial ground state broadening. In this work inelastic neutron scattering data obtained from the PELICAN time of flight spectrometer located at the OPAL reactor, Lucas Heights has allowed further refinement of the values to  $W = 0.42(1)$  K and  $x = -0.63(1)$ . In addition the CEF transitions are found to be very broad, as required for the specific heat, and suggestive of strong 4f-conduction electron coupling.

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## Multiple Magnetic Phases in DyNiAl<sub>4</sub>

R. White<sup>a</sup>, W.D. Hutchison<sup>a</sup> and M. Avdeev<sup>b</sup>

<sup>a</sup> School of Physical, Environmental and Mathematical Sciences, The University of New South Wales, Canberra ACT 2600, Australia.

<sup>b</sup> Australian Centre for Neutron Scattering, Australian Nuclear Science and Technology Organisation, Kirrawee DC NSW 2232, Australia.

Members of the orthorhombic RNiAl<sub>4</sub> series of materials are known to display variations in the character and number of ordered magnetic phases dependent on the particular rare earth ion present. In TbNiAl<sub>4</sub> there are two ordered phases, the first being an incommensurate elliptical helix type structure [1-3] and the second, lower temperature phase being a commensurate structure with magnetic moments aligned along the *a*-axis. In PrNiAl<sub>4</sub>, there are also two magnetic phases with the incommensurate phase in this case consisting of a sinusoidal modulation of the magnetic moment along the easy *a*-axis [4]. ErNiAl<sub>4</sub> only has an incommensurate magnetic phase, with the magnetic moments pointing along the *c*-axis but sinusoidal in magnitude along the perpendicular *a*- and *b*-axes [5]. The magnetic phases generally exist independently of each other for a given compound, though in TbNiAl<sub>4</sub> the incommensurate and commensurate phases have been shown to coexist in a decreasing magnetic field [2]. New neutron diffraction data recently obtained for DyNiAl<sub>4</sub> using the *ECHIDNA* High Resolution Powder Diffractometer [6] has not only confirmed two ordered magnetic phases, but that these two phases coexist in the region between the two transition points identified in the specific heat data in zero applied field [7].

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**Analysis of interfacial structure and chemistry in FeV<sub>2</sub>O<sub>4</sub>-based  
heterostructures on (001)-oriented SrTiO<sub>3</sub>**

Y. Zhou<sup>a</sup>, D. Zhou<sup>a</sup>, D. R. M. Mitchel<sup>b</sup>, N. Valanoor<sup>a</sup> and P. R. Munroe<sup>a</sup>

<sup>a</sup> *School of Materials Science and Engineering, UNSW Australia, Sydney NSW 2052,  
Australia*

<sup>b</sup> *Electron Microscopy Centre, Australian Institute for Innovative Materials, University of  
Wollongong, North Wollongong NSW 2522, Australia*

Non-collinear multiferroics (NCMs) are a new class of functional oxides which produce magnetoelectric coupling by possessing both ferroelectric and ferromagnetic ordering at low temperatures [1]. FeV<sub>2</sub>O<sub>4</sub> (FVO) is a multiferroic which undergoes successive phase transitions at low temperatures [2]. In this study, we investigate the interfacial structures and chemistry of FeV<sub>2</sub>O<sub>4</sub>/La<sub>0.33</sub>Sr<sub>0.67</sub>MnO<sub>3</sub>/SrTiO<sub>3</sub> (FVO/LSMO/STO) and FVO/STO heterostructures, in which the non-collinear multiferroic, FVO, is epitaxially grown on both (001)-oriented and LSMO-buffered STO substrates by pulsed laser deposition (PLD). By combining data from transmission electron microscopy (TEM) imaging, and high-resolution scanning transmission electron microscopy (STEM) imaging, stacking faults are discovered in the FVO film regions due to more than 8% lattice mismatch. Energy-dispersive X-ray spectroscopy (EDS) analysis suggests that localised diffusion may occur at the FVO/STO and FVO/LSMO interfaces. Electron energy-loss spectroscopy (EELS) at the FVO/LSMO interface confirms that diffusion also plays a role in retaining the epitaxy of the FVO films, despite the lattice mismatch. However, the exact nature of this interfacial diffusion at the interfaces, the chemistry and stoichiometry of the stacking fault needs further investigation.

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**Magnetic Proximity Effect in YBCO/STO/LCMO Multilayers**O. Paull<sup>a,b</sup>, G. Causer<sup>a,b</sup>, A. V. Pan<sup>a</sup> and F. Klose<sup>b</sup><sup>a</sup> *Institute for Superconducting & Electronic Materials, University of Wollongong*<sup>b</sup> *Australian Centre for Neutron Scattering (ACNS), ANSTO*

Tailoring of the electronic properties of complex oxide heterostructures, thin films, and superlattices with atomically sharp interfaces is at the frontline of materials research at present [1, 2, 3]. Interfaces exhibit novel states that are not possible in bulk materials as a result of broken symmetry, induced strains, and modified exchange interactions. In this work we examined the interaction between a superconducting  $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$  thin film layer and a ferromagnetic  $\text{La}_{2/3}\text{Ca}_{1/3}\text{MnO}_3$  layer using polarised neutron reflectometry.

The interaction at the interface between YBCO/LCMO multilayers has resulted in a variety of observed phenomena such as induced ferromagnetic moments in YBCO layers that are antiparallel to neighbouring LCMO layers, and a strong reduction in magnetization in LCMO near the interface. Prajapat et al. investigated the YBCO/LCMO interface using  $\text{SrTiO}_3$  (STO) as an intermediate insulating layer, and reported that the magnetic depletion (MD) in LCMO near the interface is dependent on the critical temperature of YBCO and the thickness of the LCMO layer, and claimed that the origin of the MD in LCMO is due to Cooper pairs tunneling through the STO interlayer across the interface [5]. Our work has verified the observation of the MD layer in LCMO near the interface as claimed in the past report, and additionally studied the effect of a magnetic field on this layer. Polarised neutron reflectometry measurements performed at ANSTO on the PLATYPUS reflectometer indicate that the effect of applying fields at 0.03 T and 1 T is to cause a small restoration of magnetization in this depleted layer. This result supports the mechanism proposed by Prajapat et al. of a superconductivity-induced MD from tunneling through STO.

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**Spatial modulation of a superconducting order in cuprates**

Y. Kharkov<sup>a</sup> and O. Sushkov<sup>a</sup>

<sup>a</sup> *School of Physics, University of New South Wales, NSW 2050, Australia.*

Discovered five years ago in cuprates a mysterious incommensurate charge density wave (CDW) state gave a new twist in physics of high temperature superconductivity. The presence of static CDW order has been confirmed in YBCO [1,2] and other cuprates [3,4] by numerous experimental groups.

The microscopic mechanism responsible for the formation of the CDW in cuprates and its relation to superconductivity is unknown. However, there are a few well established experimental/phenomenological facts about the CDW:

- The CDW is two-dimensional and constraint within CuO planes.
- The CDW has a stripe-like spatial pattern [5], the period of CDW is about  $\lambda_{\text{CDW}} = 3.2$  lattice spacings.
- The CDW competes with the *d*-wave superconductivity: the superconducting order suppresses the amplitude of CDW.

We perform analysis of available experimental data on the CDW. We suggest that the CDW induces a spatial modulation of the *d*-wave superconducting (dSC) order in cuprates. We predict a stripe-like modulation of dSC order with the period  $\lambda_{\text{CDW}}/2$ . The estimated in YBCO relative amplitude of the modulation is  $10^{-3}$ .

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**Interference effects in magnetic focusing with strong spin orbit interactions**

S. Bladwell<sup>a</sup> and O. P. Sushkov<sup>a</sup>

<sup>a</sup> *School of Physics, UNSW*

Transverse magnetic focusing is an experimental technique where charge carriers are focused from a source to a detector via a weak magnetic field; it is the direct analogue of charge mass spectroscopy in the solid state. Despite the simplicity of this experimental method, it presents exceptionally rich physics, particularly in systems with spin-orbit coupling, where the first magnetic focusing peak is split due to the spin-splitting of the momentum. Earlier work has extensively studied intermodal interference, which becomes important at higher magnetic fields [1]. In this theoretical work we analyze the interference effects in magnetic focusing systems with strong spin-orbit interactions, focusing on quantum interference that dominates for the first magnetic focusing peak. Due to the spin-orbit interaction, Berry phase can play a significant role. This poster includes already published results [2] as well as new and yet unpublished results.

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## Growth of Graphene on 3C-SiC Nanostructures by UHV Annealing

Mojtaba Amjadipour<sup>1</sup>, Jennifer MacLeod<sup>1</sup>, Josh Lipton-Duffin<sup>1</sup>, Francesca Iacopi<sup>2</sup>,  
Jose Alarco<sup>1</sup> and Nunzio Motta<sup>1</sup>

<sup>1</sup> School of Chemistry, Physics and Mechanical Engineering, Science and Engineering  
Faculty, Queensland University of Technology, QLD, Australia

<sup>2</sup> School of Computing and Communications, Faculty of Engineering and Information  
Technology, University of Technology Sydney, NSW Australia

There is a growing body of literature that recognizes the potential of graphene for use in electronics<sup>1</sup>. However, the fact that graphene is a semimetal with zero bandgap is a key issue which challenges its remarkable range of applications<sup>2</sup>. Therefore, over the past few years, a considerable literature has grown up around the theme of producing a semiconducting graphene<sup>3</sup>. Thermal decomposition of SiC has proven to be an excellent method to grow transfer-free wafer-scale graphene<sup>4</sup>. Theoretical work suggests that a bandgap might be opened in graphene through quantum confinement, for example in graphene nanoribbons. In this research we attempt to manipulate the SiC substrate dimension to grow graphene over small nanostructures with lateral sizes ranging from tens of nm to 1  $\mu\text{m}$ . To date, there has been no report about the growth of graphene on nanometer-scale SiC mesas, and very little is known about the effect of changing the dimension and characteristic of the substrate on which graphene is grown.

In order to elucidate the possibility for patterned graphene-growth in substrate-defined geometries, we have examined the effect of SiC patterning on graphene growth. SiC mesas have been fabricated by patterning SiC/Si substrates using Focused Ion Beam (FIB) milling. using X-ray photoelectron spectroscopy (XPS), scanning tunnelling microscopy (STM), scanning electron microscopy (SEM), helium ion microscopy (HIM) and Raman spectroscopy were used to investigate the surface condition and to identify surface reconstructions produced during growth. Our results indicate that without employing preventative measures, FIB milling leads to beam-related damage that prevents graphene growth on the SiC/Si milled structures. However, using a modified procedure, we succeeded to produce epitaxial graphene over the SiC nanostructures patterned by FIB.

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## CVD Synthesis of Transition Metal Dichalcogenides on Epitaxial Graphene/SiC

J. Bradford<sup>a</sup>, J. Lipton-Duffin<sup>a</sup>, M. Shafiei<sup>a</sup>, J. MacLeod<sup>a</sup> and N. Motta<sup>a</sup>

<sup>a</sup> *School of Chemistry, Physics and Mechanical Engineering and Institute for Future Environments, Queensland University of Technology, 2 George Street, Brisbane 4001, QLD, Australia.*

Van der Waals heterostructures of layered materials such as graphene, hexagonal boron nitride and transition metal dichalcogenides (TMDs) have attracted attention recently due to the ability to create synthetic materials with properties different to their constituent layers [1]. Stacked layers of graphene and semiconducting TMDs (such as MoS<sub>2</sub>) have previously been demonstrated to exhibit exceptional optoelectronic properties since graphene's high carrier mobility and broad spectrum absorption is complemented by high optical absorption of monolayer TMDs owing to their direct bandgap [2].

In this work we have grown TMD layers directly on epitaxial graphene/SiC substrate by sulfurization of metal oxide precursors. We have conducted a systematic investigation of the growth parameters for MoS<sub>2</sub> on graphene/SiC in order to develop an understanding of the domain size, areal density and thickness of the MoS<sub>2</sub> domains which have been characterised by AFM, Raman spectroscopy, XPS and STM. Direct growth on TMD layers on epitaxial graphene/SiC offers controlled growth of van der Waals materials with a pristine interface on a device-ready substrate.

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## Terahertz Spectroscopic Characterization for Carbon-based Materials

H. Zhang<sup>a</sup>, J. Horvat<sup>a</sup> and R. A. Lewis<sup>a</sup>

<sup>a</sup> *School of Physics and Institute for Superconducting & Electric Materials (ISEM),*

*University of Wollongong, New South Wales 2522, Australia.*

Terahertz (THz) spectroscopy has been used in materials characterization, particularly of lightweight molecules and semiconductors, to determine the carrier concentration and mobility [1]. The Drude-Lorentz model may be linked by the frequency-dependent dielectric response to material free-carrier dynamics [2].

Carbon can be made into very long chains of strong and stable interconnecting carbon-carbon bonds. Graphite is a semi-metallic allotrope of carbon, characterized by a high anisotropic three-dimensional (3D) band structure. THz pulses generation using highly oriented pyrolytic graphite (HOPG) samples illuminated with fs laser has also been reported [3]. Ye et al. also reported on the modulation of THz pulse radiated from a voltage biased graphite [4]. Carbon nanotubes (CNTs) hold a broad range of applications to THz photonics, including THz radiation detection by armchair CNTs in strong magnetic fields [5]. One of the outstanding features of these structures is the presence of a large number of edges, which in turn constitute sites readily available for physical or chemical interaction, particularly adsorption.

In this work, we concentrate on the seldom-used frequency range of 0.1-1.0 THz, which cannot be accessed by standard far-infrared spectrometers. THz spectra of graphite, graphite nanofibers and multi-walled carbon nanotubes are measured and compared. Our results indicate that carbon-based materials have interesting transmission properties in this frequency range, arising from the intermolecular bonds. The bands at these energies most likely occur through an extended  $\pi$ -electron system along the molecular backbone on which charge carriers are delocalized. Van der Waals forces also are likely take effect at these energies.

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**PELICAN: cold-neutron time-of-flight spectrometer at the Australian  
Centre for Neutron Scattering**

G. N. Iles<sup>a</sup>, R. A. Mole<sup>a</sup> and D. H. Yu<sup>a</sup>

<sup>a</sup> *Australian Centre for Neutron Scattering, ANSTO, Australia.*

PELICAN is a cold neutron time-of-flight neutron spectrometer located at the OPAL reactor within the Australian Centre for Neutron Scattering [1]. The instrument has been in continuous operation since 2014 and is currently available to the Australian research community for around 200 days a year. The applications of the inelastic neutron scattering techniques are diverse, ranging from the study of crystal field splitting and phonons in crystals through to the study of atomic diffusion.

A range of wavelength options are available on PELICAN from  $2.73 < \lambda < 5.97$  Å providing corresponding energy resolutions in the range  $0.6 < \text{FWHM} < 0.065$  meV. Using appropriate phasing of the two choppers also provides additional wavelength harmonics, providing versatility without the need to reconfigure the instrument.

Recent improvements to the instrument include the option to utilise polarised neutrons, *in situ* gas-loading for hydration experiments, and high temperature (up to 1600°C) capabilities. We have also designed and tested some custom-made quartz sample holders for ion diffusion studies in corrosive liquids. Future developments will allow use of a high-field magnet (< 7 T) on PELICAN as well as implementation of the software MANTID for data treatment and analysis.

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## First users on EMU, the cold-neutron backscattering spectrometer at the Australian Centre for Neutron Scattering

G. N. Iles<sup>a</sup>, N. R. de Souza<sup>a</sup> and A. Klapproth<sup>a</sup>

<sup>a</sup> Australian Centre for Neutron Scattering, ANSTO, Australia.

The cold-neutron backscattering spectrometer, EMU, one of the four spectrometers at ANSTO, received its operating licence in 2016. First spectra were obtained from measurements on laboratory standards such as polyethylene, m-Xylene and ammonia perchlorate [1]. The high energy resolution of EMU, allows dynamics in the nanosecond timeframe to be observed. This high resolution is due to backscattering from the Si (111) crystal monochromator and analyser arrays, delivering a spectrometer FWHM energy resolution in the order of 1.2  $\mu\text{eV}$ . EMU also features a linear Doppler drive modulating incident neutron energies over  $\pm 31 \mu\text{eV}$ . Scattered, analysed neutrons are counted in 3He LPSD arrays. By setting the Doppler driven backscattering monochromator to zero motion, elastic fixed window scans (EFW) can be performed. Changes in intensity of the analysed neutrons, with changing temperature, for example, correspond to changing dynamics in the system. Alternatively, when the incident energy is modulated, quasi-elastic neutron scattering (QENS) can be used to observe changes in the profile shape of the elastic peak. Finally, EMU can be used to observe purely inelastic scattering, such as observed in samples exhibiting rotational tunnelling.

The first users have now conducted experiments on EMU in a range of disciplines. We have measured the high temperature dynamics in lead-free ferroelectrics using (QENS) [2], and investigated the long-range oxygen diffusion in an ionic conductor [3]. We have also measured water diffusion in clays using (EFW) [4]. Future work will involve developing MANTID software for data treatment and analysis, and continuing to improve the signal-to-noise ratio.

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## Design of a low-energy electron source for inverse photoelectron spectroscopy

Joshua A. Lipton-Duffin<sup>a</sup> and Jennifer M. MacLeod<sup>a</sup>

<sup>a</sup> School of Chemistry, Physics, and Mechanical Engineering and Institute for Future Environments, Queensland University of Technology (QUT), Brisbane, 4000 QLD, Australia

Inverse photoelectron spectroscopy (IPES) is a surface science technique used to study the unoccupied electronic energy levels of solids. It may be thought of as the time-reversed analogue of ultraviolet photoelectron spectroscopy (UPS): a monochromatic beam of low-energy electrons is fired at the sample, and light is given off as these electrons are captured by the surface, with the photon energy being characteristic of the energy states in the solid. While significantly less efficient than UPS, IPES is the most direct method for studying unoccupied energy states between the Fermi and vacuum energies.

The latest implementations of IPES operate at very low energies ( $< 5$  eV), producing photons in the visible spectrum. This particular approach is very appealing for studies of delicate overlayers such as organic molecules, where higher energy beams cause unwanted chemical changes and/or damage to the species in question. Successful building of such an apparatus requires optimization of both the source and detector components.

Most of the knowledge and technical development in electron sources focuses on producing medium ( $E > 1$  keV) and high ( $E > 10$  keV) kinetic energy electrons, whereas development on low-energy sources remains a highly specialised and infrequently explored topic. Two main designs of electron source are found in previous implementations of IPE spectrometers, but their performance at very low energies has not yet been examined, especially as the beam current is maximised (to increase signal/noise levels) and the space-charge limit is approached.

Here, we present a simulation by finite element analysis that compares and contrasts the performance of two different IPES sources. Each source's performance can be quantified both in terms of spot size and convergence angle as a function of energy, which together dictate the ultimate performance of the spectrometer. The effect of space charge, which is not considered in most previous models, is explicitly explored here. This analysis will inform the design of a new electron source to be commissioned and installed for QUT's inverse photoelectron spectrometer.

## Investigation of the Emission of X-Rays in a Pyroelectric Micro X-Ray Generator

Emily W.J. Yap<sup>a,b</sup>, Rhys M. Preston<sup>b</sup>, James R. Tickner<sup>b</sup> and John E. Daniels<sup>a</sup>

<sup>a</sup> *School of Materials Science and Engineering, UNSW Australia, NSW 2052, Australia.*

<sup>b</sup> *CSIRO Mineral Resources, Lucas Heights Science and Technology Centre, NSW 2234, Australia.*

The continual implementation of X-rays as an analytical tool has led to numerous advancements in science and technology. Examples include X-ray crystallography, X-ray fluorescence analysis and medical imaging. The conventional method to generate X-rays requires high-voltage electronic components and a vacuum tube, making it a costly piece of equipment with limited lifetime. This has raised interest in developing a low-cost micro X-ray generator to expand the possibilities for the application of X-ray analysis methods. X-ray generator systems using pyroelectricity has become a potential candidate as it is able to develop a large electric field with low electrical power, dramatically reducing the required input power and device complexity. Despite several variations of such a system being demonstrated, there has been little exploration of the mechanism behind the emission of X-rays in pyroelectric generators [1]. The micro X-ray generator presented employs lithium niobate as its pyroelectric material where it is thermally cycled to ionise residual gas particles in a vacuum environment and accelerate electrons in order to emit X-rays. From this, characteristic and bremsstrahlung X-rays were observed when collected by a silicon drift detector. Furthermore, Monte Carlo simulations and X-ray emission experiments were conducted in this study to understand the X-ray emission mechanism as well as to improve the performance of the micro X-ray generator.

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**WWW 2017 Conference Abstracts**

**ABSTRACTS  
THURSDAY**

## Quantum Information Machines

David Reilly<sup>a,b</sup>

<sup>a</sup>*Microsoft Corporation*

<sup>b</sup>*Centre for Engineered Quantum Systems, The University of Sydney*

With the building-blocks of quantum technologies now in hand, efforts worldwide are turning to scale up devices into powerful machines. In addition to overcoming immense engineering challenges, scaling-up qubits into useful computational architectures will also require new science, with fundamental condensed matter physics (CMP) continuing to play a leading role. Combining a large and focused engineering effort with basic physics research is a key driver in Microsoft Corp establishing new laboratories on the campus of the University of Sydney. This talk will outline some of the challenges at the interface of condensed matter physics and quantum engineering and detail approaches to scale up quantum devices into machines.

**Bose-Einstein condensate of exciton-polaritons in structured microcavities**

T. Gao<sup>a</sup>, E. Estrecho<sup>a</sup>, G. Li<sup>a</sup>, O. A. Egorov<sup>b</sup>, X. Ma<sup>b</sup>, K. Winkler<sup>c</sup>, M. Kamp<sup>c</sup>, C. Schneider<sup>c</sup>,  
S. Höfling<sup>c</sup>, A. G. Truscott<sup>a</sup>, and E. A. Ostrovskaya<sup>a</sup>

<sup>a</sup>*Research School of Physics and Engineering, The Australian National University, Canberra  
ACT 2601, Australia.*

<sup>b</sup>*Institute of Condensed Matter Theory and Solid State Optics, Abbe Center of Photonics,  
Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany*

<sup>c</sup>*Technische Physik, Wilhelm-Conrad-Röntgen-Research Center for Complex Material  
Systems, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany*

The etch-and overgrowth technique for structuring in solid-state semiconductor microcavities provides a powerful tool for creating a photonic crystal-like potential landscape for a cavity photon. When the photon is strongly bound to an exciton in a quantum well embedded in the microcavity, the resulting exciton-polariton exhibits a confining potential whose scale is comparable with its wavelength [1]. We present a set of experiments and a comprehensive theory of loading exciton-polaritons into a one-dimensional periodic lattice of buried mesa traps. By increasing the excitation power, we observe transition from an incoherent Bose gas to a highly nonequilibrium polariton condensate. We are also able to load the condensate into distinct energy bands by changing the size, shape, and position of the excitation beam [2].

When high energy, weakly bound Bloch modes are excited, polaritons in the barrier region are free to propagate to the plane away from the array. These polaritons act as a source of coherent and phase-locked light-matter waves as evidenced by a formation of a Talbot pattern [3]. Furthermore, we demonstrate that the mesa array acts as both an amplitude and phase grating. Thus the mesa arrays can act as an effective 1D flat lens for shaping a two-dimensional coherent flow of polaritons.

A mean-field nonlinear model of nonequilibrium polariton condensation with stochastic treatment of quantum and thermal fluctuations adequately describes our experimental observations [2].

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**A two-dimensional hydrogen-bonded molecular substitutional solid solution**

Jennifer M. MacLeod,<sup>a,b,c</sup> Joshua A. Lipton-Duffin,<sup>a,b,c</sup> Chaoying Fu,<sup>d</sup> Tyler Taerum,<sup>d</sup>  
Dmitrii F. Perepichka<sup>d,e</sup> and Federico Rosei<sup>b,d,f</sup>

<sup>a</sup> *School of Chemistry, Physics, and Mechanical Engineering, Queensland University of Technology (QUT), Brisbane, 4000 QLD, Australia*

<sup>b</sup> *Institut National de la Recherche Scientifique, Centre Énergie, Matériaux, Télécommunications, Varennes, QC J3X 1S2, Canada,*

<sup>c</sup> *Institute for Future Environments, Queensland University of Technology (QUT), Brisbane, 4000 QLD, Australia*

<sup>d</sup> *Department of Chemistry, McGill University, Montreal, QC H3A 2K6, Canada*

<sup>e</sup> *Centre for Self-Assembled Chemical Structures, Montreal, QC H3A 2K6, Canada,*

<sup>f</sup> *Institute for Fundamental and Frontier Science, University of Electronic Science and Technology of China, Chengdu 610054, PR China*

Two-dimensional (2D) molecular self-assembly leads to the formation of well-defined supramolecular layers with tailored geometrical, compositional and chemical properties. To date, random intermixing and entropic effects in these systems have been associated with glassy phases and imperfect crystals. Here, we describe a 2D crystalline molecular self-assembled system that incorporates random substitutional defects.

The system comprises two C<sub>3</sub>-symmetric hydrogen bonding units with different sizes: terthienobenzenetricarboxylic acid (TTB) and 1,3,5-benzene tricarboxylic acid (TMA). Both of these molecules are well-studied, and self-assemble on highly oriented pyrolytic graphite (HOPG) surfaces to form hydrogen-bonded porous meshes. When combined, the TTB and TMA can spontaneously form an intermixed lattice, where a lattice comprising predominantly TMA also includes a small number of TTB-substituted sites. This system is analogous to the substitutional solid solutions formed in some alloys of metals. We combine density functional theory (DFT) calculations with Monte Carlo simulations to elucidate the thermodynamics of the system. This work provides insight into minimization of Gibbs free energy in an epitaxial molecular system, where molecule-substrate interactions, molecule-molecule interactions and the multiplicity of the available lattice configurations all play an important role.

## Modeling Conductive Domain Walls by means of Random Resistor Networks

Benjamin Wolba<sup>a,b</sup>, Jan Seidel<sup>a</sup>, Claudio Cazorla<sup>a</sup>, Christian Godau<sup>b</sup>,  
Alexander Haußmann<sup>a,c</sup> and Lukas M. Eng<sup>a,c</sup>

<sup>a</sup> *Institute of Applied Physics, TU Dresden Germany.*

<sup>b</sup> *School of Materials Science and Engineering, UNSW Australia.*

<sup>c</sup> *cfaed – center for advancing electronics Dresden, TU Dresden Germany.*

A random resistor network is an electrical network of ohmic resistors, for which the electrical resistivity of a single resistor is randomly determined according to a certain resistance distribution. They are not only intrinsically interesting, but moreover also quite useful for modeling electronic transport in systems with phase separation, like in composite media [1] or in manganites undergoing an insulator-metal-transition [2], as well as in lower-dimensional systems such as graphene [3] or even DNA-strings [4].

Here the random resistor network approach has been employed to model the conductivity of domain walls in uniaxial ferroelectrics, such as lithium niobate. Recently the inclination angle distribution of a domain wall in lithium niobate has been measured locally by Godau et al. [5], using a Cerenkov second-harmonic generation method for 3-dimensional domain wall mapping (see [6] for further information). This data has been used as input for a random resistor network model - addressing both the DC and AC case.

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## Terahertz Condensed Matter Physics

R. A. Lewis<sup>a</sup>

<sup>a</sup> *Institute for Superconducting and Electronic Materials and School of Physics,  
University of Wollongong, Wollongong, NSW 2522, Australia.*

Terahertz physics has developed rapidly recently as new sources, detectors and components have opened up this previously inaccessible region of the electromagnetic spectrum [1]. Indeed, the growth in the field, as evidenced by bibliometric data, is, literally, exponential [2]. Imaging, as well as spectroscopy, increase the utility and applicability of the new tools [3].

In condensed matter, many fundamental excitations, both mechanical and electronic, have energies of the order of millielectronvolts and consequently are amenable to being probed by terahertz-frequency photons [4]. These fundamental phenomena include phonons, plasmons and polaritons; impurity states and other confined states in structures of reduced dimensionality; and, in a magnetic field, cyclotron resonance and Zeeman splittings.

Terahertz techniques have recently been extended to a variety of practical problems, such as art conservation [5]. Our recent work on the terahertz spectrum of the synthetic pigment quinacridone illustrates this [6].

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## Molecule-Induced Conformational Change in 2D Nanomaterials with Enhanced Surface Adsorption

Ying Chen<sup>a</sup>, Qiran Cai<sup>a</sup>, Srikanth Mateti<sup>a</sup>, Aijun Du<sup>b</sup>, Rodney S. Ruoff<sup>c</sup> and Lu Hua Li<sup>a</sup>

<sup>a</sup> *Institute for Frontier Materials, Deakin University, Waurin Ponds 3216, VIC, Australia*

<sup>b</sup> *School of Chemistry Physics and Mechanical Engineering, Queensland University of Technology, Brisbane City, QLD 4000*

<sup>c</sup> *Center for Multidimensional Carbon Materials, Institute for Basic Science (IBS) Ulsan 44919, Republic of Korea*

Surface interaction is extremely important to both fundamental research and practical application. Physisorption can induce shape and structural distortion (i.e., conformational changes) in macromolecular and biomolecular adsorbates, but such phenomena have rarely been observed on adsorbents. We demonstrate theoretically and experimentally that atomically thin 2D nanomaterials as an adsorbent experience conformational changes upon surface adsorption of molecules, increasing adsorption energy and efficiency. [1, 2] The study not only provides new perspectives on the strong adsorption capability of 2D nanomaterials but also opens up possibilities for many novel applications. For example, such special surface property of boron nitride (BN) nanosheets can be used to increase sensitivity and reusability of Surface Enhanced Raman spectroscopy.

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## A Novel Vertical-type Light-Emitting Transistor and Approach to Normally-OFF Operation

Tadahiko Hirai<sup>a</sup>, Mark Bown<sup>a</sup> and Kazunori Ueno<sup>a</sup>

<sup>a</sup> Manufacturing, CSIRO, Bayview Avenue, Clayton, VIC3168, Australia

The light-emitting transistors have been studied for flat panel displays (FPD) and flexible display applications. There have been many reports on light-emitting organic field-effect transistors (OFETs) published. However, these devices have a narrow luminescence area in a planar-type structure, and require the used of special materials with high crystallinity and high mobility in many cases. On the other hand, vertical-type light-emitting transistors potentially have large luminescence area and low-voltage/high-current operation compared with planar-type light emitting OFETs. Recently, several vertical-type devices have been proposed, polymer grid triodes,<sup>[1]</sup> organic static induction transistors,<sup>[2-4]</sup> organic/inorganic hybrid transistors,<sup>[5]</sup> space-charge-limited transistors,<sup>[6-7]</sup> unique architecture vertical transistors,<sup>[8]</sup> metal-base organic transistors,<sup>[9]</sup> and carbon nanotube enabled vertical organic light emitting transistors.<sup>[10]</sup> However, these devices have problems for fine patterning on glass and compatibility of conventional backplane such as amorphous silicon (a-Si) or low temperature poly-crystalline silicon (LTPS) TFTs on glass substrate.

We proposed a novel vertical-type light emitting transistors (VLTs) with combination structure of layered metal-oxide and organic semiconductor layers included light emitting layer as normally-ON type device.<sup>[11]</sup> In this paper, we report to approach to normally-OFF VLTs.

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## Towards ARPES at the Australian Synchrotron: 4<sup>th</sup> Generation Toroidal Angle Resolving Electron Energy Spectrometer

A. Tadich<sup>a</sup>, E. Huwald<sup>a</sup> and J. Riley<sup>b</sup>

<sup>a</sup> *Australian Synchrotron, 800 Blackburn Road, Clayton 3168, Victoria, Australia.*

<sup>b</sup> *Department of Physics, La Trobe University, Bundoora, Victoria 3086, Australia*

Angle Resolved Photoelectron Spectroscopy (ARPES) is the “complete” photoemission experiment. It simultaneously measures a photoelectron’s kinetic energy, emission angle and sometimes spin, relative to the crystallographic axes, constructing a direct image of the electronic bandstructure. This makes ARPES the most powerful contemporary technique for determining the electronic structure of novel materials. ARPES has been instrumental in the discovery and understanding of new electronic phases of matter. For example, important aspects of the electronic structure of high-T<sub>c</sub> superconductors, such as the pseudogap were discovered using ARPES, as was the experimental discovery of three dimensional topological insulators Bi<sub>1-x</sub>Sb<sub>x</sub> and Bi<sub>2</sub>(Se,Te)<sub>3</sub>. Over the years, a dramatic improvement in the energy and momentum resolution possible with ARPES has occurred as a result of advances in photoelectron analysers and 2D detectors, allowing a range of new physics to be probed.

Despite the popularity of ARPES overseas, within Australia it has until now remained as a niche technique due to a small (albeit dedicated) user community. However, the continually growing local interest in studying novel materials with exotic electronic properties has led to the demand for our own synchrotron – based ARPES instrument. Here, an overview of a forthcoming ARPES instrument, an advanced 4<sup>th</sup> generation “toroidal” electron spectrometer, at the Australian Synchrotron will be given. Constructed at La Trobe University, the instrument will arrive at the soft x-ray beamline in early 2017, and will be located in an offline staging area between its times on the beamline. An advanced helium discharge lamp will allow for offline work to be carried out. In contrast to the previous 3<sup>rd</sup> generation instrument installed at BESSY2, the 4th generation Toroidal Analyser is equipped with a liquid helium cryostat and radiation shielding to allow for ARPES measurements to be conducted with the sample at cryogenic temperatures. An overview of the system’s principles of operation, and sample preparation environment will be given.

**Probing condensed matter with the modern fast electron**J. Etheridge<sup>a</sup>

*<sup>a</sup> Monash Centre for Electron Microscopy and Department of Materials Science and Engineering, Monash University, VIC 3800, Australia.*

Recent advances in electron-optics have given us the ability to generate and manipulate highly stable, phase coherent electron wavefields that can be brought to a focal point much smaller than an atom. This is enabling the exploration of fundamental phenomena in quantum physics, electron-optics and electron-atom interactions. It is also being applied to probe the atomic and electronic structure of matter with unprecedented spatial and energy resolution. In particular, electron scattering experiments can now be performed from small numbers of “important” atoms selected from within a specimen, offering powerful capabilities for determining the local structure and bonding of “nanostructured materials”.

This talk will give an overview of these developments, and will illustrate with various applications, such as mapping surface plasmon polaritons in metallic nanostructures; revealing Li-dependent 3D octahedral superlattices in Li-ion conductors; structure-property relationships in semiconducting nanostructures; understanding crystal growth and shape control in metal nanoparticles; and ‘imaging’ the distribution of electrons as they scatter within an atomic lattice.

## **Phase transformations and associated microstructural evolution during shock compression of materials**

J. P. Escobedo<sup>a</sup>, P.J. Hazell<sup>a</sup> and A.D. Brown<sup>a</sup>

<sup>a</sup> *School of Engineering and IT, UNSW Australia, Canberra 2610, Australia.*

When materials are subjected to high pressures in shock loading (high velocity impact) experiments they may undergo phase transformations. One such example is zirconium, it transforms from the hexagonal closed packed (hcp)  $\alpha$ -phase to the simple hexagonal  $\omega$ -phase at approximately 7 GPa. Through a combination of post-mortem and in situ techniques, different dynamic drive conditions are utilized to create a set of specimens with various volume fractions of retained high pressure  $\omega$ -phase and stored plastic work. The mechanical properties of these well-characterized microstructures are subsequently examined. The results indicate that while both plastic deformation and the volume fraction of the high pressure phase play important roles in determining subsequent material properties, the effect of texture evolution due to plastic work may be of critical importance in determining these properties. These findings shed insight into strength of condensed matter under pressure.

In this presentation the author (JP) will present the above work as well as briefly introduce the high and hyper velocity impact capabilities at UNSW Canberra able to perform these experiments.

## **Towards Generic Mathematical Descriptors for Structural Analysis and Their Applications in the Property Predictions for Molecular Crystals**

Jack Yang and Graeme M. Day

*School of Chemistry, University of Southampton  
Highfield, Southampton SO17 1BJ, United Kingdom*

The steady progress in the field of organic crystal structure predictions (CSP), exemplified by successes in the most recent international CSP blind test, has demonstrated great promise in using this computational tool in advancing our understanding in polymorphism. With global lattice energy exploring algorithms, the number of putative crystal structures generated is typically on the order between 10 to 100K, which poses a significant challenge in extracting structural patterns and thus generalizing useful chemical insights in an automated fashion. A more challenging task is how to correlate this structural information with the predicted physical properties, such as the charge transport parameters for organic crystals. The later is crucial for advancing computer-guided material designs. Unlike molecular conformation samplings in gas/solution phases, where a plethora of dimensionality reduction techniques had been developed to extract intriguing features from the energy landscapes, less had been developed for molecular crystals, due to a lack of generic and robust descriptor to represent molecular crystals ubiquitously.

Dimer synthons are the most widely used term in describing molecular crystals. Starting with the crystal structure landscape of a polyaromatic molecule, I will show how a simple set of Steinhardt bond order parameters can be applied to target  $\pi$ -stacking motifs in molecular crystals, and hence to predict nearest-neighbouring transfer integrals for calculating electron mobilities. I will then discuss how a more agnostic fingerprint (SOAP) can be used to describe more extended structural features in molecular crystals, not only that it leads to near-identical structural classification by human inspection, but excellent predictions on charge mobilities. Finally, building on the formalism of many-body expansion for energy evaluation in molecular crystals, it will be demonstrated that how to design different ‘similarity kernels’ for highlighting structural similarities in molecular crystals at different ‘length scales’, which is particularly important for characterising hydrogen-bondings in molecular crystals.

**Laser-induced Ignition of RDX Explosive Crystals**

X.T. Zu<sup>a, d</sup>, W. Liao<sup>b</sup>, W. Liu<sup>a</sup>, Z.H. Yan<sup>a, b</sup>, X. Xiang<sup>a</sup>, C.C. Zhang<sup>b</sup>, J.S. Li<sup>c</sup>, M. Huang<sup>c</sup>,  
J.X. Wang<sup>b</sup>, Z.W. Yang<sup>c</sup>, B.S. Tan<sup>c</sup>, Z.J. Li<sup>a</sup>, L. Li<sup>a</sup>, Wei Liao<sup>b</sup> and X.D. Yuan<sup>b</sup>

<sup>a</sup> School of Physical Electronics, University of Electronic Science and Technology of China,  
Chengdu 610054, China.

<sup>b</sup> Research Center of Laser Fusion, China Academy of Engineering Physics, Mianyang  
621900, China.

<sup>c</sup> Institute of Chemical Materials, China Academy of Engineering Physics, Mianyang 621900,  
China.

<sup>d</sup> Institute of Fundamental and Frontier Sciences, University of Electronic Science and  
Technology of China, Chengdu, 610054, China.

Focusing on laser ignition of energetic materials, researchers have succeeded in exploring influences of laser parameters, environmental pressure, and surface conditions on the initiation energy threshold of energetic materials. However, the chaotic configuration of explosive powders or as-pressed tablets makes it difficult to establish quantitative investigations on the laser ignition dynamics in aspect of crystallography discrimination.

In this work, we report the interactions between RDX single crystal and laser beam. It indicates that micro-defects on the RDX facets have significant influence on the surface roughness root mean square (RMS) of RDX crystals. Meanwhile, the parameters related with laser ignition probability are found to have an exponential relationship with the crystal surface roughness RMS [1]. Besides, it has been observed that the RDX crystal can be ignited more easily under UV laser irradiation. Laser-induced damages appear on the incident surface of RDX crystal slice irradiated at UV wavelength, while occur on the exit surface at near-IR wavelength. The dynamic process of laser igniting RDX crystals indicates that plasma fireball appears firstly. Then expansion of the plasma fireball generates shock wave which propagates through the air and RDX crystal respectively, and finally results in crystal materials ejection and bulk damages near the surface [2].

[1] Z.H. Yan, W. Liu, C.C. Zhang, et al. *J. Hazard Mater.* **313**, 103 (2016).

[2] Z.H. Yan, C.C. Zhang, W. Liu, et al. *Sci. Rep.* **6**, 20251 (2016).

**WWW 2017 Conference Abstracts**

**ABSTRACTS**

**POSTER**

**THURSDAY**

## Integration of Polarised $^3\text{He}$ Infrastructure with Sample Environment Equipment

T. D'Adam<sup>a</sup>, N. Booth<sup>a</sup>, G. Davidson<sup>a</sup>, S. Lee<sup>a</sup>, A. Manning<sup>a</sup>, N. Timperon<sup>a</sup> and P. Imperia<sup>a</sup>

<sup>a</sup> *Australian Centre for Neutron Scattering, Australian Nuclear Science and Technology Organisation, Lucas Heights, NSW, Australia*

Many challenges exist when attempting to integrate polarised  $^3\text{He}$  infrastructure with neutron beam instruments. This is often due to its sensitivity to the magnetic environment and also due to the compact geometry of many beam lines. One additional consideration is the effect that Sample Environment equipment can have on the functionality of a particular polarised neutron setup. We have been able to provide incident beam polarisation with two separate magnets providing fields at the sample position of up to 2 T. In addition, full polarisation analysis is possible over a temperature range of 30 mK to 800 K. To enable this, some pieces of Sample Environment equipment must be designed specifically for use with polarised  $^3\text{He}$  and in many cases modifications are necessary to accommodate the sensitive gas. We are also in the process of procuring an 8 T shielded asymmetric magnet suitable for use with polarised  $^3\text{He}$  infrastructure.

## **Polarised neutron diffraction study of the spin cycloid in strained nanoscale bismuth ferrite thin films**

Wai Tung Lee<sup>a</sup>, J. Bertinshaw<sup>a,b,\*</sup>, R. Maran<sup>c</sup>, S. J. Callori<sup>a,b</sup>, V. Ramesh<sup>c</sup>, J. Cheung<sup>c</sup>,  
S. A. Danilkin<sup>a</sup>, S. Hu<sup>c</sup>, J. Seidel<sup>c</sup>, N. Valanoor<sup>c</sup> and C. Ulrich<sup>a,b,\*</sup>

<sup>a</sup> *Australian Centre of Neutron Scattering, Australian Nuclear Science and Technology Organisation, Lucas Heights, NSW, Australia*

<sup>b</sup> *School of Physics, The University of New South Wales, Sydney, NSW, Australia*

<sup>c</sup> *School of Materials Science and Engineering, The University of New South Wales, Sydney, NSW, Australia.*

*\*Corresponding authors*

Polarised neutron scattering is capable of separating magnetic structure from chemical structure. Here we report an experiment using the newly available capability at ANSTO, namely polarised neutron diffraction using polarised <sup>3</sup>He neutron spin-filters to obtain the detail magnetic structure in even highly complex magnetic materials.

Magnonic devices that utilize electric control of spin waves mediated by complex spin textures are an emerging direction in spintronics research. Room-temperature multiferroic materials, such as BiFeO<sub>3</sub>, with a spin cycloidal structure would be ideal candidates for this purpose [1-4]. In order to realise magnonic devices, a robust long-range spin cycloid with well-known direction is desired. Despite extensive investigation, the stabilization of a large scale uniform spin cycloid in nanoscale (100 nm) thin BiFeO<sub>3</sub> films has not been accomplished. The polarized neutron diffraction experiment did confirm the existence of the spin cycloid in this BiFeO<sub>3</sub> film, which is an important prerequisite for the multiferroic coupling [1].

[1] Bertinshaw, J. et al., Nat. Commun. **7**:12664 doi: 10.1038/ncomms12664 (2016).

[2] Eerenstein, W., Mathur, N. D. & Scott, J. F., Nature **442**, 759–765 (2006).

[3] Ramesh, R. & Spaldin, N. A., Nat. Mater. **6**, 21–29 (2007).

[4] Chu, Y.-H. et al., Nat. Mater. **7**, 478–482 (2008).

## Direct evidence for the spin cycloid in strained nanoscale bismuth ferrite thin films

J. Bertinshaw<sup>a,b</sup>, R. Maran<sup>c</sup>, S. J. Callori<sup>a,b</sup>, V. Ramesh<sup>c</sup>, J. Cheung<sup>c</sup>, S. A. Danilkin<sup>b</sup>,  
W. T. Lee<sup>b</sup>, S. Hu<sup>c</sup>, J. Seidel<sup>c</sup>, N. Valanoor<sup>c</sup> and C. Ulrich<sup>a,b</sup>

<sup>a</sup>*School of Physics, The University of New South Wales, 2052 NSW, Australia.*

<sup>b</sup>*Australian Centre for Neutron Scattering, Australian Nuclear Science and Technology Organization, Lucas Heights, 2234 NSW, Australia.*

<sup>c</sup>*School of Materials Science and Engineering, The University of New South Wales, Kensington, 2052 NSW, Australia.*

Multiferroic materials demonstrate excellent potential for next-generation multifunctional devices, as they exhibit coexisting ferroelectric and magnetic orders. Bismuth ferrite (BiFeO<sub>3</sub>) is a rare exemption where both order parameters exist far beyond room temperature, making it the ideal candidate for technological applications. In particular, magnonic devices that utilize electric control of spin waves mediated by complex spin textures are an emerging direction in spintronics research. 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 (100 nm) thin BiFeO<sub>3</sub> films has not been accomplished. Here, we demonstrate cycloidal spin order in 100 nm BiFeO<sub>3</sub> thin films through the careful choice of crystallographic orientation, and control of the electrostatic and strain boundary conditions during growth [1]. Neutron diffraction, in conjunction with X-ray diffraction, reveals an incommensurate spin cycloid with a unique [112] propagation direction. While this direction is different from bulk BiFeO<sub>3</sub>, the cycloid length and Néel temperature remain equivalent to bulk single crystals. The discovery of a large scale uniform cycloid in thin film BiFeO<sub>3</sub> opens new avenues for fundamental research and technical applications that exploit the spin cycloid in spintronic or magnonic devices.

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

## Strain and Magnetic Field-Induced Spin Structure Transitions in Multiferroic BiFeO<sub>3</sub>

A. Agbelele<sup>a</sup>, D. Sando<sup>b,c</sup>, C. Toulouse<sup>d</sup>, R. D. Johnson<sup>e</sup>, R. Ruffer<sup>f</sup>, A.F. Popkov<sup>g</sup>,  
C. Carrétéro<sup>c</sup>, J.-M. Le Breton<sup>a</sup>, B. Dkhil<sup>h</sup>, M. Cazayous<sup>d</sup>, A. K. Zvezdin<sup>g</sup>, A. Barthélémy<sup>c</sup>,  
J. Juraszek<sup>a</sup> and M. Bibes<sup>c</sup>

<sup>a</sup> *Groupe de Physique des Matériaux, UMR 6634, CNRS-Université de Rouen, France.*

<sup>b</sup> *School of Materials Science and Engineering, UNSW Australia, Sydney 2052, Australia.*

<sup>c</sup> *Unité Mixte de Physique, CNRS, Thales, Univ. Paris-Sud, Palaiseau, France.*

<sup>d</sup> *Laboratoire Matériaux et Phénomènes Quantiques, Université Paris Diderot, France.*

<sup>e</sup> *Clarendon Laboratory, University of Oxford, United Kingdom.*

<sup>f</sup> *European Synchrotron Radiation Facility, Grenoble Cedex 9, France.*

<sup>g</sup> *Moscow Institute of Physics and Technology (State University), Russia.*

<sup>h</sup> *Laboratoire SPMS, UMR 8580, Ecole Centrale Paris-CNRS, Châtenay-Malabry, France.*

In multiferroic materials [1], the coexistence of several exchange interactions often results in competition between non-collinear spin orders which are sensitive to temperature, hydrostatic pressure, or magnetic field. In bismuth ferrite (BiFeO<sub>3</sub>) [2], a room-temperature multiferroic, the intricacy of the magnetic phase diagram is only fully revealed in thin films [3]: epitaxial strain suppresses the cycloidal spin order present in the bulk [4], transforming it into various antiferromagnetic states, modifying the spin direction and ordering patterns [5]. Here, we explore the combined effect of strain and magnetic field on the spin order in BiFeO<sub>3</sub>. Through nuclear resonant scattering [6] and Raman spectroscopy, we show that both strain and magnetic field destabilize the cycloid, resulting in a critical field sharply reduced from the bulk value. Neutron diffraction data support this hypothesis, with a cycloid period larger than the bulk value and increasing with strain and/or magnetic field. Analysis of the data in light of Landau-Lifshitz calculations [7] indicates that very small strains are sufficient to induce large modifications in magnetoelastic coupling, suggesting interesting opportunities for strain- and/or field-mediated devices which take advantage of finite-size effects in multiferroic films.

[1] W. Eerenstein, *et al.*, Nature 442, 759 (2006). [2] G. Catalan, J. F. Scott, Adv. Mater. 21, 2463 (2009). [3] D. Sando, *et al.*, J. Phys. Condens. Matter 26, 473201 (2014). [4] I. Sosnowska, *et al.*, J. Phys. C 15, 4835 (1982). [5] D. Sando, *et al.*, Nat. Mater. 12, 641 (2013); A. Agbelele, D. Sando, *et al.*, Adv. Mat., accepted (2016.) [6] R. Röhlsberger, *et al.*, Phys. Rev. B 67, 245412 (2003). [7] Z. V. Gareeva, *et al.*, Phys. Rev. B 87, 214413 (2013).

**Tuning domain structure and domain conductivity in BiFeO<sub>3</sub> thin films.**

V. Ramesh<sup>a</sup>, D. Sando<sup>a</sup>, Q. Zhang<sup>a</sup> and N. Valanoor<sup>a</sup>

<sup>a</sup> School of Material Science and Engineering, University of New South Wales, NSW-2052, Australia.

Multiferroic materials are at the center of focus of recent research due to extensive demand for the multifunctional materials and also due to the potential to investigate the fundamental physics associated with the coupling of various order parameters [1]. Among all multiferroics materials, BiFeO<sub>3</sub> (BFO) is of paramount interest as it is suitable for high temperature applications and also it has demonstrated the existence of large magneto electric coupling, both in the form of single crystal and as well as thin films [2].

In this study we investigate how the electrical boundary conditions, can be effectively used to control the domain structures and domain conductivity of BFO thin films. It is shown that, domain structure and properties can be tuned by the selection of right electrodes and by varying the thickness of electrode. X-ray diffraction (XRD) and atomic force microscopy (AFM) are employed for the morphological and structural characterizations. Structural and electronic characterization of intrinsic nanodomain structures is conducted with the aid of extensive piezo-force microscopic (PFM) studies at room temperature and also both room temperature and low temperature conductive-AFM. In addition, change in size and shape of the domains is also studied by varying the thickness of the BFO.

- [1] Ramesh, Ramaroorthy, & Spaldin, Nicola A. (2007). Multiferroics: progress and prospects in thin films. *Nature materials*, 6(1), 21-29.
- [2] Martin, Lane W, Chu, Ying-Hao, Holcomb, Mikel B, Huijben, Mark, Yu, Pu, Han, Shu-Jen, . . . Ramesh, R. (2008). Nanoscale control of exchange bias with BiFeO<sub>3</sub> thin films. *Nano letters*, 8(7), 2050-2055.

## ***In situ* Poling and the Strong Post-poling Relaxation of non-180° Domain Texture in Bismuth Ferrite Ceramics**

Lisha Liu<sup>a</sup> and John Daniels<sup>a</sup>

<sup>a</sup> School of Materials Science and Engineering, UNSW Australia, Sydney, Australia

Many of the overarching structural changes occurring in ferroelectrics under the application of an external field can be measured using diffraction. Real-time diffraction measurements (in-situ technique) offer a more complete view of time-dependent properties of such materials. Time-resolved diffraction techniques have been demonstrated to be useful for the measurement of structural changes at strong field for Bismuth Ferrite, BiFeO<sub>3</sub>, which is currently a highly investigated material due to its multiferroic properties (i.e., coexistence of magnetic and ferroelectric order).

BiFeO<sub>3</sub> has high spontaneous polarization ( $P_s \sim 100 \mu\text{C}/\text{cm}^2$ ) and high Curie temperature ( $T_c = 825^\circ\text{C}$ ). The remarkably high  $T_c$  of BiFeO<sub>3</sub> in comparison with other ferroelectrics such as BaTiO<sub>3</sub> ( $T_c \sim 130^\circ\text{C}$ ) and commercial Pb(Zr,Ti)O<sub>3</sub> (PZT) ( $T_c \sim 360^\circ\text{C}$ ) has made it attractive for high-temperature applications where the current market dominating piezoelectrics cannot be used. Moreover, the global restrictions on lead-based materials have further enhanced the potential of BiFeO<sub>3</sub> ceramic as a lead-free alternative for electro-mechanical applications.

However, the domain dynamics in BiFeO<sub>3</sub> is still not well-understood because of the difficulties in processing high-purity bulk ceramic and the high electrical conductivity. BFO ceramics with a high phase purity and reduced conductivity by doping 0.1%wt Co into the structure were obtained. A severe post-poling relaxation of switched non-180° ferroelectric domains has been observed *in situ* under strong-field poling. Detailed studies revealed that this effect is due to the configuration of defect dipoles inside the material,  $(V'_{Fe} - V''_O)$  and/or  $(V'_{Bi} - V''_O)$ . Quenching and extending the poling time are proposed as efficient ways to tackle this relaxation pitfall.

## The Wonderful World of Oxide Interfaces through the Lens of A Transmission Electron Microscopy

P. S. Musavi Gharavi<sup>a</sup> and Nagarajan Valanoor<sup>a</sup>

<sup>a</sup>*School of Materials Science & Engineering, University of New South Wales, NSW 2033,  
Australia.*

The demands placed by modern technologies has shifted the focus to nanoscale structured materials such as ultra-thin films, quantum dots etc. There is a whole new world when you go sub-nanometer and the transmission electron microscope (TEM) is perhaps the most powerful tool for direct visualization of nanoscale phenomena, particularly when it pertains to structural and chemical analysis. Here we present an investigation on the atomic structure of epitaxial Lanthanum Strontium Manganite (LSMO) thin films, grown on (001) Strontium Titanate (STO) substrates by pulsed laser deposition (PLD). The nature of this hetero interface affects the magnetic and electrical properties. Due to the difference in the lattice parameters of films ( $a_{\text{LSMO}} = 3.870 \text{ \AA}$ ) and substrate ( $a_{\text{STO}} = 3.905 \text{ \AA}$ ) at the room temperature, LSMO films are under tensile stress. This presentation demonstrates the complex correlations between the thickness of the LSMO films (<20nm, 30nm, and 40nm), and interface nature such as structural defects, misfit dislocations, and chemical diffusion at a nanostructured oxide boundary. In doing so it will provide insight into the local chemistry-defect structure correlations for archetypical perovskite interfaces.

## **Conduction Behaviour of Domains, Domain Walls, and Grain Boundaries in Pure and La-doped BaTiO<sub>3</sub> Ceramics**

Dohyung Kim<sup>a</sup>, Marty Gregg<sup>b</sup> and Jan Seidel<sup>a</sup>

<sup>a</sup> *School of Materials Science and Engineering, UNSW Australia, Sydney*

<sup>b</sup> *Center for Nanostructured Media and School of Mathematics and Physics, Queen's  
University Belfast, UK*

The electric conductivity at domain walls as well as domains of ferroelectric materials has received significant interest as these effects open new perspectives for future nanoelectronics applications. Although the conduction behavior in various standard ferroelectric thin films and single crystals has been studied recently, which includes bismuth ferrite, lithium niobate and lead zirconate titanate, there has been no report that systematically investigates this conductivity of domain walls in polycrystalline ceramics.

In our work, polycrystalline pure and La-doped barium titanate (BTO) ceramics were used for measurements of conduction mechanism at the domains, and domain walls and grain boundaries. These materials have practical application as positive thermal coefficient resistors (PTCR). Detailed domain configurations in individual grain were measured by piezoelectric force microscopy (PFM) as a function of temperature. Domain structures with 90 and 180 degree walls were found that interact with grain boundaries. In order to measure difference of conductivity at the domains, domain walls, and grain boundaries in pure and La-doped BTO, conductive atomic force microscopy (c-AFM) was used with increasing temperature. Furthermore, I-V curves from those samples were measured macroscopically which can be compared with the microscopic data. Distinct temperature-dependent electric conduction at certain grain boundaries and conductivity of the domains were observed. In particular, domain walls showed different behavior in comparison with grain boundaries.

## Reversible Polarization in PbZrTiO<sub>3</sub> Bilayers Grown Upon Silicon Substrates

R.S. Winkler<sup>a</sup> and N. Valanoor<sup>a</sup>

<sup>a</sup> *School of Materials Science and Engineering, UNSW Australia, Sydney 2033, Australia.*

Polarization rotation engineering is an effective approach to control rotational polar systems leading to giant piezoelectric and dielectric responses and can be achieved in ferroelectric ultrathin films by lowering symmetry through epitaxial strain. It has been previously shown that an underlying epitaxial 20 nm thick rhombohedral PbZr<sub>0.55</sub>Ti<sub>0.45</sub> (PZT-R) film naturally causes a canting of the polarization in a 5 nm thick tetragonal PbZr<sub>0.3</sub>Ti<sub>0.7</sub> (PZT-T) film due to an imposed in-plane tensile strain [1]. This caused a decoupling of the PZT-T layer to the STO [001] substrate giving rise to robust, reversible in- to out-of-plane rotation. Silicon substrates are much more widely used in functional devices, with considerably higher investment in industry and would therefore be a more appropriate choice of substrate for end of use applications. This work shows an optimized method for producing the PZT-T/PZT-R ferroelectric bilayer structure with reversible polarization upon silicon substrates. Epitaxial quality was assured via atomic force microscopy (AFM) and x-ray diffraction (XRD) and the effects of polarization rotation were investigated with piezoresponse force microscopy (PFM). The control of the polarization via interfacial interactions leads to more enhanced and efficient ferroelectric devices for logic and memory giving great potential for future development.

[1] G. Liu, et al. *Advanced Materials Interfaces*. **3**, 18 (2016).

**Focused Ion Beam Methodologies pave the way for “Ferroelectrics”:  
Release the Kraken**

S.R. Burns<sup>a</sup>, J.M. Gregg<sup>b</sup> and N. Valanoor<sup>a</sup>

<sup>a</sup> *School of Materials Science and Engineering, University of New South Wales, Sydney 2052, Australia.*

<sup>b</sup> *Centre for Nanostructured Media, School of Mathematics and Physics, Queen’s University Belfast, University Road, Belfast BT7 INN, United Kingdom.*

As we reach the physical limit of Moore’s law and silicon based electronics, alternative schemes for memory and sensor devices are being proposed on a regular basis. The properties of ferroelectric materials on the nanoscale are key to developing device applications of this intriguing material class, and nanostructuring has been readily pursued in recent times. Focused ion beam (FIB) microscopy is one of the most significant techniques for achieving this. When applied in tandem with the imaging and nanoscale manipulation afforded by proximal scanning force microscopy tools, FIB-driven nanoscale characterization has demonstrated the power and ability which simply may not be possible by other fabrication techniques in the search for innovative and novel ferroic phenomena. At the same time the process is not without pitfalls; it is time-consuming and success is not always guaranteed thus often being the bane in progress. A level of sophistication using nanostructuring to control domain dynamics has been established in nanomagnetism that is far beyond the equivalent state-of-the-art in ferroelectrics.

For ferroelectrics, completely new forms of domain wall nanoelectronics could be created in which “now-you-see-it, now-you-don’t” conducting channels would entirely dictate device function. Merging the two ideas above, that is using FIB to pattern ferroelectrics and then PFM to create interesting domain wall functionality and domain wall device control paves the way for next generation “ferroelectrics”

**Epitaxial PbZr<sub>x</sub>Ti<sub>1-x</sub>O<sub>3</sub> ferroelectric bilayers with giant electromechanical properties**

Guangqing Liu<sup>a</sup>, Hsin-Hui Huang<sup>a</sup>, Qi Zhang<sup>a</sup>, Esther Huang<sup>a</sup>, Ronald Maran<sup>a</sup>, Hugh Simons<sup>b</sup>, Zijian Hong<sup>c</sup>, Osami Sakata<sup>d</sup>, Yoshitaka Ehara<sup>a,d</sup>, Takahisa Shiraishi<sup>d</sup>, Hiroshi Funakubo<sup>d</sup>, Long-Qing Chen<sup>c</sup>, Paul Munroe<sup>a</sup> and Valanoor Nagarajan<sup>a</sup>

<sup>a</sup>*School of Materials Science and Engineering, The University of New South Wales,*

<sup>b</sup>*Department of Physics, Technical University of Denmark, Lyngby kgs 2800, Denmark*

<sup>c</sup>*Department of Materials Science and Engineering, Materials Research Institute, The Pennsylvania State University, University Park, PA 16802-5006, USA*

<sup>d</sup>*Department of Innovative and Engineered Materials, Tokyo Institute of Technology, J2-1508, 4259 Nagatsuda-cho, Midori-ku, Yokohama, Kanagawa, 226-8502, Japan*

Giant electromechanical response via ferroelastic domain switching and polarization rotation is achieved in epitaxial (001) ferroelectric tetragonal (T) PbZr<sub>0.30</sub>Ti<sub>0.70</sub>O<sub>3</sub> (T-PZT)/rhombohedral (R) PbZr<sub>0.55</sub>Ti<sub>0.45</sub>O<sub>3</sub> (R-PZT) bilayers, grown on La<sub>0.67</sub>Sr<sub>0.33</sub>MnO<sub>3</sub> (LSMO) buffered SrTiO<sub>3</sub> (STO) substrates. Three different PZT bi-layer configurations are studied in this report: (a) Thick PZT (100 nm T-PZT/100 nm R-PZT/20 nm LSMO/STO(001)); (b) Thin PZT (30 nm T-PZT/100 nm R-PZT/20 nm LSMO/STO(001)) and (c) Ultra-Thin PZT (5 nm T-PZT/20 nm R-PZT/15 nm LSMO/STO(001)).

For Thick and Thin PZT, high-resolution x-ray diffraction and transmission electron microscopy show that the domain structure of the T-PZT films is tuned as a function of its thickness, from a fully in-plane *a1/a2*-domains (for a 30 nm T-PZT layer) to a three domain stress-free *c/a1/c/a2* polytwin state (for a 100 nm thick T-PZT layer). Polarization switching experiments find large switchable polarizations of up to 65  $\mu\text{C}/\text{cm}^2$ . Quantitative piezoelectric force microscopy reveals enhanced piezoelectric coefficients, with  $d_{33}$  coefficients ranging from 250 to 350 pm/V, which is up to 7 times higher than the nominal PZT thin film values. These large numbers are attributed to the motion of nanoscale ferroelastic domains, confirmed by piezoresponse force microscopy images. For the Ultra-Thin PZT, an underlying 20 nm thick PZT-R layer reduces the symmetry in a 5 nm-thick PZT-T layer by imposing an in-plane tensile strain while simultaneously decoupling the PZT-T layer from the substrate. This prevents clamping and facilitates large-scale polarization rotation switching ( $\sim 60 \mu\text{C}/\text{cm}^2$ ) and an effective  $d_{33}$  response 500% ( $\sim 250 \text{ pm}/\text{V}$ ) larger than the PZT-R layer alone. All bi-layer films present a stable ferroelectric switching for up to  $10^7$  cycles.

The study thus reports a fundamental understanding of the origin of giant piezoelectric coefficients in epitaxial ferroelectric bilayers, and the precise control of the subtle interface-driven interactions between the lattice and the external factors that control polarization opens a new door to enhanced – or completely new – functional properties.

## Combinatorial high resolution scanning X-ray diffraction in lead-free piezoelectrics

F. Marlton<sup>a</sup>, O. Standard<sup>a</sup> and J. Daniels<sup>a</sup>

<sup>a</sup> *School of Materials Science and Engineering, University of New South Wales, NSW 2033, Australia.*

Piezoelectrics are used in a wide variety of technology applications and currently their best performing compositions are lead-based. Legislative requirements will impose serious restrictions on the use of these lead-based materials in consumer devices over the coming years. Currently no viable lead-free alternative exists that operate over similar environmental ranges to existing lead-based materials.

It is well accepted that the electro-mechanical properties of piezoelectrics are maximised at Morphotropic Phase Boundaries (MPBs). Locating these phase boundaries can be difficult using traditional routes due to the vast numbers of samples required. A potential pathway for the discovery of otherwise unknown phase boundaries in higher order (ternary and quaternary) solid solutions is through combinatorial techniques. This involves the rapid synthesis and analysis of large numbers of compositions, through many combinations of a relatively small number of starting compounds.

A powder layering method was used to prepare binary combinatorial samples within the lead-free ternary system  $\text{BT}_x\text{ST}_y\text{BNT}_{(1-x-y)}$  (where  $\text{BT} = \text{BaTiO}_3$ ,  $\text{ST} = \text{SrTiO}_3$ ,  $\text{BNT} = \text{Bi}_{0.5}\text{Na}_{0.5}\text{TiO}_3$ ). Scanning beam synchrotron x-ray diffraction was then used to analyse the structure as a function of composition to map out potential phase boundaries where the piezoelectric properties of the ceramics are expected to be a maximum.

## Disordered structures in lead-free piezoelectrics from diffuse x-ray and neutron scattering

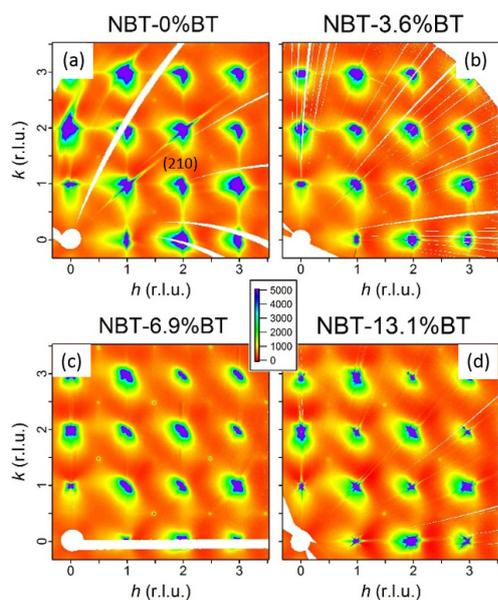
P. Tung<sup>a</sup>, M. Major<sup>b</sup>, J. Hudspeth<sup>c</sup> and J. Daniels<sup>a</sup>

<sup>a</sup> School of Materials Science and Engineering, UNSW, Sydney, Australia.

<sup>b</sup> Institute of Materials Science, Technische Universität Darmstadt, Darmstadt, Germany

<sup>c</sup> Structure of Materials Group, European Synchrotron Radiation Facility, Grenoble, France

With global environmental policies being enforced, it is crucial to replace the dominant lead-based piezoelectrics with lead-free alternatives. One potential candidate that shows promising properties is the perovskite solid-solution of  $\text{Na}_{1/2}\text{Bi}_{1/2}\text{TiO}_3\text{-xBaTiO}_3$  (NBT-xBT). [1] In particular, the composition of NBT-7BT shows heightened piezoelectric properties, where the material sits on a phase boundary between a ferroelectric rhombohedral and a ferroelectric tetragonal phase, known as a morphotropic phase boundary. [2] However, elucidating the origins of the electro-mechanical mechanisms of such materials is not straightforward, as there are numerous disordered structures that contribute to the functional properties. [3]



**Figure 1.** Segments of  $(hk0)$  reciprocal space planes from diffuse x-ray scattering for (a) NBT-0%BT (b) NBT-3.6%BT (c) NBT-6.9%BT and (d) NBT-13.1%BT.

Single crystal compositions of NBT-0BT, NBT-3.6BT, NBT-6.9BT and NBT-13.1BT were chosen to resolve the local structures across the morphotropic phase boundary. To analyse the local structures, diffuse x-ray and neutron scattering was utilised. Diffuse scattering arises from correlated short-range order in materials and thus can provide unique information that differs from the long-range average atomic structure provided by Bragg scattering. Synchrotron x-ray and neutron scattering

experiments were performed with *in-situ* electric fields and temperature variations, respectively. This presentation provides an overview of the structural features giving rise to the diffuse scattering signals and how these may affect the macroscopic functional properties of the material.

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[3] J.E. Daniels, W. Jo and W. Donner, *JOM*, **64** [1] 174-80 (2012).

**Electron Diffraction from Micro- and Nano-structured cubic zirconia**Chris Yu Chen<sup>a,\*</sup> and J R Sellar<sup>a</sup><sup>a</sup> *Department of Materials Science and Engineering, Monash University**\*Permanent Address: Pyrotek Products, East Tamaki, New Zealand 2013*

Pure zirconia ( $\text{ZrO}_2$ ), when alloyed with  $\sim 10$  mole percent or more of metal oxides such as those of Mg, Sc, Ca or Y, can “stabilize” its cubic form down to room temperature for engineering applications, often in harsh conditions. The diffraction patterns of these various stabilized zirconias are strikingly similar in appearance and their phase equilibria are also topologically quite similar, hinting at a common structural origin. The structure, however, of these oxide alloys has been hotly contested over a long period, with a consensus emerging only recently that the alloys consist essentially of nanometric regions of known single-crystal line phases containing crystallographic vacancies, embedded coherently in a matrix of pure, distorted cubic  $\text{ZrO}_2$ , first identified in the lime (CaO)-stabilized alloy by Allpress and Rossell (AR). In the present note we demonstrate how the AR model can account for the appearance of a distinctive ring-shaped feature in the selected-area diffraction patterns of alloy specimens which have been prepared at high temperature and very slowly cooled to equilibrium.

## In-situ studies of $\gamma$ -based Ti-Al alloys using synchrotron X-ray and neutron diffraction

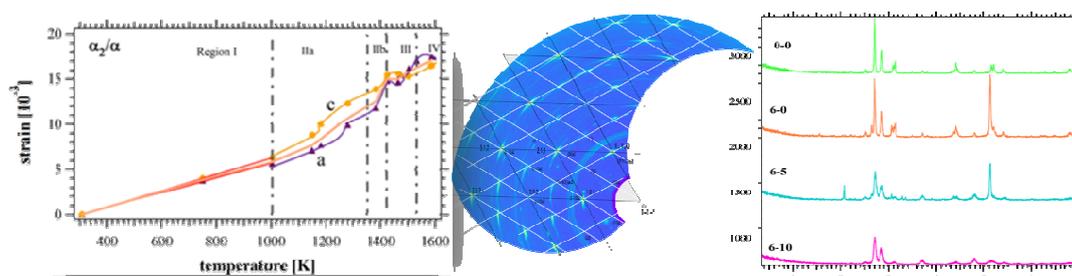
Xi Li<sup>a,b</sup>, Klaus-Dieter Liss<sup>a,b</sup> and Rian Dippenaar<sup>b</sup>

<sup>a</sup> Australian Nuclear Science and Technology Organisation, Lucas Heights, NSW 2234, Australia

<sup>b</sup> School of Mechanical, Materials & Mechatronic Engineering, University of Wollongong, NSW 2522, Australia.

Email:xl910@uowmail.edu.au

Because of their low density, good strength, corrosion resistance and high service temperature  $\gamma$ -based titanium aluminides are being considered as materials of choice in the aerospace and automobile industry. In our study, we focus on a series of interesting  $\gamma$ -based Ti-Al alloys with respect to the lattice evolution of Ti-45Al-7.5Nb-0.25C (at. %) during heating under a pressure of 10 GPa followed by synchrotron radiation; order-disorder transitions and short-range-order in polysynthetic twinned Ti-Al single crystals using neutron scattering and phase transformation and texture evolution of high pressure torsion samples of Ti-45Al-7.5Nb by using complementary X-ray and neutron diffraction. Lattice parameter evolution can be separated into four contributions: thermal expansion, composition, order parameter and pressure. Diffuse scattering at reciprocal lattice positions provides evidence of short-range order, even in the disordered phase at very high temperature. Structural and atomic disorder is largely introduced by severe plastic deformation. These findings are fundamental to develop an improved understanding of the complex phase transformations. We report our first results of experiments performed under extremely high-pressure, relevant to advanced manufacturing processes.



## High-Pressure Single-Crystal Neutron Diffraction

G.J. McIntyre<sup>a</sup>, J. Binns<sup>b</sup> and S. Parsons<sup>c</sup>

<sup>a</sup> *Australian Nuclear Science and Technology Organisation, Lucas Heights NSW 2234, Australia*

<sup>b</sup> *Centre for High-Pressure Science & Technology Advanced Research, Shanghai, PRC*

<sup>c</sup> *Centre for Science at Extreme Conditions, School of Chemistry, University of Edinburgh, Edinburgh EH9 3JJ, UK*

High-pressure neutron diffraction is always challenging, but it can offer several advantages over high-pressure X-ray diffraction to make meeting those challenges worthwhile. In addition to the usual higher sensitivity to low-Z elements, notably hydrogen, and to magnetic moments, the low absorption by many pressure cell materials can yield greater reciprocal-space coverage for single crystals. The low scattering power usually requires considerably larger sample volumes than with X-rays, but for the same reason the cell-wall materials can be quite thick.

Common cell designs include He-gas cells and simple clamp cells, opposed piston cells (e.g. Bloch, McWhan), opposed-anvil cells (e.g. diamond anvil cell, Paris-Edinburgh cell), and multi-anvil cells, each adapted to sample volume, accessibility, pressure, and other external parameters, especially temperature, that suit the scientific question of interest. State-of-the-art experiments using each cell type will be described.

A special challenge in high-pressure diffraction is to perform neutron and X-ray experiments on the same material under the same conditions. Previously, this meant using different cells and samples with achieving identical pressures largely a hit-or-miss affair. This has all changed with the recent demonstration on KOALA on the OPAL research reactor that modern neutron Laue diffraction can be performed on the same sample in the same diamond-anvil cell as used for laboratory X-ray experiments [1].

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## Use of the Isolated Atom Model in Quantitative Convergent Beam Electron Diffraction

A.E. Smith<sup>a</sup>, T. Liu<sup>b</sup>, D. Peng<sup>b</sup>, L. Bourgeois<sup>b,c</sup> and P N.H. Nakashima<sup>b</sup>.

<sup>a</sup> *School of Physics, University of Melbourne, Monash University, Victoria, 3168, Australia.*

<sup>b</sup> *Department of Materials Science and Engineering, Monash University, Victoria, 3168, Australia.*

<sup>c</sup> *Monash Centre for Electron Microscopy, Monash University, Victoria, 3168, Australia.*

Quantitative Convergent Beam Electron Diffraction (QCBED) is that experimental technique which probes the bonding in metals and ceramics with highest resolution, e.g. the first unequivocal determination of bonding in aluminium [1]. At present QCBED uses background subtraction employing the Fourier transform of the electronic charge density of an isolated atom model (IAM) based on a Relativistic Hartree Fock atomic calculation [2].

Computational crystalline material property programs establish the cohesive energy, one of the most fundamental quantities, by a super cell that mimics the IAM. This then enables the determination of various defect and surface energy properties [3]. The present work employ IAMs found by WIEN2k [4] to compare with QCBED results over a wide range of materials [5]. The requirement of a charge density Fourier transform necessitates an all-electron method such as WIEN2k.

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[5] X. Sang, A. Kulovits, G. Wang and J. Wiezorek, *J. Chem. Phys.* **138**, 084504 (2013).

**In-situ study of solid state dewetting in single crystal Ni films**S. Jahangir<sup>a</sup>, C. V. Thompson<sup>b</sup> and N. Valanoor<sup>a</sup>

<sup>a</sup> *School of Materials Science and Engineering, University of New South Wales, NSW 2052, Australia.*

<sup>b</sup> *Department of Materials Science and Engineering, Massachusetts Institute of Technology, MA, USA.*

Thin films are fabricated in conditions far from the equilibrium and they bear a high surface to volume ratio. Therefore, when thermally activated, they transform to a stable morphology of isolated islands to reduce their free energy associated with surfaces. This phenomenon is called “solid state dewetting”.

Dewetting of thin films can lead to formation of complex sub-micron or nano structures, depending on the initial geometry of the film. In single crystal thin films, dewetting leads to formation of ordered assembly of the islands. This is due to the structural symmetry, anisotropic surface energy and anisotropic diffusivity of single crystal films. The morphological characteristics of these ordered structures are manifested by instabilities that happen spontaneously during dewetting. For instance, fingering instability that is the result of local differences in retraction rate of the edge of a thin film. Clear identification of these instabilities leads to enhanced inference of the underpinning kinetic mechanisms that govern the formation of complex dewetting morphologies. In this study, we use pre-patterned single crystal Ni film on single crystal MgO substrate as a model system to investigate the effect of various parameters on final morphology of dewetted structures. More specifically, we probe the effect of in-plane crystallographic orientation of film patches and annealing temperature on fingering instability. We also demonstrate that solid state dewetting can be exploited as a self-assembly method to achieve a desired morphology via introducing a template to the patches of single crystal Ni films. The template is systematically designed to facilitate the fingering instability and control the spacing of void fingers.

**Arsenic Removal from Groundwater by a Goethite-Coated Mineral Sand**

S. Kahn<sup>a</sup>, J.D. Cashion<sup>b</sup>, A.F. Patti<sup>a</sup>, W.P. Gates<sup>c\*</sup> and S. Adeloju<sup>a</sup>,

<sup>a</sup> *School of Chemistry, Monash University, Victoria 3800, Australia.*

<sup>b</sup> *School of Physics and Astronomy, Monash University, Victoria 3800, Australia.*

<sup>c</sup> *Department of Civil Engineering, Monash University, Victoria 3800, Australia..*

Arsenic (As) contamination of groundwater is a world-wide problem. There are many sources and causes including geothermal activity, mining operations and smelting of arsenopyrite mineral ores, coal burning and use in industrial processes. Approximately 50 million people in Bangladesh are exposed to As contamination above the UN standard of 10 µg/L. Up until the 1970's, surface water was the principal source for potable water, but health issues associated with bacteriological contamination has resulted in large scale replacement by ground water accessed by tube wells. Groundwater in Bangladesh suffers from arsenic contamination due to draw-down and oxidation of arsenopyritic minerals in the aquifers. Thus an urgent need for simple and cheap purification systems suitable for village use and maintenance exists.

Poorly crystalline iron hydroxides are effective at adsorbing As, but there are problems with sorptive capacity, pore blocking and in regenerating it periodically. One solution is to use iron hydroxide coated materials, such as silica. We have tested a range of potential materials sourced from around Australia and also some synthetic materials. The best results in a test rig were obtained with Skye brick sand, of ~0.1-1 mm, sourced from near Cranbourne, Victoria.

Mössbauer spectroscopy has been used to identify the active phase. A room temperature spectrum of the raw material showed a doublet, potentially clay or poorly crystalline oxyhydroxide, and a poorly resolved sextet, probably hematite. Adding As caused a marked increase in the doublet spectral area and since we had not added any iron, it must be due to an increased recoilless fraction caused by an increase in the mass. Thus the arsenic is attached to the iron particles and the particles must be nanoparticulate. Spectra in a small field and at 78 K showed that the active phase was goethite and that the hematite did not participate.

\* Present address: Institute for Frontier Materials, Deakin University, Burwood, Vic, 3125 Australia

## Boron Nitride Nanosheets Improve Sensitivity and Reusability of Surface-Enhanced Raman Spectroscopy

Ying Chen<sup>a</sup>, Qiran Cai<sup>a</sup>, Srikanth Mateti<sup>a</sup>, Aijun Du<sup>b</sup> and Lu Hua Li<sup>a</sup>

<sup>a</sup>*Institute for Frontier Materials, Deakin University, Waurin Ponds 3216, VIC, Australia*

<sup>b</sup>*School of Chemistry Physics and Mechanical Engineering, Queensland University of Technology, Brisbane City, QLD 4000*

Atomically thin boron nitride nanosheets have been used to fabricate highly sensitive, reproducible, and reusable Surface-Enhanced Raman Spectroscopy (SERS) substrates. When used to cover plasmonic silver nanoparticles (Ag NPs), boron nitride nanosheets can enhance the sensitivity by up to two orders of magnitude. The impermeability and thermal stability of boron nitride nanosheets protects the Ag NPs from oxidation so that the substrates can be regenerated by heating in air and reused. They are efficient in adsorption of aromatic molecules to improve Raman sensitivity, especially at extremely low concentrations. [1] The synergistic effect of the atomic thickness, high flexibility, stronger surface adsorption capability, electrical insulation, impermeability, high thermal and chemical stability of BN nanosheets can increase the Raman sensitivity and in the meantime attain long term stability and extraordinary reusability not achievable by other materials. These advances will greatly facilitate the wider use of SERS in many fields. [2]

[1] Cai Q, Mateti S, Yang W, Jones R, Watanabe K, Taniguchi T, Huang S, Chen Y, Li LH, *Angewandte Chemie International Edition*, **55(29)** (2016) 8405-9, (Cover)

[2] Cai, Q; Mateti, S; Watanabe, K; Taniguchi, T; Huang, S; **Chen, Y**; Li, LH, *ACS Applied Materials & Interfaces*, **8** (2016) 15630–15636



## Surface Modification of Fused Silica Optics with CO<sub>2</sub> Laser for Improving Optical Performance

W. Liao<sup>a</sup>, C. C. Zhang<sup>a</sup>, X. Xiang<sup>b</sup>, X. D. Yuan<sup>a</sup> and X. T. Zu<sup>b</sup>

<sup>a</sup>*Research Center of Laser Fusion, China Academy of Engineering Physics, Mianyang, China*

<sup>b</sup>*School of Physical Electronics, University of Electronic Science and Technology of China, Chengdu, China*

Inertial confinement fusion (ICF) class laser systems require a large area of high quality fused silica optics, which may be exposed to laser irradiation in a certain high fluences. Unavoidably, defects such as scratches and contamination are formed on the optical surface during the mechanical fabrication. Those defects may lead to laser induced damage (LID) by absorbing laser energy and thus affect the overall performance of laser system. Previous research of our group has shown that, since the material was heated to several thousand degrees by CO<sub>2</sub> laser, defects would be removed with surface melting and reconstruction so that the damage resistance could be enhanced. But the surface profile might be changed after laser treatment because of the material flowing driven by thermal expansion effects or surface tension force. Moreover, non-uniform temperature fields can cause changes of local structure which may weaken the surface strengths and degrade the polarization state of laser owing to the stress birefringence. In this work, interaction mechanism between CO<sub>2</sub> laser and fused silica was studied and the response law of the material under different laser parameters such as beam spot size, pulse duration and cumulative treating time was analyzed in detail. Experiment results showed that the damage threshold of CO<sub>2</sub> laser treated area was approximately 40% higher than before without nearly all adverse effects by reasonable control of CO<sub>2</sub> laser energy deposition. And not only that, the surface roughness was also improved.



**WWW 2017 Conference Abstracts**

**ABSTRACTS**

**FRIDAY**

## Vortices, Vortex Lattices and the possibility of exotic superfluidity in dipolar quantum gases

Andy Martin

*University of Melbourne*

In this talk I will summarize the recent progress in dipolar quantum gas research. I will then consider the properties of dipolar Bose-Einstein condensates, focusing on the properties of a vortex, pairs of vortices [1] and vortex lattices in these systems [2]. In the case of pairs of vortices I will show that their dynamics can be significantly altered in the presence of dipolar interactions. For vortex lattices I will show that dipolar interactions can significantly alter the structure of the lattice, away from the traditional triangular, Abrikosov, vortex lattice. I will then move on to consider the properties of a quantum gas of Fermions, with strong dipolar interactions. I will argue that in these systems it may be possible to have an exotic BCS like transition. However, the results presented will show that this is experimentally challenging [3].

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[2] *Vortices and vortex lattices in quantum ferrofluids*, A.M. Martin, **N.G. Marchant**, N.G. Parker and D.H.J. O'Dell, arXiv:1606.07107

[3] *Effect of anisotropic exchange interactions and short-range phenomena on superfluidity in a homogeneous dipolar Fermi gas*, **I. Corro** and A.M. Martin, Physical Review A **94**, 023603 (2016)

## Novel magnetism, superconductivity, and spintronics potential in rare earth nitrides

B.J. Ruck<sup>a</sup>

<sup>a</sup> *The MacDiarmid Institute for Advanced Materials and Nanotechnology, School of Chemical and Physical Sciences, Victoria University of Wellington, Wellington, New Zealand*

The rare earth nitrides offer a fascinating mix of magnetic and conduction properties [1]. Most members of the series have been recognised as ferromagnetic for over 40 years, with the magnetism originating in both the spin and orbital moments of the 4*f* shell. Their electronic states have been less well characterised, with even basic questions such as whether they are metals or semiconductors adequately addressed only recently. Several are now recognised as intrinsic ferromagnetic semiconductors, with potential use in spintronics devices. Here I will focus on three members of the series: GdN, EuN, and SmN.

GdN has the highest Curie temperature (~70 K), and it has a strong spin-only magnetic moment. By contrast SmN has a near-zero magnetic moment due to almost complete cancellation of the spin moment by an equally strong orbital moment. EuN should not be magnetic at all because the Eu<sup>3+</sup> ion has a total angular momentum quantum number  $J = 0$ . We have found that doping these compounds through nitrogen vacancies not only allows control of the conductivity, but it can render EuN ferromagnetic at temperatures above 100 K [2], and even give rise to superconductivity deep within the ferromagnetic state in SmN [3]. I will discuss the reasons for these surprising properties. I will also present a novel magnetic tunnel junction made with GdN and SmN electrodes [4]. The strong spin polarisation and contrasting magnetic properties lead to a surprisingly large magnetoresistance with an unusual field dependence.

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[3] E.-M. Anton, et al., *Superconductivity in the ferromagnetic semiconductor SmN*, Phys. Rev. B 94, 024106 (2016).

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## Approaching the Bose glass-superfluid quantum phase transition using nano-structured chains of Josephson junctions

K. Cedergren<sup>a</sup>, Roger Ackroyd<sup>a</sup>, A. Shnirman<sup>b</sup> and T. Duty<sup>a</sup>

<sup>a</sup> *EQuS - ARC Centre of Excellence for Engineered Quantum Systems*

*School of Physics, University of New South Wales, NSW 2052, Australia.*

<sup>b</sup> *Karlsruhe Institute of Technology (KIT)*

*Institut für Theorie der Kondensierten Materie (TKM), D-76128 Karlsruhe Germany*

The low-temperature states of bosonic fluids exhibit fundamental quantum effects at the macroscopic scale. When bosons interact, disorder can destroy condensation, leading to a Bose-Anderson glass. This phase has been very elusive in experiments, but is thought to describe helium-4 in porous media, cold atoms in disordered optical potentials, disordered magnetic insulators, and thin superconducting films. The ubiquity of such a glass phase in Josephson-junction array devices has important implications for the proposed use of such devices as the basis for a fundamental quantum current standard. Unlike the Mott insulator, the insulating state of the Bose glass is compressible, and therefore AC synchronisation of charge, as required for well-defined current steps, may not be possible. Although mesoscopic superconducting systems present significant disorder, it has not been sufficiently addressed in the context of the dual Josephson effect.

We have measured the critical voltage for a large number of single-junction chains of mesoscopic Josephson junctions. We establish Bose glass behaviour in these devices by observing universal scaling of critical voltage with single-junction Bloch bandwidth. The measurements reveal a localisation length exponent that steepens with the Luttinger constant  $K$ , as one moves toward the quantum phase transition. This is in contrast to the fixed exponent found for classical pinning of charge density waves, vortex lattices, and disordered spin systems. We have recently extended our measurements to SQUID chains, finding somewhat unexpected behaviour.

## Mechanisms of the in-plane g-factor anisotropy in p-type quantum point contacts

D. S. Miserev<sup>a</sup>, A. Srinivasan<sup>a</sup>, I. Farrer<sup>b</sup>, D. A. Ritchie<sup>c</sup>, A. R. Hamilton<sup>a</sup> and O. P. Sushkov<sup>a</sup>

<sup>a</sup> *School of Physics, University of New South Wales, Australia*

<sup>b</sup> *Department of Electronic and Electrical Engineering, University of Sheffield, United Kingdom*

<sup>c</sup> *Cavendish Laboratory, University of Cambridge, United Kingdom*

A quantum point contact (QPC) is a narrow constriction linking two two-dimensional reservoirs with electrons or holes. Experimental studies of electron based QPCs started three decades ago with the discovery of the conductance quantization [1-2]. A decade ago advanced technologies made it possible to study hole based systems that provide a variety of complex spin-orbital effects. Spin-orbit interaction (SOI) in hole systems is much stronger and complex than in electron systems. It makes p-type systems important for spintronics and spin based quantum information applications.

The effect of anisotropy of the hole in-plane g-factor in QPCs has been discovered a decade ago in [3] and later confirmed in several publications [4]. However, the mechanism under the effect has remained unclear. All previous theoretical models either predict no anisotropy of the in-plane g-factor or predict the anisotropy opposite to experimental data [5]. In the present work, we explain the physical mechanism of the g-factor anisotropy. We identify the additional SOI which has been ignored in all previous studies but which results in strong anisotropy of the in-plane g-factor. We also performed systematic experimental studies which confirm the legitimacy of our new theory.

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- [2] D. A. Wharam et al, *J. Phys. C: Solid State Phys.* **21**, L209 (1988).
- [3] R. Danneau et al, *Phys. Rev. Lett.* **97**, 026403 (2006).
- [4] F. Nichele et al, *Phys. Rev. Lett.* **113**, 046801 (2014).
- [5] Y. Komijani et al., *EPL* **102**, 3 (2013).

## **Structural Evolution of Metals at High Temperature: Complementary Investigations with Neutron and Synchrotron Quantum Beams**

Klaus-Dieter Liss<sup>a,b</sup>

<sup>a</sup> *Australian Nuclear Science and Technology Organisation,  
Lucas Heights, NSW 2234, Australia*

<sup>b</sup> *School of Mechanical, Materials & Mechatronic Engineering, University of Wollongong,  
Wollongong, NSW 2522, Australia*

*Email: kdl@ansto.gov.au, liss@kdliss.de, web site: <http://liss.freeshell.org>*

In-situ neutron and synchrotron X-ray diffraction deliver unique and complementary insight into the microstructural evolution of metals at high temperature, during thermo- mechanical processing or under high pressure. Neutrons illuminate a larger bulk volume and reveal quantitative phase abundance, bulk texture, lattice parameter changes and other ensemble averaged quantities. They are particularly sensitive to characterize atomic order and disorder in titanium aluminides. Extinction effects can be investigate to reveal the defect kinetics of a metal at high temperature. In contrast, fine- bundled synchrotron high-energy X-rays deliver reflections from a number of individual grains. For each constituting phase, their statistics and behavior in time reveal information about grain growth or refinement, subgrain formation, static and dynamic recovery and recrystallization, slip systems, twinning, etc. Grain orientation correlation can be revealed and lattice strain gives complementary insight to the transformation and reaction processes. This presentation reviews pioneering experiments on metals in reciprocal space, which nowadays serve the wider community.

## Spectroscopic Studies of Glycine/Alumina Surfaces

A.P.J. Stampfl<sup>a</sup> and J. E.M. Pereira<sup>a</sup>

<sup>a</sup> *Australian Centre for Neutron Scattering, Australian Nuclear Science and Technology Organisation, NSW 2234, Australia*

The basic field of surface adsorption and complexation of amino-acids on various oxide surfaces is an interesting area of investigation that has direct relevance in such diverse fields as chemistry (geochemistry, biochemistry), biotechnology (medical implants, biosensors, tissue engineering, bioelectronics, biomimetics and artificial photosynthesis), radiation technology (radiation damage and detection), colloid chemistry, surface chemistry and physics

The combination of both photoemission and neutron spectroscopy is quite rare and yet extremely powerful as these techniques directly yield the electronic and vibrational structure of a material respectively: two of the most basic properties of materials. Photoemission spectroscopy is clearly surface sensitive and hence is an ideal probe to study surface chemistry. While neutron spectroscopy is the domain of vibrational spectroscopy on bulk materials. There are exceptions to this rule where the surface dominates the scattered signal due to huge surface to volume ratios and large scattering cross-sections from adsorbate molecules. This study aim to exploit such ideas.

The deposition of glycine onto alumina from solution is investigated by both inelastic neutron spectroscopy and high resolution photoemission. Studies focused on the extent of adsorption at various pH's, the character of each adsorbate (zwitterionic, basic, acidic), and the number of discrete surface sites of adsorption. Results show strong chemisorption of glycine through an ester type bond with the alumina surface across a range of pH. Direct sorption of the amine group with alumina is observed only at pH 9. Formation of multilayers and/or peptides is postulated to also occur which may have implications in the area of prebiotic chemistry.

## Pressure-induced valence transitions: squeezing electrons from big orbitals to smaller ones

C.D. Ling<sup>a</sup>, M. Avdeev<sup>b</sup> and B.J. Kennedy<sup>a</sup>

<sup>a</sup> School of Chemistry, The University of Sydney, Sydney 2006, Australia.

<sup>b</sup> Australian Centre for Neutron Scattering, ANSTO, Menai 2232, Australia.

While bonds in solid-state compounds always have some degree of covalent character, the ionic approximation is usually sufficient to understand their “crystal chemistry” using concepts like the effective ionic radius (IR). IR predicts that an atom will shrink as its oxidation state increases. This occurs gradually as electrons are removed within a shell (e.g.,  $\text{IR}(\text{Ir}^{3+}) = 0.68$ ,  $\text{IR}(\text{Ir}^{4+}) = 0.625$ ,  $\text{IR}(\text{Ir}^{5+}) = 0.57$  Å in 6-fold coordination), but removing the last electron of a shell produces a much more pronounced change (e.g.,  $\text{IR}(\text{Bi}^{3+}) = 1.03$ ,  $\text{IR}(\text{Bi}^{5+}) = 0.76$  Å). For a compound with a suitable combination of cations, it should therefore be possible to effect a net reduction in volume by transferring an electron from one to the other. Temperature and/or pressure could drive such a valence state transition; but in practice, this is extremely rare, with only three cases reported until recently. We tested this idea systematically in a series of high-pressure X-ray and neutron diffraction and spectroscopy experiments on six candidate materials containing  $\text{Bi}^{3+}$  with 4d or 5d metal cations. We observed a valence state transition in every case, suggesting that they are far more common than previously thought. This talk will present both published [1,2] and unpublished experimental results, as well as *ab initio* calculations that shed light on the finely balanced electronic states of these compounds. The potential for tuning these transitions closer to ambient pressures, and of inverting the effect to give a volume change with an electronic stimulus, will be discussed.

- [1] W. Müller, M. Avdeev, Q. Zhou, B.J. Kennedy, N. Sharma, R. Kutteh, G.J. Kearley, S. Schmid, K.S. Knight, P.E.R. Blanchard, C.D. Ling, *Journal of the American Chemical Society* **134**, 3265-3270 (2012).
- [2] Z. Huang, J.E. Auckett, P.E.R. Blanchard, B.J. Kennedy, W. Müller, Q. Zhou, M. Avdeev, M.R. Johnson, M. Zbiri, G. Garbarino, W.G. Marshall, Q. Gu, C.D. Ling, *Angewandte Chemie – International Edition* **53**, 3414-3417 (2014).

## Hydrogen bond dynamics, conformational flexibility and polymorphism in antipsychotics

José E.M. Pereira<sup>a</sup>, Juergen Eckert<sup>b</sup>, Dehong Yu<sup>c</sup>, Richard Mole<sup>c</sup> and Heloisa N. Bordallo<sup>a,d</sup>

<sup>a</sup> *Niels Bohr Institute, University of Copenhagen, DK-2100, Copenhagen, Denmark.*

<sup>b</sup> *Department of Chemistry, University of South Florida, Florida 33620, United States.*

<sup>c</sup> *Australian Nuclear Science and Technology Organisation, Lucas Heights, 2233 NSW.*

<sup>d</sup> *European Spallation Source ESS AB, PO Box 176, SE-22100 Lund, Sweden.*

This work is related to the investigation of three different antipsychotics, one of each generation: aripiprazole ( $C_{23}H_{27}Cl_2N_3O_2$ ), haloperidol ( $C_{21}H_{23}ClFNO_2$ ) and quetiapine hemifumarate ( $C_{23}H_{27}N_3O_4S$ ) using a combination of Inelastic Neutron Scattering (INS) and Density Functional Theory (DFT). These substances were selected because their crystalline structure and the concerns related to their polymorphism are somehow known [1]. We report on data obtained using the direct geometry spectrometer PELICAN, located at the Australian Centre for Neutron Scattering (ACNS, formerly the Bragg Institute) at the Australian Nuclear Research and Technology Organisation (ANSTO). Polymorphic transformations and purity of the samples were determined by calorimetric studies, while their structures were verified by X-rays diffraction. Furthermore, the origin of each of the observed modes is supported by theoretical data provided by Density Functional Theory calculations (DFT).

- [1] G.L. Destri et al, *J. Pharmaceutical Sciences* 2011, 100, 4896; K. Ravikumar and B. Sridhar, *Acta Cryst.* 2005, E61, o3245 & JB Nanubolu et al, *CrystEngComm.*, 2012, 14, 4677.



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<b>Tuesday 31/01/2017</b>	<b>Wednesday 1/02/2017</b>	<b>Thursday 2/02/2017</b>	<b>Friday 3/02/2017</b>
	Breakfast 7:30 - 8:30	Breakfast 7:30 - 8:30	Breakfast 7:30 - 8:30
	Conference Opening 8:40 - 8:50		
	WM1 - WM4 8:50 - 10:30	TM1 - TM4 8:50 - 10:30	FM1 - FM4 8:50 - 10:30
	Morning Tea 10:30 - 11:00	Morning Tea 10:30 - 11:00	Morning Tea 10:30 - 11:00
	WN1 - WN4 11:00 - 12:30	TN1 - TN4 11:00 - 12:30	FN1 - FN4 11:00 - 12:20
	Lunch 12:30 - 14:00	Lunch 12:30 - 14:00	Lunch 12:40 - 14:00
Registration Desk OPEN 14:00 -	WA1 - WA5 14:00 - 15:40	TA1 - TA4 14:00 - 15:30	
	Poster Slam (WP) 15:40 - 16:00	Poster Slam (TP) 15:30 - 16:00	
	Wednesday Poster Session (WP) incl. afternoon tea and conference bar 16:00 - 18:00	Thursday Poster Session (TP) incl. afternoon tea and conference bar 16:00 - 18:00	
Welcome Reception 16:00 - 18:00			
Dinner 18:00 - 19:30		Dinner 18:00 - 19:30	
Wine Tasting & Reception Drinks 19:30 - 21:30	Conference Dinner incl. After Dinner Talk 18:30 - 22:00	Trivia Night (Lindsay Davis Cup) 19:30 - 22:00	
			Awards & Closing

