PRIFYSGOL ABERYSTWYTH UNIVERSITY

PRIFYSGOL BANGOR UNIVERSITY

Centre for Advanced Functional Materials and Devices

Annual Report

2008

Centre for Advanced Functional Materials and Devices

www.cafmad.ac.uk

Annual Report

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Executive summary

Welcome to the second report for the Centre for Advanced Functional Materials and Devices (CAFMaD) that reports the Centre's activity during 2008.

The £2.9M Centre for Advanced Functional Materials and Devices (CAFMaD) is part of the Aberystwyth University and Bangor University Research & Enterprise Partnership. The Partnership was awarded HEFCW funding of £10.9M from 2007 to 2011 to provide research and entrepreneurship support across the Universities and to create four internationally recognised research Centres, of which CAFMaD is one.

CAFMaD brings together leading academics from the Institute of Mathematics and Physics (IMAPS) and the Welsh Visualisation Centre at Aberystwyth University, and the College of Physical and Applied Sciences at Bangor University, which includes the School of Chemistry, the School of Electronic Engineering and the School of Computer Science.

CAFMaD's strengths are in materials, sensors, mathematics, space physics, synthesis and catalysis, molecular modelling, visualisation, image recognition, characterisation, photovoltaics, biological chemistry, optoelectronics and high performance computing. Aberystwyth leads in glasses and ceramics, semiconductor surfaces and interfaces, advanced characterisation techniques and stereo reconstruction and modelling of solids and surfaces. Bangor leads developments in optoelectronics and solar cell technology, materials synthesis and catalysis, polymer processing, polymer electronics, micro-nano-fabrication and molecular modelling.

CAFMaD's Vision is to be an international centre of excellence for the development, characterisation and application of advanced materials and devices, and CAFMaD's Mission is to be an international centre of research excellence, which is based on pure science and capable of delivering sustainable economic growth in Wales, the UK and beyond.

CAFMaD is managed by an executive group consisting of the Co-Directors, Professor Neville Greaves and Professor Geoff Ashwell, and is Chaired by Gary Reed, the Head of the Partnership Office. This group meets every other month, and a management group consisting of all CAFMaD members meets every six months. The External Advisory Board

(EAB) was drawn from leading Physics, Chemistry and Engineering Institutes across the UK, with representation from the Welsh Assembly Government and industry. The EAB is Chaired by Professor Mike Scott from IQE Plc.

This Annual Report presents the activities of the research streams, the publications and conference attendance by CAFMaD members, and research grants awards.

	2008	2007
Publications	38	54
Conferences/Seminars	49	40
Workshops	2 (+2)	4

Grant Capture	Total to end of 2008	Total to end of 2007
Total Awards core CAFMaD	£4,475,000	£2,272,000
Joint AU and BU	£443,000	£77,000
CAFMaD Members	£1,850,211	£793,000

During 2008, CAFMaD has continued on its early successes, with positive and encouraging reports from the External Advisory Board and the Research and Enterprise Partnership Board. It is progressing well with funding in the core CAFMaD areas, and some of the highlights have included:

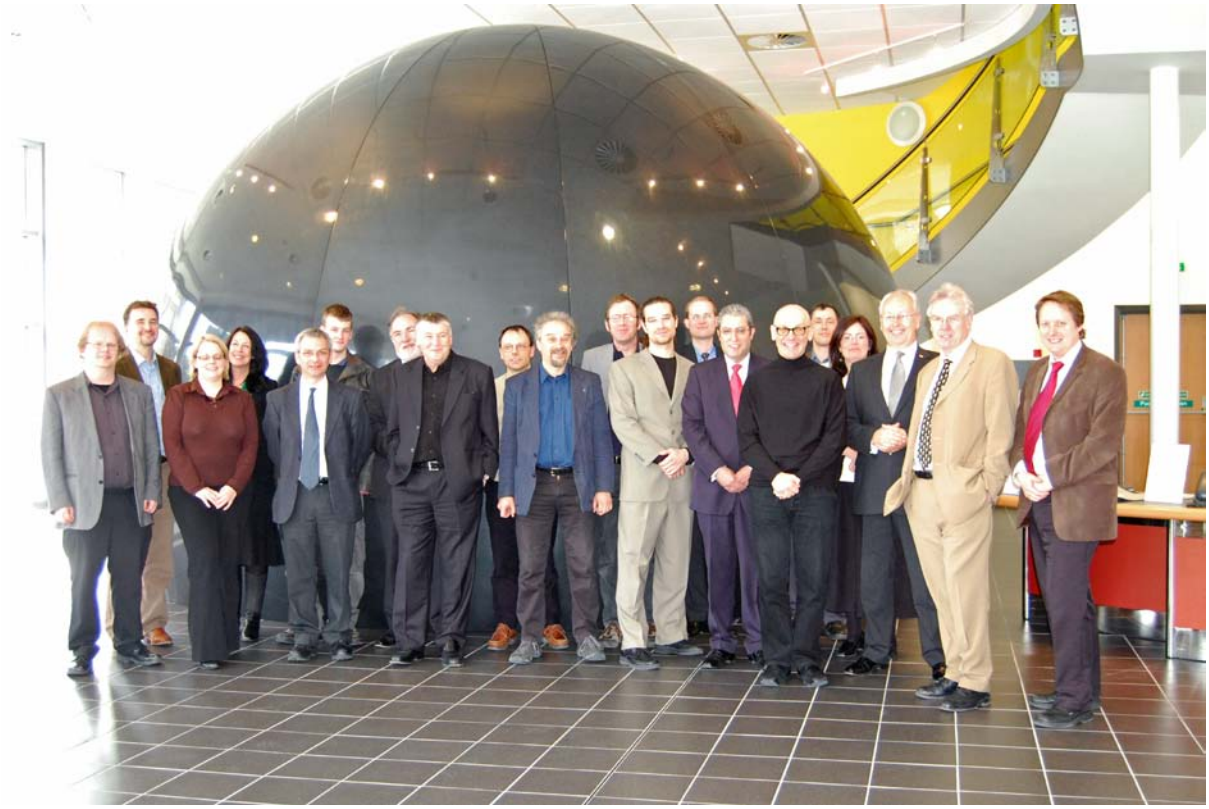
- World Class Science evidenced, for example:
    - Research led by Professor Neville Greaves with six CAFMaD, and five international colleagues on Detection of First Order Liquid-Liquid Phase Transitions in Yttrium Oxide – Aluminium Oxide Melts, which was published in Science, a Journal with an impact factor of 30, and it was reviewed in Nature Materials by Paul McMillan, which has an international impact factor of 20.
    - A breakthrough in molecular rectification with a 1000 fold increase in the single molecule rectification ratio by Professor Geoff Ashwell and his team.
    - First characterisation of the conductance of a single molecule contacted by silicon electrodes by Professor Geoff Ashwell and his team.
- Grant income across all research streams since the conception of the project in 2006 of £4.5M, an additional £2.3M from the 2006-7 report.
- A successful joint CAFMaD seminar series, both academic, and in conjunction with industry
- Participation in the Optoelectronics Industry Development Association (OIDA) conferences in the USA.
- High level of Joint Central Facilities access at Diamond Light Source, ISIS (Rutherford Appleton Laboratory) and ILL, Genoble.
- A range of international research collaboration and strong links developed with the

National University of Singapore and Nanyang Technical University in Singapore, which has led to the Development of the British Council International Network of Young Scientists initiative and conference in Singapore in July 2009.

- Progression on two Commercialisation projects: the Charge Detector Array and the Ellipsometer, the latter was awarded £50,000 PPOC money.
- New links were forged with the EPSRC funded Innovative Electronics Manufacturing Centre, based at Loughborough University.

It is a pleasure to report successful midterm progress for CAFMaD.

Gary Reed
Chair of CAFMaD Executive Committee
Partnership Development Manager and Head of the Partnership Office



CAFMaD

Research Groups

2008

Organic Conductors and Molecular Electronics

Team Leaders: Professor Martin Taylor; Professor Andy Evans

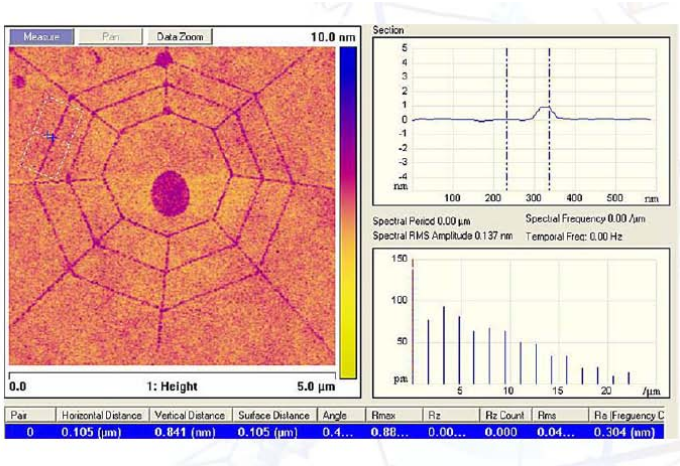
Members: Professor Geoff Ashwell; Professor Paul Spencer; Dr Justin Lawrence; Dr Dave Langstaff; Dr Nigel Poolton

Areas of Focus:

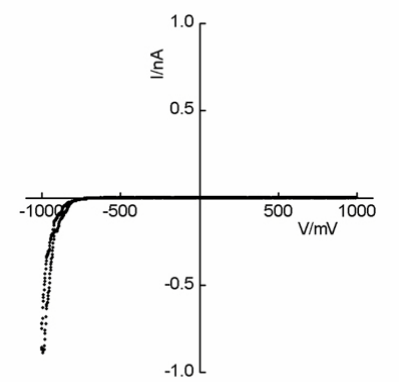
- Polymer Electronics
- Organic Lasers
- Contact Formation
- Nanolithography
- Molecular wire and diodes

The intense organic electronics research activity of the last decade is beginning to come to fruition with new products entering the marketplace, with more in the pipeline. The key materials in this research field, small organic molecules and polymers, are electrically and optically active leading to a range of applications in displays, circuits and tunable lasers. Despite this success, significant effort is still required to optimise the devices in these products.

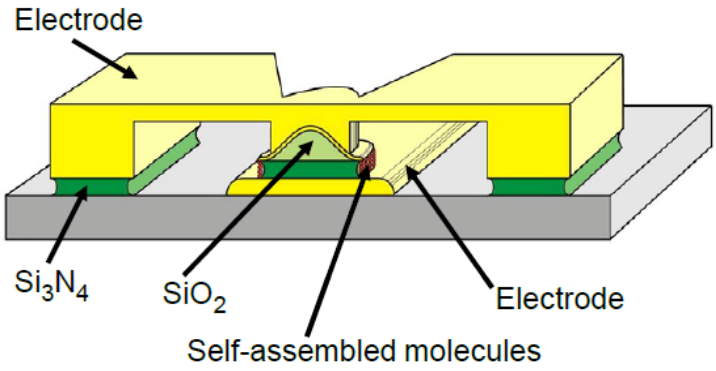
Research in this CAFMaD stream is directed towards understanding the nature of interfaces e.g. insulator-semiconductor and contact-semiconductor interfaces, which are a source of device instability and degradation in organic MISFETs and OLEDs. Significant effort is also being devoted to next generation devices where nanolithography and self-assembly techniques are being exploited to fabricate and characterise single molecule rectifiers.



50 nm wide x 1 nm high lines of molecules "written" onto a gold surface



I-V characteristics of molecular diode



Electrode device for measuring I- V characteristics

Extreme Materials

Team Leaders: Professor Neville Greaves; Dr Peter Holliman

Members: Professor Andy Evans; Dr Florian Kargl; Dr Rudi Winter; Dr Martin Wilding; Dr Edwin Flikkema; Dr Mike Beckett; Professor Stuart Irvine

Areas of Focus:

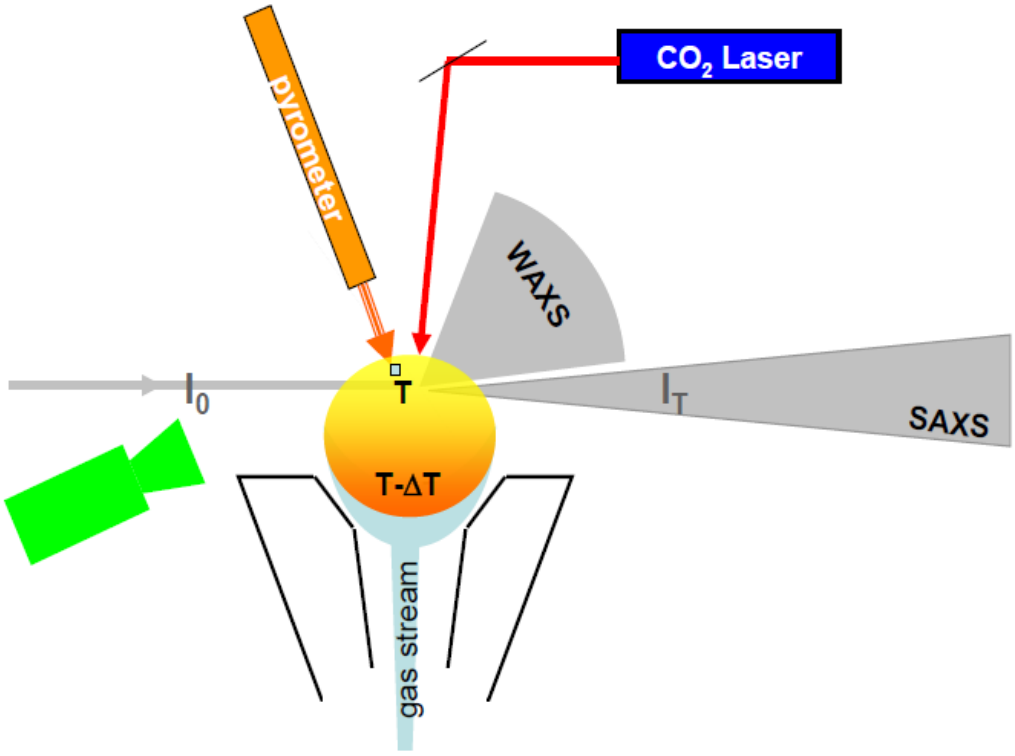
- Fast ion diffusion
- Glasses at HT and HP
- Melting and amorphisation
- Nanoceramics and sintering
- Radiation-hard semiconductors

The researchers in this stream study inorganic materials, which are interesting from a fundamental point of view as well as for applications under extreme conditions such as ultra-high temperatures, high pressure, and in hostile chemical environments.

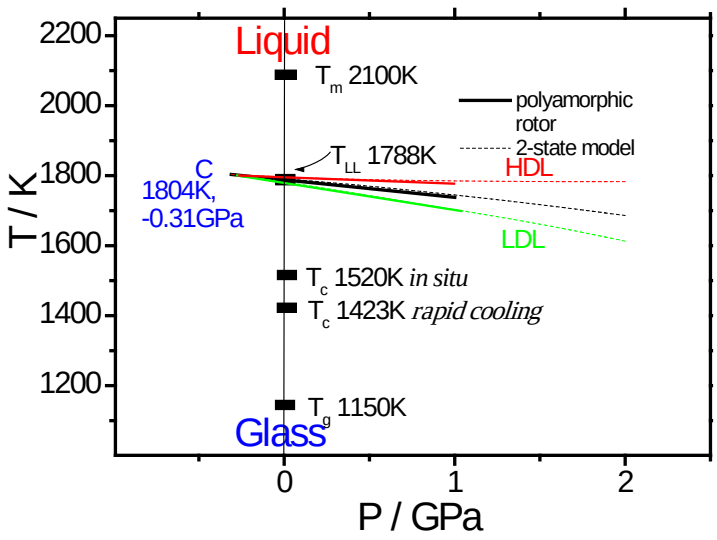
A primary aim of this stream's research is to understand how melting and freezing impacts on the structure and properties of materials. Container-less processing employing levitation laser-heating techniques prevents heterogeneous nucleation which is beneficial in extending the range of ceramics and glasses that can be fabricated. These include perfect or low entropy glasses that are likely to have mechanical and chemical properties superior to glasses made conventionally.

Applying high pressure and high temperature simultaneously allows materials to be studied under deep Earth conditions as well as the severe changes encountered in volcanic eruptions.

The same principles involved in fabricating under extreme conditions are being used to improve and tailor the properties of nano-structured materials so that they can sustain extreme thermal, chemical, and mechanical environments. This is being enabled through novel in situ characterisation methods capable of identifying new routes of synthesis. Likewise research on the atomic and electronic structure of coatings and surfaces of oxides, nitrides and carbides aims to generate the outstanding macroscopic properties needed for robust radiation-hard photovoltaic devices.



Aberystwyth aerodynamic levitator furnace configured for synchrotron radiation SAXS/WAXS experiments.



Measured phase diagram for liquid-liquid transitions in yttria-alumina melts.

Sensors and Devices

Team Leaders: Professor Maher Kalaji; Dr Dave Langstaff

Members: Dr Dave Barnes; Dr Tony Cook; Professor Andy Evans; Dr Peter Holliman; Dr Stuart Irvine

Focus Areas:

- Electrochemical sensors for explosives and drugs detection
- Semiconductor solar cells
- Charge detectors for electrons and ions
- Smart end-station for combined electron and light spectroscopies
- Space robotics for planetary exploration

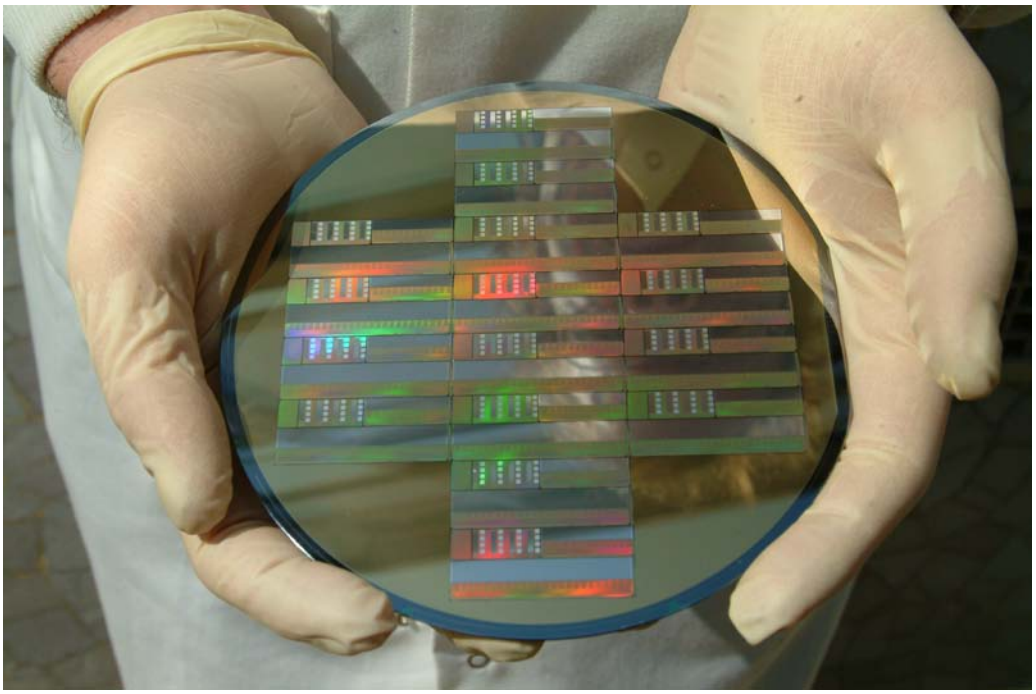
From a sensitive electronic nose to sniff out drugs and explosives to solar cells that can be printed onto buildings, researchers in this stream are working with novel materials and devices that have the power to transform the way we live.

Sensors have been developed to detect a range of pollutants such as heavy metals and carbon monoxide. This analytical skill is coupled with a strong research base in environmental rehabilitation, such as the development of new clays and gel materials for allowing plant growth in slag heaps.

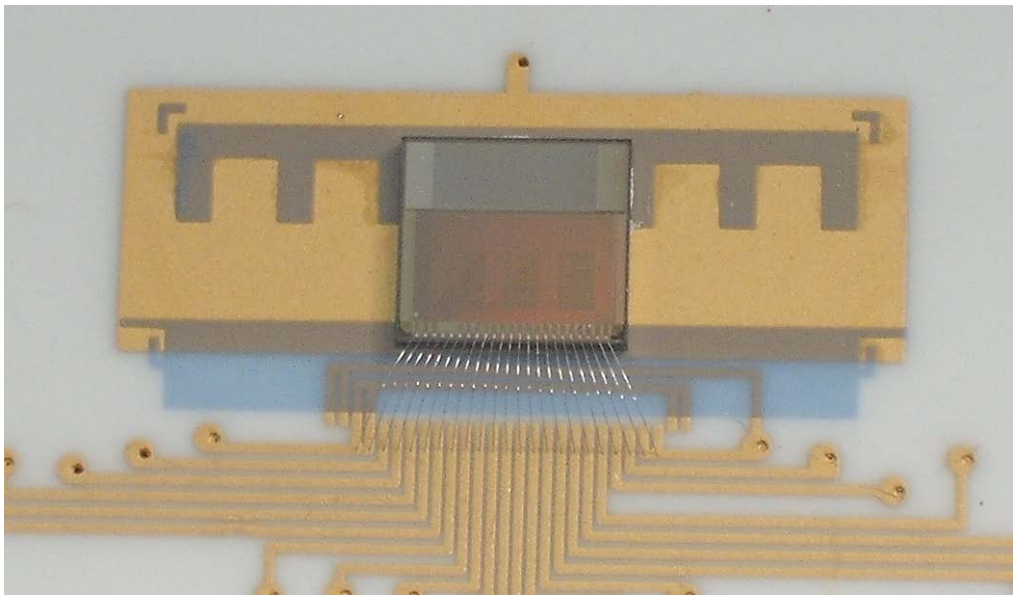
A novel charge counting detector has been developed which enables changes occurring at the surfaces of materials to be studied in-situ for the first time. This has been applied to the study of how contacts may be formed between organic materials and metal wires used to connect devices to form electronic systems.

The collaboration between researchers in chemistry, electronics and physics brings together expertise in designing and producing, characterising and applying these new devices and opening up new areas of science.

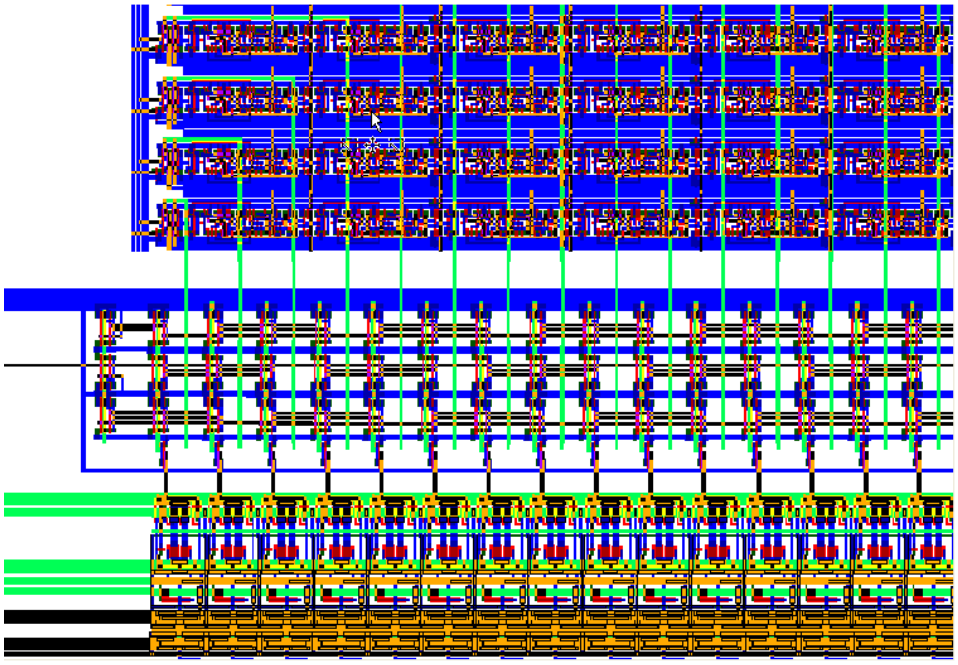
Expertise in robotics is being applied to instrumentation for areas as diverse as space exploration and earth bound x-ray science.



A silicon wafer containing the latest generation of electron detector array devices, recently fabricated from designs produced by Aberystwyth University.



An electron detector with the prototype on-chip image enhancement circuitry mounted on a ceramic substrate ready for testing.



Layout for a portion of the electron detector chip with circuitry to eliminate multiple triggering of adjacent pixels.

Characterisation and Modelling

Team Leaders: Professor Andy Evans; Dr Greg Chass

Members: Dr Simon Cox; Dr Edwin Flikkema; Professor Neville Greaves; Mr Matt Gunn; Dr Tudor Jenkins; Dr Florian Kargl; Dr Dave Langstaff; Dr Nigel Poolton; Dr Rudi Winter; Dr Martin Wilding; Dr Peter Holliman; Dr Keith Hughes; Dr Lorrie Murphy; Professor Ron Pethig; Mr Denis Williams.

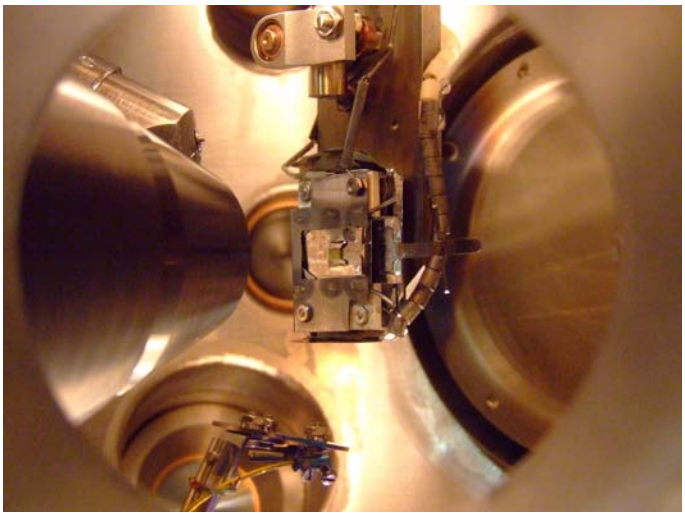
Focus Areas:

- Real time photoemission
- Optical luminescence
- Elastic and inelastic X-ray and neutron scattering
- X-ray and optical imaging
- Scanned probe microscopy
- Computer simulation and visualisation

A broad swathe of characterisation, measurement and modelling facilities are available through researchers in CAFMaD:

- The standard chemistry techniques of mass spectroscopy, chromatography, X-ray diffraction and Nuclear Magnetic Resonance are complemented with a wide range of optical techniques covering wavelengths from the Infra-red to the Ultra-violet.
- Thin film and device characterisation is catered for using spectroscopy (Raman spectroscopy, ellipsometry, luminescence, photoelectron spectroscopy), microscopy (optical, scanned probe and electron microscopy) and electrical measurements (IV/CV, impedance).
- Nanostructures fabricated in the CAFMaD laboratories are characterised by optical, electron and x-ray methods and by scanned probe techniques (scanning tunnelling microscopy, atomic force microscopy and related techniques (STS, EFM, SCM, I-AFM).

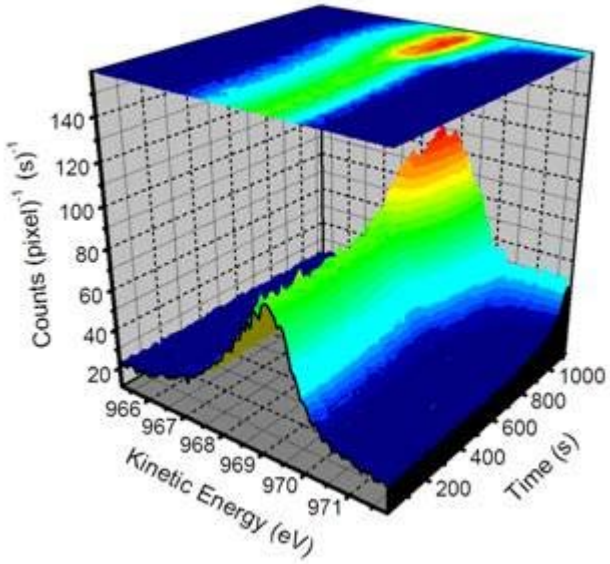
Many of these facilities have been enhanced and extended by researchers within CAFMaD to offer unique measurement techniques, in particular the in-situ study of processes as they occur.



Ultrahigh vacuum thin film deposition chamber for multi-technique processing and characterisation by in-situ UV, x-ray, optical and electron techniques.

In addition to the in-house facilities, researchers in CAFMaD have considerable expertise in the use of large scale national facilities for the study of materials using such techniques as x-ray and neutron scattering and advanced x-ray techniques.

The measurement and characterisation instrumentation is complemented by extensive computational and modelling facilities. Immersive 3D visualisation permits researchers to combine their knowledge and expertise with experimental results to derive accurate models of the integrated processes taking place within complex materials.



Correlating changes in carbon chemistry and device performance by real-time spectroscopy during high temperature (1000°C) annealing of a diamond-metal contact.

CAFMaD

Publications

2008

CAFMaD Publications 2008

ID	Paper title	CAFMaD Author 1	Other Authors	Journal	Volume	Date	Page Number
27	Characterization and conductivity of Langmuir-Blodgett films prepared from an amine-substituted oligo(phenylene ethynylene)	G.J. Ashwell	A. Villares, D.P Lydon, P.J. Low B.J. Robinson, F.M. Royo, and P. Cea	Chem. Mater.	20	2008	258-264
82	Charge Storage in Pentacene/Polymethylmethacrylate Memory Devices	M. F. Mabrook	Y. Yun, C. Pearson, D. A. Zeze, M.C. Petty	IEEE Electron Device Letters		in press	
85	Fabrication and characterisation of MIS organic memory devices	M. F. Mabrook	D. Kolb, C. Pearson, D. A. Zeze, and M. C. Petty	Adv. Sci. Tech	54	2008	474-479
86	Memory effects in hybrid silicon-metallic nanoparticle-organic thin film structures	M. F. Mabrook	C Pearson, D Kolb, D A Zeze, and M C Petty	Organic Electronics	9, No. 5	2008	816-820
84	Memory effects in MIS structures based on silicon and polymethylmethacrylate with nanoparticle charge-storage elements	M. F. Mabrook	A. S. Jombert, D. Kolb, D. A. Zeze, and M. C. Petty	Matt. Sci. Eng. B.		in press	
24	Response of the transmission spectrum of tapered optical fibres to the deposition of a nanostructured coating.	G.J. Ashwell	R. Jarzebinska, C.S. Cheung, S.W. James, R.P. Tatam	Proc. Soc. Photo-Optical Instr. Eng. (SPIE)	7004	2008	L45
38	Switching in polymeric resistance random-access memories (RRAMs)	D. M. Taylor	H. L. Gomes, A. R. V. Benvenho, D. M. de Leeuw, M. Cölle, P. Stallinga, F. Verbakel	Organic Electronics	9	2008	119-128
25	Synthesis and properties of functionalized 4 nm scale molecular wires with thiolated termini for self-assembly onto metal surfaces	G.J. Ashwell	C.S. Wang, M.R. Bryce, J. Gigon, I. Grace and C.J. Lambert	J. Org. Chem.	73	2008	4810-4818
56	A quantitative scale for the extent of conjugation of carbonyl groups. Carbonylicity percentage as a chemical driving force 9153-9165	Gregory A. Chass	Zoltán Mucsi, Imre G. Csizmadia	JPCA	112 (38)	2008	

ID	Paper title	CAFMaD Author 1	Other Authors	Journal	Volume	Date	Page Number
52	Amidity change as a significant driving force and thermodynamic selection rule. A synergy between experiment and theory in the study of transamidation reactions	Gregory A. Chass	Zoltan Mucsi, Imre G. Csizmadia	JPCB	112(26)	2008	7885-7893
18	An in situ amperometric biosensor for the detection of vapours from explosive compounds	M. Kalaji	Gwenin, CD; Kay, CM; Williams, PA; Tito, DN	ANALYST	133 (5)	2008	621-625
79	Azine Bridge Formation During the Electrografting of Acrylonitrile	D.M. Taylor	P.A. Easter	J. Polymer Sci A		in press	
54	Conversion of Combustible Municipal Solid Waste to Methanol	Gregory A. Chass	Imre G. Csizmadia	Int. J. Env. Stud.	65(5)	2008	655-665
5	Detection of First Order Liquid-Liquid Phase Transitions in Yttrium Oxide – Aluminium Oxide Melts	G.N. Greaves	M.C. Wilding; D. Langstaff; S. Fearn, F. Kargl, S. Cox, O. Majérus, Q. Vu Van, C.J. Benmore, R. Weber, C.M. Martin, L. Hennet	Science	322	2008	566-570
71	Determination of the optical band-gap energy in cubic and hexagonal boron nitride using luminescence excitation spectroscopy	D.A. Evans	R. Winter; N.R.J. Poolton; A.G. McGlynn; D. Jones; T.E. Jenkins; M. Gunn; B.M. Towlson	J Phys: Condensed Matter	20	2008	075233
40	Determining the interfacial density of states in metal-insulator-semiconductor devices based on poly(3-hexylthiophene	D. M. Taylor	N. Alves	Appl. Phys.	92	2008	10331
87	Electrical behaviour of memory devices based on fluoren-containing organic thin films	M. F. Mabrook	P Dimitrakis, P Normand, D Tsoukalas, C Pearson, J H Ahn, D A Zeze, M C Petty, K T Kamtekar, C Wang, M R Bryce and M Green	J. Appl. Phys		in press	
45	Electroluminescent colloidal inks for flexographic roll-to-roll printing	J. R. Lawrence	Huebner CF, Carroll JB, Evanoff DD, Ying Y, Stevenson BJ, Houchins JM, Foguth AL, Sperry J, and Foulger SH	Journal of Materials Chemistry	18	2008	594
65	Electronic and optical properties of magnesium phthalocyanine (MgPc) solid films studied by soft x-ray excited optical luminescence and x-ray absorption spectroscopies	N R J Poolton	N. Peltekis, B. Holland, S. Krishnamurthy, I. T. McGovern, S. Patel (STFC Daresbury Laboratory) and C.McGuinness (Trinity College, Dublin) S. Patel (STFC Daresbury Laboratory)	Journal of the American Chemical Society	130	2008	13008-13012

ID	Paper title	CAFMaD Author 1	Other Authors	Journal	Volume	Date	Page Number
68	Feasibility of in situ neutron diffraction studies of non-crystalline silicates up to pressures of 25 Gpa	M Wilding	Guthrie, M, Bull, C. L., Tucker, M. G. And McMillan, P. F.	Journal of Physics, Condensed Matter	20(24)	2008	244122
17	FTIR spectroscopic investigation of pyruvate electroreduction on copper in alkaline medium - On the mechanistic aspects	M. Kalaji	Martin, C ; Hahn, F ; Servat, K; Huser, H; Tito, D; Kokoh, KB	CANADIAN JOURNAL OF CHEMISTRY - REVUE CANADIENNE DE CHIMIE	86 (10)	OCT 2008	992-995
26	Functional Molecular Wires	G.J. Ashwell	P. Wierzchowiec, Piotr, L.J. Phillips, C.J. Collins, J. Gigon, B.J. Robinson, C.M. Finch, I.R. Grace, C.J. Lambert, P.D. Buckle, K. Ford, B.J. Wood, I.R. Gentle	Phys. Chem. Chem. Phys.	14	2008	1859-1866
92	High pressure effects on liquid viscosity and glass transition behaviour, polyamorphic phase transitions and structural properties of glasses and liquids	M Wilding	McMillan, P. F.	Journal of non-crystalline solids		in press	
53	High-level ab initio exploration on the conversion of carbon dioxide into oxazolidinones: The mechanism, and regioselectivity 6708-6714	Gregory A. Chass	Wei-Hua Mu, De-Cai Fang	JPCA	112(29)	2008	
69	In situ diffraction studies of magnesium silicate liquids	M Wilding	Benmore, C. J. and Weber, J. K. R	Journal of Materials Science	43	Published online: 30 April 2008	4707-4713
23	Langmuir-Blodgett films incorporating molecular wire candidates of ester-substituted oligo(phenylene-ethynylene) derivatives	G.J. Ashwell	A. Villares, D.P Lydon, B.J. Robinson, F.M. Royo, P.J. Low and P. Cea,	Surface Science	602	2008	3683-3687
4	Liquids, Glasses, Density Fluctuations and Low Frequency Modes	G.N. Greaves	M.C. Wilding; F. Kargl; L. Hennet and O. Majérus	Advanced Materials Research	39-40	2008	3-12
1	Melting and Amorphisation	G.N. Greaves		J. Mater. Chem.	18	2008	166-180
74	Na-relaxation and intermediate range structure in sodium-potassium silicate melts	F.Kargl	A. Meyer	Chemical Geology	256	2008	278-285

ID	Paper title	CAFMaD Author 1	Other Authors	Journal	Volume	Date	Page Number
75	Neutron Applications in Earth, Energy, and Environmental Sciences	F.Kargl	A. Meyer, J. Horbach, Liang L, Rinaldi R, Schober H (Eds.)	Springer, Heidelber		2008	
19	Nickel dithiolenes containing pendant thiophene units: precursors to dithiolene-polythiophene hybrid materials	M. Kalaji	Robertson, N; Mount, AR; Coles, SJ; Hursthouse, MB; Anjos, T; Roberts-Bleming, SJ Charlton, A; Murphy, PJ	JOURNAL OF MATERIALS CHEMISTRY	18 (4)	2008	475-483
66	Optically detected X-ray absorption spectroscopy (ODXAS) measurements as a means to monitor corrosion layers on copper	N R J Poolton	M. G. Dowsett, G.K.C. Jones (Warwick University) A. Adriaens (Ghent University, Belgium) S. Fiddy (STFC, Daresbury) S. Nikitenko (ESRF, France)	Analytical Chemistry	80	2008	8717-8724
55	Pd-NHC (PEPPSI) Complexes: Synthetic Utility and Computational Studies into their Reactivity	Gregory A. Chass	Michael G. Organ, De-Cai Fang, Alan C. Hopkinson, Cory Valente	Synthesis	17	2008	2776-2797
39	Separating interface state response from parasitic effects in conductance measurements on organic metal-insulator-semiconductor capacitors	D. M. Taylor	N.Alves	J. Appl. Phys	103	2008	054509
73	Solvent and lipid dynamics of hydrated lipid bilayers by incoherent quasielastic neutron scattering	F.Kargl	J. Swenson, P Berntsen, C. Svanberg	Journal of Chemical Physics	129	2008	045101
78	Structural, Optical and Electrical Properties of Co-evaporated CuCl/KCl films	D.M. Taylor	F. O. Lucas, P.J. McNally, A. Cowley, S. Daniels, L. Bradley, D. Danieluk	Phys. Stat. Solid-C		in press	
51	Test and modification of the van der waals radii employed in the default PCM model	Gregory A. Chass	Wei-Hua Mu, De-Cai Fang	Int. J. Quant. Chem.	108(9)	2008	1422-1434
6	Two million hours of science	G.N. Greaves	C.R.A. Catlow; G.E. Derbyshire, M.I. McMahon, R.J. Nelmes and G. Van der Laan	Nature Materials	7	2008	827-830

CAFMaD

Conference Participation

2008

CAFMaD Conferences 2008

ID	Title	CAFMaD Author	Conference	Location	Date	Capacity	Other Authors
27	Detecting sp2-bonded carbon in natural and synthetic diamond using Optically-Detected X-ray Absorption Spectroscopy Imaging X-ray Absorbtion and Optical Luminescence Studies of Diamond	Andrew Evans	59th Diamond Conference	Oxford	July 2008	Talk	
22	Organic semiconductor interfaces	Andrew Evans	CLEO/PHAST Conference	San Jose, USA	May 2008	Invited talk	
30	Measurement of energy band alignment and thin film morphology in an organic photovoltaic cell structure using photoelectron spectroscopy	Andrew Evans	Excitonic Solar Cell Conference	Warwick	September 2008	Talk	
24	Growth and morphology of SnPc films on GaAs(001) surfaces and their role as organic modifiers of diode performance	Andrew Evans	ICSFS-14 Conference	Dublin, Ireland	July 2008	Talk	
25	Energy band alignment and thin film morphology in an organic photovoltaic cell structure	Andrew Evans	ICSFS-14 Conference	Dublin, Ireland	July 2008	Poster	
26	Diamond-metal contact formation monitored by real-time electron spectroscopy	Andrew Evans	ICSFS-14 Conference	Dublin, Ireland	July 2008	Poster	
21	Optically-detected X-ray Absorption Spectroscopy and X-ray Excited Optical Luminescence studies of diamond and boron nitride.	Andrew Evans	SBDD XVIII	Hasselt, Belgium	February 2008	Poster	
28	Imaging X-ray Absorbtion and Optical Luminescence Studies of Diamond	Andrew Evans	SR Users Meeting	Daresbury	September 2008	Poster	
29	Real-time Spectroscopy at MPW6.1: Application to the Fabrication of Organic Devices	Andrew Evans	SR Users Meeting	Daresbury	September 2008	Poster	
23	Science Issues in OLED fabrication: materials and interfaces	Andrew Evans	UK Displays and Lighting KTN Workshop		June 2008	Invited talk	

ID	Title	CAFMaD Author	Conference	Location	Date	Capacity	Other Authors
32	Historical observations of effects that might be associated with impacts on the Moon	Anthony Charles Cook	4th Europlanet Meteor Workshop	Cologne, Germany	26-27 Sep 2008	Invited talk	
31	Observational Techniques for Detecting Lunar Impacts	Anthony Charles Cook	European Planetary Science Conference	Munster, Germany	26 Sep 2008	Invited talk	
33	Mapping Coverage Around a Lander Using passive Structured Ligh	Anthony Charles Cook	Lunar and Planetary Science Conference	League City, Houston, Texas	March 2008	Poster presentation	
20	Metal-diamond interface formation monitored by real-time photoelectron spectroscopy.	D. Andrew Evans	SBDD XVIII	Hasselt, Belgium	February 2008	Talk	
76	Admittance Measurements on Organic MIS Capacitors, TFTs and Heterojunction Solar Cells	D. Martin Taylor	Cambridge Display Technology	Cambridge	May 2008	invited talk	
72	Interface States – A Source of Threshold Voltage Instability in Organic Transistors	D. Martin Taylor	Cranfield Multistrand Conference.		May 2008	invited oral	
68	Determining the density of states for interface hole traps in MIS capacitors based on P3HT	D. Martin Taylor	Int. Conf. On Organic Electronics	Eindhoven	June 2008	Oral	N. Alves
69	Plastic memories: A small signal impedance study	D. Martin Taylor	Int. Conf. On Organic Electronics	Eindhoven	June 2008	Oral	H. L. Gomes, A. R. V.Benvenho, D. M. de Leeuw, M. Cölle, P. Stallinga and F. Verbakel
77	Determining the density of states for interface traps in MIS capacitors based on P3HT	D. Martin Taylor	Massachusetts Institute of Technology	Massachusetts	June 2008	invited talk	
71	Determining the Density of Interface States in MIS Devices Based on P3HT	D. Martin Taylor	Materials Research Society Fall Meeting	Boston	December 2008	Poster	
70	Small-signal electrical response of organic MIS devices	D. Martin Taylor	Proc 11th European Conference on Organised Films	Potsdam	July 2008	Oral	
73	Interface States - The Origin of Threshold Voltage Instability	D. Martin Taylor	UK Display and Lighting (UKDL) KTN	Pot Shrigley	February 2008	invited talk	

ID	Title	CAFMaD Author	Conference	Location	Date	Capacity	Other Authors
34		David Philip Langstaff	8th International Conference on Position Sensitive Detectors	Glasgow	1-5 September 2008	Conference Organisation	
36	Progress on the Aberystwyth Electron Counting Array	David Philip Langstaff	8th International Conference on Position Sensitive Detectors	Glasgow	1-5 May 2008	Oral Presentation	
37	Reduction of Multiple Triggering in Counting Detectors	David Philip Langstaff	8th International Conference on Position Sensitive Detectors	Glasgow	1-5 May 2008	Poster Presentation	
35	The Design, Operation and Application of an Electron Counting Detector for Photoemission Spectroscopy	David Philip Langstaff	workshop on Detectors as part of “2008 NSLS/CFN Users' Meeting”	Brookhaven National Laboratory, NY, USA	19-21 May 2008	Invited Presentation	
43	Linking structure and microscopic dynamics to understand macroscopic properties	Florian Kargl	British Council International Network of Young Scientists Scoping visit, talk to members of SSLS, NUS and NTU	Singapore	January 2008	Talk	
40		Florian Kargl	Co Organiser of the Satellite Meeting: “Materials at High Pressures and High Temperatures”, as part of the 2008 SR Users Meeting	Daresbury	11-12 September 2008	Conference Organisation	
44	Comparing experiment and theory to understand catalytic activity in solution	Florian Kargl	German Neutron Scattering Conference 2008	Physics Department, Technical University Munich, Garching, Germany	14-17 September 2008	Poster	G. Chass, C. J. O'Brian, D.-C. Fang, and M. G. Organ
41		Florian Kargl	ISIS Molecular Spectroscopy User Meeting	Cosener’s House, Abingdon	4-5 November 2008	Conference Organisation	
15	The detection of first order liquid-liquid Phase Transitions	G. Neville Greaves		Cavendish laboratory, Cambridge	24 October 2008	Invited Seminar	
16	Glasses, perfect glasses and zeolite amorphisation	G. Neville Greaves		Department of Materials Science, Cambridge	27 October 2008	Invited Seminar	
17	Liquid unmixing at white heat	G. Neville Greaves		Department of Chemistry, Cambridge	27 October 2008	Invited Seminar	
8	Vibrational spectra of NaY and NaA zeolites investigation using Fourier transform infrared synchrotron radiation	G. Neville Greaves	6th International Conference on Synchrotron Radiation in Materials Science	Campinas, Brazil	20-23 July 2008	Oral Presentation	M. Bahou

ID	Title	CAFMaD Author	Conference	Location	Date	Capacity	Other Authors
10	Inelastic X-ray Scattering Studies of Zeolite Amorphisation	G. Neville Greaves	6th International Conference on Synchrotron Radiation in Materials Science	Campinas, Brazil	20-23 July 2008	Oral Presentation	F. Kargl
11	Structure factor changes during the liquid-liquid phase transition in supercooled Y2Al8O16	G. Neville Greaves	6th International Conference on Synchrotron Radiation in Materials Science	Campinas, Brazil	20-23 July 2008	Poster presentation	M.C. Wilding
12	Characterising density fluctuations in liquid yttria aluminates with small angle x-ray scattering	G. Neville Greaves	6th International Conference on Synchrotron Radiation in Materials Science	Campinas, Brazil	20-23 July 2008	invited talk	Quang Vu Van
18		G. Neville Greaves	6th International Conference on Synchrotron Radiation in Materials Science	Campinas, Brazil	20-23 July 2008	Conference Organisation	
6	Liquids, Glasses, Density Fluctuations and Low Frequency Modes	G. Neville Greaves	ESG09	Trencin, Slovakia	22-25 June 2008	Plenary Lecture	
14	Low entropy glasses from zeolite amorphisation	G. Neville Greaves	Fragility of Viscous Liquids: Cause(s) and Consequences	International Workshop, Carlsberg Academy, Copenhagen, Denmark	8-10 October 2008	Invited talk	
13	Detecting the parameters that define first order liquid-liquid transitions	G. Neville Greaves	High Pressure High Temperature Symposium, UK Synchrotron Radiation Users Meeting	Daresbury Laboratory, Warrington, UK	11-12 September 2008	Invited talk	
7	Zeolite collapse and polyamorphism	G. Neville Greaves	International Workshop on Glass and Entropy	Trencin, Slovakia	24-26 June 2008	Invited Lecture	
53	The high pressure structure of magnesium silicate liquids: insight from in situ diffraction studies	Martin Charles Wilding	American Geophysical Union Conference	San Fransisco, USA	15-19 December 2008	invited contribution	
52	High pressure effects on liquid viscosity and glass transition behaviour, polyamorphic phase transitions and structural properties of glasses and liquids	Martin Charles Wilding	International Workshop on Glass and Entropy	Trencin	24-26 June 2008	contribution (two papers)	
50	Changes in the structure of silicate glasses with pressure.	Martin Charles Wilding	SNAP/COMPRESS meeting	Oak Ridge National Laboratory, TN, USA	April 11-13 2008	oral contribution	

ID	Title	CAFMaD Author	Conference	Location	Date	Capacity	Other Authors
47		Martin Charles Wilding	Synchrotron Radiation Source (SRS) users meeting , co-convener of Satellite Session on Extreme Conditions, STFC	Daresbury Laboratory	11-12 September 2008		
54	Optical Detection of X-ray Absorption: a direct link between chemistry, structure and luminescence	Nigel Robert Poolton	6th International Conference on Synchrotron Radiation in Materials Science	Campinas, Brazil	20-23 July 2008	Oral Contribution	
58	Anomalous small angle scattering to probe the formation of nanoceramics and glasses	Rudolf Winter	6th International Conference on Synchrotron Radiation in Materials Science	Campinas, Brazil	20-23 July 2008	invited talk	
57		Rudolf Winter	International Conference on Solid Films and Surfaces	Dublin	July 2008		
59		Rudolf Winter	Society of Glass Technology Annual Conf	Cambridge	September 2008	Conference Organisation & Contribution	
55		Rudolf Winter	Society of Glass Technology Annual Conference	Cambridge	September 2008	Chair, programme committee	

CAFMaD

Joint Workshops

2008

CAFMaD Workshops 2008

ID	Date	Place	Talk 1	Talk 2	Talk 3	Talk 4	Talk 5	Talk 6	Talk 7
1	22 January 2008	Bangor University	Towards a synergy betweem experiment and theory: From algorithms and data-sets (biological) building blocks and functional materials: Greg Chass;	Landfill monitoring - developing sensor devices for optimising power generation and reducing pollution: Louise Jones; Ellipsometry - a Panacea?: Tudor Jenkins;	Optical probing of organic semiconductor devices using high-k dielectrics: Janet Lancaster, Electronic Engineering, Bangor; Polythiophene based metal-insulator-semiconductor devices with an organic dielectric: Maria Lada, Electronic Engineering, Bangor;	Polythiophene based metal-insulator-semiconductor devices with an organic dielectric: Maria Lada, Electronic Engineering, Bangor; Oh, what a virtual world!: Andrew Davies, Chemistry, Bangor;	Titania thin films for sensing and photocatalytic detoxification: Sian Masson, Chemistry, Bangor; Dipole reversal in molecular rectifiers: Benjamin Robinson, Chemistry, Bangor;	Characterising liquids, liquid-liquid transitions and polyamorphism at extreme temperatures: Neville Greaves; Characterising liquids, liquid-liquid transitions and polyamorphism at extreme temperatures: Neville Greaves;	The ExoMars Rover Inspection Mirror (RIM): New opportunities for Mars surface science: Dave Barnes
2	6 October 2008	Physical Sciences Building, Aberystwyth University	Janet Lancaster: Resistive Switching in organic metal insulator semiconductor devices; Gruffudd Williams: Dynamical studies of photovoltaic systems; Quang Vu Van: Rheological and Thermal Studies of Alumina;	Nigel Poolton: Optical Luminsecence Spectroscopy with Synchrotron Radiation; Greg Chass: Design Rules, Mechanistic Studies and Neutron Spectroscopy of Pd-Carbene Cross-Coupling Catalysts: A Synergy between Experiment and Theory;	Florian Kargl: Inelastic Neutron Scattering for Materials Characterisation; Dave Langstaff: Detectors for Real Time Photoemission; Colin Watson: Organic near-field detector for integrated surface plasmon resonance biosensing;	Chris Gwenin: An overview of Nanosecure: A European Security Consortium;			

CAFMaD

Grant Capture Data

2008

CAFMAD Grant Capture Data 2008

ID	Project Title	Status	Principal Investigator 1	PI 1 Aber or Bangor?	Prinicpal Investigator 2	PI 2 Aber or bangor?	Joint AU/BU Project	Investigator funded by Partnership	CAFMaD core activity	Funder	Total Value to Partnership	Comments
71	Molecular diodes and an approach to single molecule electronics	Award	Geoff Ashwell	Bangor			☐	☑	☑	EPSRC	£329,000.00	Organic conductors & semiconductors
73	Basic technology: controlled electron transport through single molecules	Award	Geoff Ashwell	Bangor			☐	☑	☑	EPSRC	£97,047.00	Organic conductors & semiconductors
74	RCUK Academic Fellowship	Award	Martin Taylor	Bangor			☐	☑	☑	RCUK	£125,000.00	Organic conductors & semiconductors
75	Determining sp2 and sp3 bonding in natural and synthetic diamonds	Award	Andrew Evans	Aberystwyth			☐	☑	☑	DTC	£18,000.00	Extreme Materials
77	RCUK Academic Fellowship	Award	Neville Greaves	Aberystwyth			☐	☑	☑	RCUK	£125,000.00	Extreme Materials
78	Charge detector array	Award	Dave Langstaff	Aberystwyth			☐	☑	☑	PPOC-KEF	£70,000.00	Sensors & Devices
80	Continuation of CETIC funding	Award	Martin Taylor	Bangor	Alan Shore	Bangor	☐	☑	☑	WAG	£100,000.00	Sensor & Devices
82	Collaborative Visits between Potsdam and Bangor	Award	Martin Taylor	Bangor			☐	☑	☑	British Council	£1,800.00	Sensors & Devices
124	Photo-electron Spectroscopy & Electron emission study as function of Temp. of synthetic Diamonds	Award	Andrew Evans	Aberystwyth			☐	☑	☑	Element Six	£19,940.00	Characterisation & Modelling
175	Diamonds	Award	Andrew Evans	Aberystwyth			☐	☑	☑	Element Six	£19,940.00	Extreme Materials

ID	Project Title	Status	Principal Investigator 1	PI 1 Aber or Bangor?	Prinicpal Investigator 2	PI 2 Aber or bangor?	Joint AU/BU Project	Investigator funded by Partnership	CAFMaD core activity	Funder	Total Value to Partnership	Comments
183	Optical Pump Probe Studies of the Boron-K Edges in BN using a Tuneable Laser Probe	Award	Andrew Evans	Aberystwyth			☐	☑	☑	CCLRC	£310.00	Characterisation & Modelling
184	Organic Semiconductors	Award	Andrew Evans	Aberystwyth			☐	☑	☑	CCLRC	£850.00	Organic conductors & semiconductors
185	Threshold Voltage Instability in Polymer MIS Structures	Award	Andrew Evans	Aberystwyth			☐	☑	☑	EPSRC	£5,000.00	Organic conductors & semiconductors
206	CHARGED PARTICLE DETECTOR	Award	Dave Langstaff	Aberystwyth			☐	☑	☑	WAG	£49,624.00	Sensors & Devices
268	Technology programme project: molecular electronic sensors	Award	Geoff Ashwell	Bangor			☐	☑	☑	DTI QinetiQ	£24,000.00	Organic conductors & semiconductors
269	Single molecule electronics	Award	Geoff Ashwell	Bangor			☐	☑	☑	QinetiQ	£20,000.00	Organic conductors & semiconductors
271	Royal Academy of Engng Travel Grant 2008	Award	Martin Taylor	Bangor			☐	☑	☑	Royal Academy	£400.00	Organic conductors & semiconductors
272	Exchange visit with MIT	Award	Martin Taylor	Bangor			☐	☑	☑	Drapers Wynn Humphrey Davies Trust Fund	£6,000.00	Organic conductors & semiconductors
273	3M contract for IDB	Award	Martin Taylor	Bangor			☐	☑	☑	3M	£15,000.00	Organic conductors & semiconductors

ID	Project Title	Status	Principal Investigator 1	PI 1 Aber or Bangor?	Prinicpal Investigator 2	PI 2 Aber or bangor?	Joint AU/BU Project	Investigator funded by Partnership	CAFMaD core activity	Funder	Total Value to Partnership	Comments
275	British-Polish Young Scientist Programme,	Award	Martin Taylor	Bangor			☐	☑	☑	British Young Scientist Programme	£1,100.00	Organic conductors & semiconductors
305	'Flash Bang' The Chemistry Show	Award	Geoff Ashwell	Bangor			☐	☑	☑	EPSRC	£2,081.00	Organic conductors & semiconductors
308	International Travel Grant - Plastic Memories: A Small Signal Impedance Study	Award	Martin Taylor	Bangor			☐	☑	☑	The Royal Academy of Engineering	£400.00	Organic conductors & semiconductors
469	NERC DTG DR A COOK	Award	Anthony Cook	Aberystwyth			☐	☑	☑	NERC	£68,543.00	Charaterisation and Modelling
471	STFC QUOTA STUDENTSHIP	Award	Neville Greaves	Aberystwyth			☐	☑	☑	STFC	£132,045.00	Extreme Materials
497	Inert Environment Fabrication and Characterisation Facility	Award	Martin Taylor	Bangor			☐	☑	☑	WAG A4B	£200,003.00	Organic conductors & semiconductors
											£1,431,083.00	

CAFMaD

CAFMaD Flyer and list of core members research interests

2008

CAFMaD

PRIFYSGOL ABERYSTWYTH UNIVERSITY

PRIFYSGOL BANGOR UNIVERSITY

Prifysgol Aberystwyth a Phrifysgol Bangor

Aberystwyth University and Bangor University

Centre for Advanced Functional Materials and Devices
www.cafmad.ac.uk

The £2.9M Centre for Advanced Functional Materials and Devices (CAFMaD) is part of the Aberystwyth University and Bangor University Research & Enterprise Partnership. The Partnership was awarded HEFCW funding of £10.9M from 2007 to 2011 to provide research and entrepreneurship support across the Universities and to create four internationally recognised research Centres:

- Centre for Advanced Functional Materials and Devices (CAFMaD)
- Centre for Integrated Research in the Rural Environment (CIRRE)
- Centre for Catchment and Coastal Research (CCCR)
- Institute for Medieval and Early Modern Studies (IMEMS)

CAFMaD brings together leading academics from the Institute of Mathematics and Physics (IMAPS) and the Welsh Visualisation Centre at Aberystwyth University, and the College of Physical and Applied Sciences at Bangor University, which includes the School of Chemistry, the School of Electronic Engineering and the School of Computer Science.

CAFMaD's strengths are in materials, sensors, mathematics, space physics, synthesis and catalysis, molecular modelling, visualisation, image recognition, characterisation, photovoltaics, biological chemistry, optoelectronics and high performance computing.

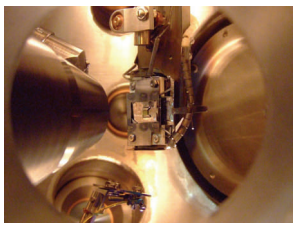
Aberystwyth leads in glasses and ceramics, semiconductor surfaces and interfaces, advanced characterisation techniques and stereo reconstruction and modelling of solids and surfaces. Bangor leads developments in optoelectronics and solar cell technology, materials synthesis and catalysis, polymer processing, polymer electronics, micro-nano-fabrication and molecular modelling.

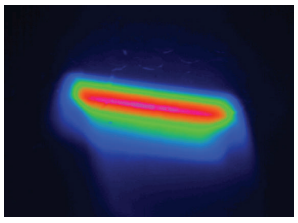
CAFMaD's Vision

To be an international centre of excellence for the development, characterisation and application of advanced materials and devices.

CAFMaD's Mission

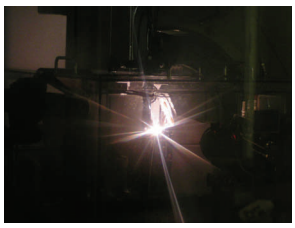
To be an international centre of research excellence, which is based on pure science and capable of delivering sustainable economic growth in Wales, the UK and beyond.

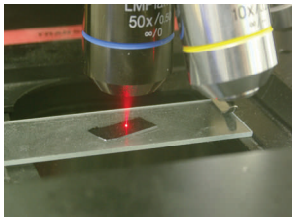




Research Facilities and Equipment available at CAFMaD include:

- Sopra Spectroscopic Ellipsometer
- JY Raman spectrometer (high resolution)
- The X-ray Diffractometer (with fast position sensitive detector)
- The REES XPS kit with bespoke detector enabling real time measurements
- CLASSIX luminescence kit (unique and soon to be upgraded)
- Laser heated aerodynamic levitation furnace
- Bespoke imaging ellipsometer under development
- Bruker microTOF mass spectrometer
- Waters GCT TOF mass spectrometer
- Philips X-PERT pro XRD
- HPC and visualisation facilities
- Nano-arrayer
- Surface probe microscopy
- Polymer electronic device prototyping
- Surface analysis
- Electrical characterisation

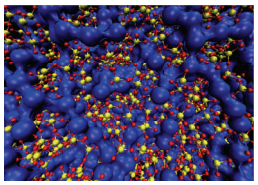




Research Streams

CAFMaD is a Research Centre that has its values embedded in pure science and seeks to increase funding in this area, but also embraces commercialisation opportunities by developing links with other universities, industry, government and third mission organisations.

1. Organic conductors & Molecular Electronics, which includes:

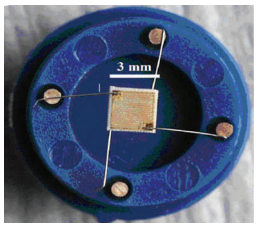


- Polymer Electronics
- Organic Lasers
- Contact Formation
- Nanolithography
- Molecular Wires and Diodes
- Sustainable Energy

2. Extreme Materials, which includes:

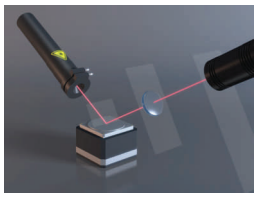
- Fast Ion Diffusion
- Glasses at HT and HP
- Melting and Amorphisation
- Nanoceramics and sintering
- Radiation-hard Semiconductors
- Planetary Exploration

3. Sensors and Devices, which includes:



- Semiconductor Solar Cells
- Charge Detectors for Electrons and Ions
- Smart end-station for combined electron and light spectroscopies

4. Characterisation & Modelling, which includes:



- Real Time Photoemission
- Optical Luminescence
- Elastic and Inelastic X-ray and Neutron scattering
- X-ray and Optical Imaging
- Computer simulation and visualisation

CAFMaD Members

CAFMaD is led by a Management Group, which is currently steered by Professor Neville Greaves at Aberystwyth University and Professor Geoff Ashwell at Bangor University. As well as many academic members researching in the CAFMaD research streams, there are a number of directly funded Chairs and Researchers; their contact details are below. For information about their research interests and the wider CAFMaD community, please visit www.cafmad.ac.uk. If you wish to contact to someone about CAFMaD, please contact Gary Reed, Partnership Development Manager on +44 (0)1970 62 1789 or gar@aber.ac.uk

Prof Geoff Ashwell	g.j.ashwell@bangor.ac.uk	Single molecule electronics: singe molecule Schottkey diode.
Dr Ben Robinson	b.robinson@bangor.ac.uk	Organic Photovoltaics and Molecular Electronics - particularly molecular diodes, rectifying junctions and functional single molecules on silicon testbed structures
Dr Tony Cook	atc@aber.ac.uk	Change detection on the Moon's surface: impact flashes and transient lunar phenomena, automated digital planetary cartgraphy, and robotic telescopes
Dr Greg Chass	g.chass@bangor.ac.uk	Formulation of effective computational methods including the design and construction of PC-Unix clusters and 'smart' data-sets for scientific computations
Prof Andrew Evans	a.evans@aber.ac.uk	Semiconductor physics, in particular using carbon-based materials (organic molecules and diamond)
Prof Neville Greaves	gng@aber.ac.uk	Materials Physics: Glass structure and glass properties: semiconductors: Syncotron Radiation and Neutron Techniques and applications.
Mr Matthew Gunn	mmg@aber.ac.uk	Optical measuring techniques and related instrumentation systems. Developing sampling environments in low and high temperatures and from vacuums to underwater.
Dr Florian Kargl	ffk@aber.ac.uk	Relationship between microscopic dynamics and structure.
Dr David Langstaff	dpl@aber.ac.uk	The design, implementation and application of advanced detectors for electron spectroscopy applications
Dr Justin Lawrence	ees40e@bangor.ac.uk	Organic optoelectronics devices such as lasers and LEDs
Dr Mohamed Mabrook	m.f.mabrook@bangor.ac.uk	Plastic Technology: Organic Transistors, Memory Devices, Sensors and organic Solar Cells
Dr Hongyun Tai	h.tai@bangor.ac.uk	Functional polymers for tissue engineering and drug delivery applications
Prof Martin Taylor	d.m.taylor@bangor.ac.uk	Electrical properties of thin films including insulating polymers, silicon dioxide, Langmuir-Blodgett films and semi conducting polymers: organic electronics
Mr Denis Williams	d.j.williams@bangor.ac.uk	Chief Technician, School of Chemistry, Bangor University