16th International conference on materials chemistry (MC16) 3-6 July 2023, Dublin, Ireland

OVERVIEW PROGRAMME

Monday 3 July 2023

11:30			Refreshments & registration								
12:00		Lunch O'Reilly Hall									
12:45		Welcome & Introductions									
		Silvia Vignolini, University of Cambridge and David Scanlon, University College London (Co-chairs)									
			Session chair: David Scanlon								
40.00	Diama	DI OI			Electrocatalytic Materials and Interfaces	for the	Production of Solar Fuels and Chemicals				
13:00	Pienary	PL01			Peter Strasser						
44.00					Technical Univ	ersity B	erlin, Germany				
14:00			George Moore Auditorium		O'Reilly Hall	nove be	Theatre D		Theatre F		
		Ар	proaches to material design and discovery		Future materials		Materials for energy		Materials for life		
			Session chair: Miriam M. Unterlass	Session chair: Itziar Oyarzabal Epelde		Session chair: Alex Cowan		Session chair: Susan Quinn			
14:10	Keynote	K01	Data-driven chemical understanding and machine learning of materials properties Janine George Federal Institute for Materials Research and Testina, Friedrich-Schiller University Jena	K02	New Materials from High Pressure Paul Attfield CSEC and School of Chemistry, University of Edinburgh, UK	K03	Renewable Fuels and Chemicals Maria Escudero-Escribano ICREA and Catalan Institute of Nanoscience and Nanotechnology, Spain	K04	New materials-based strategies for advanced therapeutics and ultrasensitive biosensing Molly Stevens		
			Germany		Winner: 2022 John B Goodenough Award		Winner: 2021 Journal of Materials Chemistry Lectureship		Imperial College London, UK		
14:40	Contributed	DD01	Autonomous millimeter scale high throughput battery research system (Auto- MISCHBARES) Fuzhan Rahmanian Helmholtz Institute Ulim at the Karlsruhe Institute of Technology, Germany	F01	Computer-aided understanding of phase changes in two-dimensional transition motal dichalcogenides Katherine Inzani University of Nottingham, UK	E01	Templated synthesis of porous single atom electrocatalysts with high atomic utilization Jesus Barrio Imperial Callege London, UK	L01	Morphogenetically active polyphosphate, an unexpected nano-/bio-material for successful tissue regeneration Werner E.G. Müller University Medical Center of the Johannes Gutenberg University Mainz, Germany		
15:00	Contributed	DD02	On the Largest Possible Mobility of Molecular Semiconductors and How to Achieve It Tahereh Nematiaram University of Strathclyde, UK	F02	New high-entropy oxides in a mulite-type structure Andrea Kirsch University of Copenhagen, Department of Chemistry and Nanoscience Center, Denmark	E02	Rational design of cathode materials for the electrocatalytic hydrogenation of organic substrates by modulating the binding strength of H surface coverages Anna Ciotti Trinity College Dublin, Ireland	L02	Inorganic-Organic Hybrid Nanoparticles as Theranostic High-Load Drug Carriers Claus Feldmann Karlsruhe Institute of Technology (KIT), Germany		
15:20	Contributed	DD03	Locating novel polyanionic cathode materials for Li-ion batteries in underexplored chemical spaces Bonan Zhu University College London, UK	F03	Epitaxial growth, optical and electrical conductivity and electronic structure of metallic pyrochlore Bi2Ru2O7 heterostructures Marita O'Sullvan University of Liverpool, UK	E03	Tuning the Catalytic Activity of Bifunctional Metal Boride Nanoflakes for Overall Water Splitting Veronica Sofianos University College Dublin, Ireland	L03	In-situ FTIR monitoring of sarcosine N- carboxyanhydride from a lysine dendrimer macroinitiator Richard England AstraZeneca, UK		
15:40					Refres	nments	nents				
		Ap	George Moore Auditorium proaches to material design and discovery	<u>O'Reilly Hall</u> Future materials		Ineatre D Materials for energy		Materials for life			
		. 4	Session chair: Andrew Beale	Session chair: Paul Attfield		Session chair: David Scanlon		Session chair: Cameron Alexander			
16:20	Contributed	DD04	Exploring the configurational space of amorphous graphene with machine- learned atomic energies Zakariya El-Machachi University of Oxford, UK	F04	Thermally conductive h-BN/polymer composites for textiles thermal management Chengning Yao Imperial College London, UK	E04	Phase segregation and nanoconfined fluid O2 in a layered lithium rich oxide cathode material Kit McColl University of Bath, UK	L04	Controlled polymerisation of water-soluble monomers towards the fabrication of soft cellular scaffolds Maria Chiara Arno University of Birmingham, UK		
16:40	Contributed	DD05	Combining Theoretical Approaches in Understanding the Ionisation potentials of Metal Oxides Xingfan Zhang University College London, UK	F05	Characterisation of cation order in A-site doped polar hexagonal multiferroic MnAMo308 (A2+ = Fe, Co, Zn) Holly L. McPhillips University of Kent, UK	E05	Room Temperature Electrochemical Cycling of F-ions in CSMnFoF6 Brent Melot University of Southern California, USA	L05	3D printing, wet spinning and cell culture on carbohydrate low molecular weight supramolecular hydrogels Juliette Fitremann CNRS - IMRCP - University of Toulouse, France		
17:00	Contributed	DD06	Density Functional Theory (DFT): A tool for rational design of crystalline piezoelectrics Geetu Kumari University Of Limerick, Ireland	F06	Weaving the future: dynamic designs of active textiles using liquid crystalline elastomer yarn Pedro Emanuel Santos Silva Aalto University, Finland	E06	The Baseline of Prussian White: Exploring the Electrochemical and Physical Properties for Thick Structured Electrodes Halima Khanom University of Birmingham, UK	L06	Magnetically responsive hydrogels with high and reproducible hyperthermic performance Karina Nigoghossian University College Dublin, Ireland		
17:20	Contributed	DD07	Investigating oxygen reduction kinetics at Au-water interfaces via neural network potential accelerated metadynamics Xing Yang Technical University of Denmark, Denmark	F07	Computational prediction and experimental realisation of earth-abundant transparent conducting oxide Ga-doped ZnSb2O6 Joe Willis University College London, UK	E07	Best practices for photo-assisted batteries: Decoupling Heat and Light Arvind Pujari Cavendish Laboratory, Department of Physics, University of Cambridge, UK	L07	Fabrication of Polysaccharide-based pH Responsive Anti-inflammatory Nanofibers and Their Characterization for Wound Dressing Applications Beste Elveren University of Maribor, Slovenia		
17:40					Poster session (sponsored by	lournal o	of Materials Chemistry)				
19:30	1	Close									

Tuesday 4 July	Tuesday 4 July 2023										
			Session chair: Andrew Dove O'Reilly Hall								
09:00	Plenary	PL02	Polymers and nanocomposites to treat vascular disease without a trace								
			Junia voltimia California Institute of Technology, USA								
10:00			George Moore Auditorium		Time for delegates to r O'Reilly Hall	nove bet	tween theatres Theatre D	Theatre F			
		Ар	proaches to material design and discovery	Future materials		Materials or energy		Materials for life			
10:10	Keynote	K05	Digital Polymer Chemistry on The Rise Tanya Junkers Monash University, Australia	K06	Controlling Polymer Properties with Stereochemistry Andrew Dove University of Birmingham, UK	K07	Understanding Operation of Halide Perovskite Photovoltaics on Different Longth Scales Sam Stranks	K08	Material and Devices for Bioelectronic Medicine George Maliaras University of Cambridge, UK		
10:40	Contributed	DD08	On-demand upgrading of material properties with universal polymer crosslinkers Jeremy Wulff University of Victoria, Canada	F08	Winner: 2022 Corday-Morgan Prize Hydroaminoalkylation As a Sustainable Process to Amine Functionalized Materials Sabrina S. Scott University of British Columbia, Canada	E08	University of Cambridge, UK Nanostructured coordination polymers for high performing solar cells Kezia Sasitharan Newcastle University, UK	L08	Hybrid fabrication of multimodal intracranial implants for electrophysiology and local drug delivery Johannes Gurke University of Potsdam. Germany		
11:00	Contributed	DD09	Autonomous optimization of liquid- handling parameters for accurate transfer of viscous liquids using automated pipette robots Pablo Quijano Velasco Institute of Materials Research and Engineering, A*STAR (Agency for Science, Technology and Research). Singapore	F09	Switchable spin crossover material for passive control of temperature fluctuations in buildings Esther Resines-Urien IMDEA Nanociencia, Spain	E09	Efficiency Bottleneck in Antimony Chalcogenide Solar Cells Xinwei Wang Imperial College London, UK	L09	Laser-fabricated sustainable porous carbon electrodes for electrochemical biosensing Sanghwa Moon Max Planck Institute of Colloids and Interfaces, Germany		
11:20			Contra Mana Auditarium		Refres	hments	The also D		Theodor C		
		Ар	proaches to material design and discovery		U Kelliy Hall Future materials	Theatre D Materials for energy			Theatre F Materials for life		
			Session chair: Paul Attfield		Session chair: Kyoko Nozaki		Session chair: Kevin Sivula		Session chair: Julia Kornfield		
12:00	Contributed	DD10	Hyperfluorescence from 2,1,3- benzothiadiazole-containing oligomers Christopher Riggs University of Glasgow, UK	F10	Exploiting supramolecular chemistry for self-healing organic semiconductors Bob Schroeder University College London, UK	E10	Asymmetric Supercapacitors using Hybrid Bi and Ni-based Materials Neil Roberston University of Edinburgh, UK	L10	ninimally invasive biomarker monitoring and drug delivery Hannah Leese University of Bath, UK		
12:20	Contributed	DD11	System-based product design: An integrative paradigm for the realisation of sustainable and scalable functional nanomaterials Robert Pilling University of Sheffield, UK	F11	New strategies for self-healing electronics Fabio Cicoira Polytechnique Montreal, Canada	E11	Covalently attached ruthenium- popypyridyl complexes on aminated reduced graphene oxide for enhancing stable photocatalysis Roberto Gonzalez Commez University of Galway, Ireland	L11	Flexible, transparent electrodes based on AgNW/ZnO nanocomposites for localized heating of lab-on-chip devices David Muñoz-Rojas Laboratoire des Materiaux et du Genie Physique GRenoble INP-CNRS, France		
12:40	Contributed	DD12	Sizing up Materials Design: Predicting the Effect of Particle Size on the Optical Properties of Nanoparticles Martijn A. Zwijnenburg University College London, UK	F12	Two-dimensional Semiconductive Ni3TeO6: From Theoretical Prediction to Shape-controlled Synthesis Javier Fernández-Catalá* UOULU-NANOMO Unit, Finland	E12	Electrochemical formation of ammonia from nitrates in wastewater using a liquid metal electrode Anthony O'Mullane Queensland University of Technology, Australia	L12	Magnetic motors in inhomogeneous environments Miguel A Ramos Docampo Aarhus University, Denmark		
13:00			Lunch and posters								
14:00					Making science greener – Comm	unity pe	erspectives and solutions				
		Ap	George Moore Auditorium proaches to material design and discovery		<u>O'Reilly Hall</u> Future materials		Theatre D Materials for energy		Theatre F Materials for life		
			Session chair: Jamie Neilson		Session chair: Jenni Garden		Session chair: Alex Cowan		Session chair: Cameron Alexander		
14:30	Keynote	K09	Syntheses or complex halide perovskites: mosaic perovskites and perovskite heterostructures Hema Karunadasa Stanford University, USA	K10	Polymer Synthesis and Degradation for Sustainability Kyoko Nozaki The University of Tokyo, Japan	K11	The development of new ionic electrolytes for energy storage devices Jenny Pringle Deakin University, Australia	K12			
15:00	Contributed	DD13	Phase behaviour and driving forces behind ferroelectricity in MDABCO-based perovskites Hamish Yeung University of Birmingham, UK	F13	Sustainability and quality: Hydrothermal injection synthesis of magnetic nanomaterials for medicine Annie Regan Trinity College Dublin, Ireland	E13	Ion-Conductive Metal-Organic Framework Membranes for Lithium Metal Batteries Rui Tan Imperial College London, UK	L13	Polyvalent glycan-nanoparticles as a powerful new biophysical platform for multivalent lectin glycan interactions Dejian Zhou University of Leeds, UK		
15:20	Contributed	DD14	Structural Chemistry of Molecular Perovskites: Towards the Design of Stimuli Responsive Behaviour Gregor Kielish Technical University of Munich, Germany	F14	Piezoelectric Biomolecules for Lead-Free, Reliable, Eco-Friendly Electronics Sarah Guerin University of Limerick, Ireland	E14	Structural Complexity in Prussian Blue Analogue K-ion Cathode Materials John Cattermull University of Oxfrod, UK	L14	Multimodal theranostic amyloid-β targeted upconversion gadolinium-based nanoprobe for Alzheimer's disease Man Shing Wong Hong Kong Baptist University, Hong Kong		
15:40	Contributed	DD15	Identifying the ground state structures of point defects in solids Irea Mosquera Lois Imperial College London, UK	F15	Aluminum formate, Al(HCOO)3: An earth- abundant, scalable, and highly selective material for CO2 capture Hayden Evans NIST Center for Neutron Research, USA	E15	Improving Lithium metal battery performance by pulsed current charging and discharging Katarina Cicvaric Helmholtz Institute Ulm, Karlsruhe Institute of Technology, Germany	L15	Lignin-based polymers and colloids for functional bio-based materials Mohammad Morsali Stockholm University, Sweden		
16:00	Contributed	DD16	Quantitative detection of Force- Fluroscence correlation by self-assembled nanostructures at Nanoscale Bratati Das University of Tokyo, Japan	F16	SUPRABEADS for Catalysis Susanne Wintzheimer Friedrich-Alexander-Universität Erlangen- Nürnberg, Germany	E16	Low Temperature Graphitic Carbon from Cellulose for Li-ion Batteries Ernily Hayward* University of Birmingham, UK	L16	Antimicrobial and degradable triazolinedione (TAD) crossilinked polypeptide hydrogels Scott Kimmins Pontificia Universidad Católica de Valparaiso, Chile		
16:20			Refreshments Session chair. Susan Ouinn								
17:00	Plenary	PL03	Chad Mirkin Chad Mirkin Northwestern University, USA Winner: 2021 de Gennes Prize								
18:00			Poster session (sponsored by Journal of Materials Chemistry)								

Wednesday 5	Nednesday 5 July 2023									
			Session chair: David Scanlon <u>O'Reilly</u> Hall							
09:00	Plenary	PL04	Computation-guided discovery of supramolecular materials							
			Imperial College London, UK							
10:00			Time for deleg George Moore Auditorium O'Reilly Hall				Theatre D	Theatre F		
		Ар	proaches to material design and discovery Session chair: Miriam M. Unterlass		Future materials Session chair: Nicholas Chilton		Materials for energy Session chair: David Scanlon		Materials for life Session chair: Susan Quinn	
							Coordination complexes and polymers for			
			Finding Thermodynamic Shortcuts with		Unlocking the potential of molecule-based		Marina Freitag		Polymer Therapeutics – New Materials with Applications from Oncology to	
10:10	Keynote	K13	Jamie Neilson	K14	Itziar Oyarzabal	K15	Newcastle University, UK	K16	Infection Cameron Alexander	
			Colorado State University, USA		BCMaterials, Spain		Winner: 2022 Harrison-Meldola Memorial		University of Nottingham, UK	
			The layering and subsequent patterning of		Impact of Finite Phonon Lifetimes on the		Cation Disorder in ABZ Chalcogenide		Designer therapeutic and diagnostic tools:	
10:40	Contributed	DD17	electrospun polymer matts to improve membrane properties	F27	Spin Dynamics of Single-Molecule Magnets	E17	Photovoltaics (NaBiS & AgBiS) Seán Kavanagh	L17	From cancer to chemical weapons	
			Graham Reid School of Chemical Sciences, Ireland		Rizwan Nabi		University College London & Imperial College		Gemma-Louise Davies University College London, UK	
			Computational analysis and design of		Magnetised MOFs – an attractive solution		Luminescent waveguide-encoded lattices			
11:00	Contributed	DD18	precursors for thin film deposition Simon Elliott	F28	to carbon capture Luke Woodliffe	E18	for light harvesting Takashi Lawson	L18		
11:20			Schrödinger, USA		University of Nottingham, UK Refres	hments	University of Cambridge, UK			
		An	George Moore Auditorium		<u>O'Reilly Hall</u> Future materials		Theatre D Theatre F Materials for energy Materials for life			
			Session chair: Miriam M. Unterlass		Session chair: Nicholas Chilton	Session chair: Kevin Sivula			Session chair: Cameron Alexander	
			Resonant Properties of Polycrystalline		Stimuli responsive complex salts with ferroelectric switching and thermistor		Atomistic Simulations of Microporous Polymer Membranes for Energy Storage			
12:00	Contributed	DD19	Tara Ryan	F19	properties Lidija Andros Dubraja	E19	and Conversion Charlotte Breakwell	L19		
		-	University of Limerick, Ireland		Rudjer Boskovic Institute, Croatia		Imperial College London, UK			
					Symmetry-Induced Singlet-Triplet		A New Generation of Designed (Elettro-		Functional mesoporous silica nanoparticles towards oral delivery of	
12:20	Contributed	DD20	Interstitial Hydrides of High Entropy Alloys Aaron Keith	F20	Molecular Emitters from Known Chemistry	E20)Catalysts for Sustainable Energy Production	L20	insulin Claudia Iriarte-Mesa*	
			Queen Mary, University of London, UK		J. Terence Blaskovits École polytechnique fédérale de Lausanne,		Cristina Giordano Queen Mary University of London, UK		Department of Inorganic Chemistry – Functional Materials, Faculty of Chemistry	
					Switzerland		Queen many entretenty of Lentent, ert		University of Vienna, Austria	
			mechanochemical formation of		Stability and diffusion dynamics of TiW/Cu		Nanocellulose Electrolyte Membranes for		crystalline emulsions phase on the	
12:40	Contributed	DD21	luminescent complexes directly from metal (hydr)oxide precursors	F21	photoelectron spectroscopy	E21	Fuel Cells Stephen Lyth	L21	penetration rate of active ingredients into the skin	
			Thomas Auvray University of Birmingham, UK		University College London, UK		University of Strathclyde, UK		Mateo Michel Torino* University of Buenos Aires, Argentina	
13:00			Come loss Automation Denais Lunch and posters							
			George Moore Auditorium		O'Reilly Hall	a poster	s Theatre D		Theatre F	
		Ар	George Moore Auditorium proaches to material design and discovery Session chair. Tania, Junkers		<u>O'Reilly Hall</u> Future materials	a poster	s <u>Theatre D</u> Materials for energy Session chair: Alexander Cowan		Theatre F Materials for life Session chair: Cameron Alexander	
		Ар	George Moore Auditorium proaches to material design and discovery Session chair: Tanja Junkers		<u>O'Reilly Hall</u> Future materials Session chair: Itziar Oyarzabal Epekle	a poster	s Theatre D Materials for energy Session chair: Alexander Cowan Materials for direct solar-to-fuel energy		Theatre F Materials for life Session chair: Cameron Alexander Sustainable Mono-Material Product Design	
14:00	Keynote	Ap K17	George Moors Auditorium proaches to material design and discovery Session chair: Tanja Junkers High-Throughput Approaches for the Discovery of Organic Materials	K18	OTRelly Hall Future materials Session chair: Itziar Oyarzabal Epekle Dissolving Boundaries: Water as Near- Universal Solvent for Materials	K19	s <u>Theatre D</u> Materials for energy Session chair: Alexander Cowan Materials for direct solar-to-fuel energy conversion using semiconductor photoelectrochemistry	K20	Theatre F Materials for life Session chair: Cameron Alexander Sustainable Mono-Material Product Design with Biodegradable and Recyclable Polymers	
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Thursday 6 Ju	ly 2023									
		George Moore Auditorium		O'Reilly Hall		Theatre D		Theatre F		
		Approaches to material design and discovery		Future materials		Materials for energy		Materials for life		
	Session chair: Olli Ikkala			Session chair: Itziar Oyarzabal Epelde		Session chair:		Session chair:		
09:00	Keynote	K21	Green Chemistry through the Solid State: Sky is the Limit Tomislav Friscic University of Birmingham, UK	K22	Practising Reticular Chemistry with Titanium-Organic Frameworks Carlos Marti-Gastaldo Universidad de València/Instituto de Ciencia Molecular, Spain	K23	Hyperdimensional imaging of functional materials under operando conditions Andy Beale University College London, UK Winner: 2022 Peter Day Award	K24	Carbon nano-onions for biomedical applications Silvia Giordani Dublin City University, Ireland	
09:30	Contributed	DD26	Structure control using bioderived solvents in electrochemical metal-organic framework synthesis Stephen Worral Aston University, UK	F26	Metal Organic Frameworks : A novel material for the detection of radioactive gases Sharvanee Mauree CEA Saclay/LIST/Université Paris-Saclay, France	E26	Controlling the heat transport in thermoelectric materials Jonathan Skelton University of Manchester, UK	L26	DNA binding and luminescent response of carbon dots Clara Zehe University College Dublin, Ireland	
09:50					Refres	hments				
10:30					George Moo Publishing	re Audito with imp	<u>rium</u> pact			
			George Moore Auditorium	O'Reilly Hall		Theatre D		Theatre F		
		Approaches to material design and discovery		Future materials		Materials for energy		Materials for life		
			Session chair: Olli Ikkala		Session chair: Susan Quinn		Session chair: Martijn Zwijnenburg		Session chair:	
11:10	Contributed	DD27	Sustainable water treatment solution: 3D printed and fully biobased water purification filters Natalia Fjol Stockholm University, Sweden	F27	Enhancement of Circularly Polarized Luminescence (CPL) Dissymmetry Factor by a Guest–Host Interaction in Chromophore Encapsulated Homochiral Gyroidal MOFs Kazuya Nakashima Nadova University, Japan	E27	Tailoring the Properties of Luminescent Downshifting Layers with POSS Nanoparticles Helen Tunstall-Garcia University of Cambridge, Dept. Materials Science & Metailurgy, UK	L27	Zirconium-based MOFs and their biodegradable polymer composites for controlled and sustainable delivery of herbicides Sanjit Nayak University of Bradford, UK	
11:30	Contributed	DD28	A near-universal design concept for waterborne high-performance polyimides Daniel Alonso Cerron Infantes Universität Konstanz, Germany	F28	How does the spin transition affect electrical transport in 3D crystalline MOFs? Ana Martinez IMDEA Nanociencia, Spain	E28	Understanding aluminium graphite dual- ion batteries: anode-electrolyte interface evolution Anastasia Teck Imperial College London, UK	L28		
11:50	Contributed	DD29	Stability of single metal atoms on defective and doped diamond durfaces Shayantan Chaudhuri University of Warwick, UK	F29	Development of luminescent forensic security materials utilising ionic liquid technology Anthory Fitzpatrick Nottingham Trent University, UK	E29	Exploring the Potential of 2D Chalcogenide Films to Operate at Scale as Electrocatalysts for Hydrogen Production in Proton Exchange Membrane Electrolysers Arun Kumar Samuel University of Glasgow, UK	L29	Nano-Structured Poly amic acid Membranes for Enhanced Water Filtration Naumih Noah School of Pharmacy and Health Sciences, United States International University, Kenya	
12:10			Time for delegates to move between theatres							
					Session chair: I	Nicholas	Chilton			
12:20	Plenary	PL06	<u>O'Reilly Hall</u> Magnetic molecules in quantum nanoscience Roberta Sesoli <i>Università degli Studi di Firenze, Italy</i>							
13:20		Chairs' summary								
13:30		Close of conference								
14:00-17:00	1	Post-event online networking								