E-MRS European Materials Research Society
Spring Meeting 2022
May 30 | June 3
Virtual Conference

SYMPOSIUM G

Materials for sustainable energy technologies (M-SET)

Symposium Organizers :

Adam F. LEE, RMIT University

Arumugam MANTHIRAM, University of Texas at Austin

Pierre RUTERANA, Centre de Recherche sur les ions les matériaux et la photonique

Yuping WU, Nanjing University of Technology

Selected papers will be published
in a Special Issue of Materials Today Chemistry (Elsevier).

Monday may 30

08:45 **Welcome and Introduction to the Symposium, Symposium Organizers**

Electrodes : Vincenzo PALERMO, Yuping Wu

09:00 INV **Deciphering the electrode behavior of lithium metal under supergravity** — G E.1
Yuliang Gao, Fahong Qiao, Jingyuan You, Zengying Ren, Nan Li, Kun Zhang, Chao Shen, Ting Jin, Keyu Xie*
State Key Laboratory of Solidification Processing, Center for Nano Energy Materials, School of Materials Science and Engineering, Northwestern Polytechnical University

09:30 **Disentangling the origin of charge storage in laser-deposited nitrogen-doped nanocarbon-NiO electrodes** — G E.2
Pablo García Lebière, (a) Ángel Pérez del Pino, (a) Enikö György, (a,b) Constantin Logofatu, (c) Denys Naumenko, (d) Heinz Amenitsch, (d) Piu Rajak, (e) Regina Ciancio, (e)
(a) Institute of Materials Science of Barcelona, ICMAB-CSIC, Spain, (b) National Institute for Lasers, Plasma and Radiation Physics, Romania, (c) National Institute for Materials Physics, Romania, (d) Institute of Inorganic Chemistry, Graz University of Technology, Austria, (e) Instituto Officina dei Materiali-CNR, Trieste, Italy

09:45 **The Proton Surface Transfer Property in BZY from Density Functional Theory** — G E.3
ZhaoWenjuan, ZhuBin*, Wangjun*, LinBin
Southeast University, University of Electronic Science and Technology of China.

10:00 **Impact of the Iron-Doping on the structural integrity of Co-free Li-Rich Layered oxides (LRLO) for positive electrodes in Lithiu** — G E.4
Mariarosaria Tuccillo (a), Arcangelo Celeste (a), Laura Silvestri (b), Sergio Brutti (a)
(a) University of Rome La Sapienza (b) ENEA Research Center Casaccia

10:15 **Discussion Electrodes I**

10:30 **Effect of partial conductivities on the polarisation resistance of positrodes for proton ceramic fuel cells and electrolysers** — G E.6
Ragnar Strandbakke, Kalpana Singh, Truls Norby
Centre for Materials Science and Nanotechnology, Department of Chemistry, University of Oslo, FERMiO, Gaustadalléen 21, NO-0349 Oslo, Norway

10:45 **Thermoelectric performance of nanostructured ??FeSi2 alloys synthesized by ?in situ? SPS** — G E.7
Linda Abbassi a,b, David Mesguich b, David Berthebaud c, Bhuvanesh Srinivasan c,d, Sylvain Le Tonquesse c, Takao Mori d, Geoffroy Chevalier b, Claude Estournès b, Emmanuel Flahaut b, Romain Viennois a, Mickaël Beaudhuin a* *presenting person
a ICGM, Univ. Montpellier, CNRS, ENSCM, Montpellier, France, b CIRIMAT, Université de Toulouse, CNRS, France, c CNRS-Saint Gobain-NIMS, IRL 3629, LINK, Tsukuba, Japan, d WPI-MANA, NIMS, Tsukuba ? 1-1 Namiki Tsukuba, Ibaraki 305-0044, Japan

11:00 **Unveiling the electrochemistry of conjugated alkali-ion disulfonyl-methide as organic positive electrode materials** — G E.8
Yan Zhang a,b, Petru Apostol a, Xiaohua Chen b, Xiaolong Guo a, Xuelian Liu a, Jiande Wang a,*, Alexandru Vlad a,*
a Institute of Condensed Matter and Nanosciences, Molecular Chemistry, Materials and Catalysis, Université catholique de Louvain, Louvain-la-Neuve, Belgium, b College of Materials Science and Engineering, Hunan Province Key Laboratory for Advanced Carbon Materials and Applied Technology, Hunan University, Changsha 410082, Hunan, P. R. China.

11:15 **Electrophoretic coating of LiFePO4/Graphene oxide on carbon bers as cathode electrodes for structural lithium ion batteries** — G E.9
Jaime S. Sanchez a, Johanna Xu a, Zhenyuan Xia a, b, *, Jinhua Sun a, Leif E. Asp a, Vincenzo Palermoa,b,**
a) Industrial and Materials Science, Chalmers University of Technology, Hosalsvagen 7B, 41258, Goteborg, Sweden b) Istituto per la Sintesi Organica e la Fotoreattivita`, CNR, via Gobetti 101, 40129, Bologna, Italy

11:30 INV **Effect of pre-lithiation on solid electrolyte interphase of SiCx electrodes combined with Ni-rich cathodes for electric vehicles** — G E.10
Esen, E.* (1), Diddens, D. (1), de Meatza, I. (2), Schmuck, M. (3), Winter, M. (1,4), & Paillard, E. (5).
(1) Helmholtz-Institute Münster IEK-12, Forschungszentrum Jülich GmbH, Corrensstraße 46 48149 Münster, Germany, (2) CIDETEC, Basque Research and Technology Alliance (BRTA), Paseo Miramon 196, 20014, Donostia-San Sebastian, Spain, (3) VARTA Micro Innovation GmbH, Stremayrgasse 9, 8010 Graz, Austria, (4) MEET - Münster Electrochemical Energy Technology, Corrensstraße 46, 48149 Münster, (5) Politecnico di Milano, Dept. of Energy Via Lambruschini 4, 20156 Milan, Italy.

12:00 **Discussion Electrodes II**

Peroskytes : Judith Driscoll, Pierre Ruterana

13:30 INV **The Electronic Structure of MAPI-Based Perovskite Solar Cells: Detailed Band Diagram Determination by Photoemission Spectroscopy** — G PER.1
Tim Hellmann, Chittaranjan Das, Tobias Abzieher, Clément Maheu, Michael Wussler, Ulrich Paetzold, Thomas Mayer, Wolfram Jaegermann
Tim Hellmann, Chittaranjan Das, Clément Maheu, Michael Wussler, Thomas Mayer, Wolfram Jaegermann: Surface Science Group Materials Science Department Technical University of Darmstadt Alarich-Weiss-Straße 2, 64287 Darmstadt, Germany Tobias Abzieher, Ulrich Paetzold: Light Technology Institute Karlsruhe Technology Institute Engesserstraße 13, 76131 Karlsruhe, Germany

14:00 **Nickel oxide and copper-based inorganic hole transport layers in perovskite solar cells: a first-principles study.** — G PER.2
A. Pecoraro (1), P. Delli Veneri (2), M. Pavone (3), A. B. Muñoz-García (1)
(1) Department of Physics “E. Pancini”, University of Naples “Federico II”, Naples, Italy (2) Italian National Agency for New Technologies, Energy and Sustainable Economic Development (ENEA)- Portici, Research Centre, Piazzale E. Fermi 1, Portici, NA, Italy (3) Department of Chemical Science, University of Naples “Federico II”, Naples, Italy

14:15 **Strong Excitonic Effects in Zero-Dimensional Vacancy-Ordered Perovskites (Cs2TiX6)** — G PER.3
Seán R. Kavanagh, Shanti Liga, Christopher N. Savory, Gerasimos Konstantatos, Aron Walsh, David O. Scanlon
Thomas Young Centre and Department of Chemistry, University College London, London WC1H 0AJ, U.K, Thomas Young Centre and Department of Materials, Imperial College London, London SW7 2AZ, U.K, ICFO-Insitut de Ciencies Fotoniques, The Barcelona Institute of Science and Technology, Casteldefels, 08860 Barcelona, Spain, Department of Materials Science and Engineering, Yonsei University, Seoul 03722, Republic of Korea, ICREA-Institució Catalana de Recerca i Estudia Avançats, Lluis Companys 23, 08010 Barcelona, Spain

14:30 **Synthesis, crystal structure, band gap energy and Seebeck coefficient of trigonal Srx+1TiS3-y chalcogenide perovskites** — G PER.4
Jinan Hussein Awadh Alshuhaib 1, Jose Francisco Fernández1,2, Julio Bodega1, José R. Ares 1, Isabel J. Ferrer 1,2, Fabrice Leardini 1,2
1 Departamento de Física de Materiales, Universidad Autónoma de Madrid, Campus de Cantoblanco, E-28049 Madrid, Spain. 2 Instituto Nicolás Cabrera, Universidad Autónoma de Madrid, Campus de Cantoblanco, E-28049 Madrid, Spain.

14:45 **Disorder Enhanced Raman Scattering** — G PER.5
Menahem, Matan*(1), Asher, Maor(1), Olle Hellman(1), Safran, Sam(1), Benshalom, Nimrod(1), Aharon, Sigalit(1), Korobko, Roman(1), Yaffe, Omer(1)
(1) Weizmann Institute of Science, Israel * lead presenter

15:00 **Discussion Perovskytes I**

15:15 **Impact of small compositional and nanoscale morphology variations on the efficiency and stability of perovskite solar cells** — G PER.6
Lyubov A. Frolova (1), Nikita A. Emelyanov (1), Victoria V. Ozerova (1), Olga A. Kraevaya (1), Gennady V. Shilov (1), Sergey M. Aldoshin (1) and Pavel A. Troshin (2, 1)
(1) Institute for Problems of Chemical Physics of Russian Academy of Sciences (IPCP RAS), Semenov ave. 1, 142432, Chernogolovka, Moscow region, Russia (2) Faculty of Chemistry, Silesian University of Technology, Strzody 9, 44-100 Gliwice, Poland

15:30 **Low-cost scalable synthesis of efficient HTL materials for perovskite solar cells via oxidative polymerization of triarylamines** — G PER.7
O.A. Kraevaya,1 A.F. Latypova,1 A.A. Sokolova,1,2 A.A. Seleznyova,1,2 L. A. Frolova,1 P.A. Troshin3,1
1Institute for Problems of Chemical Physics of Russian Academy of Sciences, Chernogolovka, Russia 2Faculty of Fundamental Physics & Chemical Engineering, Lomonosov Moscow State University, Moscow, Russia 3Silesian University of Technology, Gliwice, Poland

15:45 **First-principles investigation of optoelectronic and transport properties of double perovskite Cs2TiX6 (X = Cl, Br)** — G PER.8
M. Khuili (1,2), G. El Hallani (3), N. Fazouan(3), El Houssine Atmani (3), El Hassan Abba (1), Adil Es-Smairi (3), Elhoussaine Maskar (4), Samah Al-Qaisi (5)
(1)Higher School of Technology, Sultan Moulay Slimane University, 54000 Khénifra. Morocco (2) CRMEF of Beni Mellal-Khénifra, Morocco (3) Laboratory of Physics of Condensed Matters and Renewables Energies, Faculty of Sciences and Technologies, Hassan II University of Casablanca, B.P 146, 20650 Mohammedia, Morocco (4) Nanomaterial and Nanotechnology Unit. E. N. S. Rabat. Energy Research Center, Faculty of Sciences, Mohammed V University, B.P. 1014 Rabat, Morocco (5) Palestinian Ministry of Education and Higher Education, Nablus, Palestine

16:00 **Efficient and stable copper-based hole transport layers for perovskite solar cells** — G PER.9
Alexander W. Stewart, Bernabé Marí Soucase
Universidad Politécnica de Valencia

16:15 INV **Towards High-Performance, Low-Temperature Solid Oxide Cells with Vertically Aligned Nanocomposite Films** — G PER.10
Matthew P. Wells, Adam J. Lovett & Judith L. MacManus-Driscoll
Department of Materials Science and Metallurgy, University of Cambridge, Cambridge CB3 0FS, United Kingdom

16:45 **Discussion Perovskytes II**

: Adam Lee, Arumugam Mathiram, Pierre Ruterana, Yuping Wu

17:00 **The Polycationic Doping Effect on the Ionic Conductivity Properties of LATP Solid Electrolyte** — G P1.1
A. Mashekova1,2, Ye. Baltash1, M. Yegamkulov1,2, Z.Bakenov1,2, I. Trussov1, A. Mukanova1,2
1Institute of Batteries, 53, Kabanbay Batyr Avenue, Z05P4X0 Nur-Sultan, Kazakhstan, 2Nazarbayev University, 53, Kabanbay Batyr Avenue, Z05P4X0 Nur-Sultan, Kazakhstan

17:00 **Composite Anode Based on Red Phosphorus for Lithium-Ion Batteries** — G P1.2
Z.Yelemessova, A.Nauryzbaeva, A. Mashekova, Z. Bakenov, A. Mukanova
Institute of Batteries, 53, Kabanbay Batyr Avenue, Z05P4X0 Nur-Sultan, Kazakhstan

17:00 **Enhancing the Ionic Conductivity in Li-Garnet Thin Film Solid State Electrolytes** — G P1.3
M. Yegamkulov, A. Shongalova, B. Uzakbaiuly, A. Mukanova, Zh. Bakenov
School of Engineering and Digital Science, Nazarbayev University, Z05P4X0 Nur-Sultan, Kazakhstan

17:00 **Piezoelectric devices for generation of electrical energy** — G P1.4
Irinela Chilibon
National Institute of Research and Development for Optoelectronics, INOE-2000 409 Atomistilor Street, P.O. Box MG-5, 077125, Magurele, Romania

17:00 **Deep insights into kinetics and structural evolution of dimension-engineered TiNb2O7 anode for lithium storage** — G P1.5
Wenlei Xu[1], Yaolin Xu[2], Veronika Grzimek[2], Thorsten Schultz[3], Yan Lu[2], Norbert Koch[3], Nicola Pinna[1]
[1] Institut für Chemie and IRIS Adlershof, Humboldt-Universität zu Berlin, Brook-Taylor-Str. 2, 12489 Berlin, Germany [2] Department of Electrochemical Energy Storage, Helmholtz-Zentrum Berlin für Materialien und Energie, 14109 Berlin, Germany [3] Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Albert-Einstein Str. 15, 12489 Berlin, Germany

17:00 **Computational Design of Thermoelectric Alloys** — G P1.6
Jiaxing Qu
University of Illinois at Urbana-Champaign

: Adam Lee, Arumugam Mathiram, Pierre Ruterana, Yuping Wu

17:00 **Cu2P/nickel foam as a bifunctional electrocatalyst for urea and hydrazine assisted water splitting** — G P1.7
Harshad A. Bandal, Hern Kim*
Department of Energy Science and Technology, Environmental Waste Recycle Institute, Myongji University, Republic of Korea

17:00 **Laser-pyrolysis Ge-Si based nanoparticles and their composites with reduced Graphene oxide for Li-ion battery anodes** — G P1.8
C. Fleaca 1, F. Dumitrache 1, V. Craciun 1, M. Dumitru 1, L. Gavrila-Florescu 1, C. Ungureanu 2, M. Buga 2
1 NILPRP – National Institute for Lasers, Plasma and Radiation Physics, Atomistilor str. No.409, Magurele-Bucharest, Romania, 2 ICSI – National Institute for Isotopic and Cryogenic Technologies, Uzinei str. No.4, Rm. Valcea, Romania

17:00 **Preparation of a Wearable Single Electrode Triboelectric Nanogenerator** — G P1.9
Y. Nurmakanov, G. Kalimuldina, R. Kruchinin
Y. Nurmaknov and R. Kruchinin: Nazarbayev University, School of Engineering and Digital Sciences, Nazarbayev University, Kabanbay Batyr Ave. 53, Nur-Sultan 010000 Kazakhstan G. Kalimuldina: Nazarbayev University, Department of Mechanical and Aerospace Engineering, School of Engineering and Digital Sciences, Nazarbayev University, Kabanbay Batyr Ave. 53, Nur-Sultan 010000 Kazakhstan

17:00 **Design of a membrane-less decoupled amphoteric Zn-MnO2 battery using immobilised pH gels** — G P1.10
Durena, R.*(1), Zukuls, A.(1), Vanags, M.(1)
(1) The Institute of Materials and Surface Engineering, Riga Technical University, Latvia

17:00 **PAN-(PAN-PVA)-PVA based layered solid polymer electrolyte for lithium-ion batteries** — G P1.11
a)Anar Arinova, a)Yer-Targyn Tleukenov, a)Nurbolat Issatayev, a)Gulnara Basharova, a)Arailym Nurpeissova, b)Gulnur Kalimuldinab, a,c) Zhumabay Bakenova
a National Laboratory Astana, 53 Kabanbay Batyr Ave., Nur-Sultan, 010000, Kazakhstan b Department of Mechanical and Aerospace Engineering, School of Engineering and Digital Sciences, Nazarbayev University, 53 Kabanbay Batyr Ave., Nur-Sultan, 010000, Kazakhstan c Department of Chemical and Materials Engineering, School of Engineering and Digital Sciences, Nazarbayev University, 53 Kabanbay Batyr Ave., Nur-Sultan, 010000, Kazakhstan

17:00 **Synthesis and characterization of band gap tuned Cu2Zn(Sn1 – xGex)S4 monograin powders** — G P1.12
I. Mengü, M. Kauk-Kuusik, K. Muska, V. Mikli, R. Kaupmees, J. Krustok, M. Grossberg
Department of Materials and Environmental Technology, Tallinn University of Technology, Ehitajate tee 5, 19086 Tallinn, Estonia

17:00 **Silicon Clathrates films for Photovoltaic Appplications Investigated by Surface Photovoltage** — G P1.13
Vollondat, R.*(1), Roques, S.(1), Chevalier, C.(2), Bartringer, J.(1), Rehspringer, J.-L.(3), Slaoui, A.(1), Fix, T.(1)
(1) Laboratoire des Sciences de l'Ingénieur, de l'Informatique et de l'Imagerie (ICube), CNRS and University of Strasbourg, 23 rue du Loess, 67037 Strasbourg, France (2) Université de Lyon, Institut des Nanotechnologies de Lyon INL-UMR5270, CNRS, INSA Lyon, 7 Avenue Jean Capelle, 69621 Villeurbanne, France (3) Institut de Physique et Chimie des Matériaux de Strasbourg (IPCMS), UMR7504, CNRS and University of Strasbourg, 23 rue du Loess, 67034 Strasbourg, France

17:00 **Continuous hydrothermal flow synthesis of Li-ion batteries' cathodic materials** — G P1.14
Federico Barbon(1), Dario Mosconi(2), Silvia Gross(1)
(1)Università degli Studi di Padova, Italy (2)Particular Materials srl, Cadoneghe(Padova), Italy

17:00 **Alloying leads to drastic reduction of lattice thermal conductivity of half-Heusler compounds** — G P1.15
Rasmus Tranås, Ole Martin Løvvik, Kristian Berland
Department of Mechanical Engineering and Technology Management, Norwegian University of Life Sciences, SINTEF Sustainable Energy Technology, Department of Mechanical Engineering and Technology Management, Norwegian University of Life Sciences

17:00 **Bioconstruction of electro active Cu morphologies with possible application in CO2 reduction** **G P1.16**
*Iacob, M.T. (1, 2), Stamatin, I. (1,2), Ghinea, A. (3), Diac, C. (1), Nechita, C. (2), Moisescu, C. (3), Ardelean, I. (3), Stamatin, S.N (1,2)
(1) 3Nano-SAE Research Centre, PO Box MG-38, Bucharest – Magurele, Romania (2) University of Bucharest, Physics, ICUB, Bucharest, Romania (3) Institute of Biology Bucharest, Romanian Academy, Splaiul Independentei 296, Bucharest 060031, Romania

17:00 **Coupling electrochemical active Li4Ti5O12 with PVDF as a composite solid electrolyte for solid state lithium metal battery** **G P1.17**
Qi Zhou1, Rui Sun1, Xiaosong Xiong1, Bohao Peng1, Yusong Zhu1, Yuhui Chen1, Zhaogeng Wang1, Yuping Wu1,2*
1State Key Laboratory of Materials-oriented Chemical Engineering, School of Energy Science and Engineering, Nanjing Tech University, Nanjing, Jiangsu 211816, P. R. China,2School of Energy and Environment, South East University, Nanjing, Jiangsu 211189, P. R. China

17:00 **The ionic conductive propterties of two-dimensional ZnO-Zn6Al2O9 nanocomposite membrane used for advanced fuel cells** **G P1.18**
Liwen Huang, Xin Chen, Yan Wu*
Engineering Research Center of Nano-Geo Materials of Ministry of Education, Faculty of Materials Science and Chemistry, China University of Geosciences, 388 Lumo Road, Wuhan 430074, China

17:00 **Interface channels accelerate ion transport through solid carbonate coated Gd0.1Ce0.9O1.9 (GDC)** **G P1.19**
Hao Wang, Wenjuan Zhao, Jingjing Liu, Enyi Hu, Yifei Zhang, Shuo Wan, Bin Zhu, Qi Fan, Faze Wang
Jiangsu Provincial Key Laboratory of Solar Energy Science and Technology/Energy Storage Research Center, School of Energy and Environment, Southeast University, No. 2 Si Pai Lou, Nanjing, Jiangsu 210096, P. R. China

17:00 **High-quality electrolytes for low-temperature solid oxide fuel cells** **G P1.20**
Yingbo Zhang, Jiamei Liu, Xin Jia, Decai Zhu, Xinfang Li, Yuzhao Ouyang, Xiaowei Gao, Jie Yu, Chengjun Zhu*
Key Laboratory of Semiconductor Photovoltaic Technology of Inner Mongolia Autonomous Region, School of Physical Science and Technology, Inner Mongolia University, 235 West Daxue Street, Hohhot, 010021, China

17:00 **Research on Composite Oxide Materials as Composite Electrolytes for Low Temperature Solid Oxide Fuel Cells** **G P1.21**
Yuzhao Ouyang, Jiamei Liu, Yingbo Zhang, Xin Jia, Decai Zhu, Xinfang Li, Xiaowei Gao, Jie Yu, Chengjun Zhu*
Key Laboratory of Semiconductor Photovoltaic Technology of Inner Mongolia Autonomous Region, School of Physical Science and Technology, Inner Mongolia University, 235 West Daxue Street, Hohhot, 010021, China

17:00 **Improvement of solid oxide fuel cell performance by semiconductor-ionic conductor composite electrolyte** **G P1.22**
Xinfang Li, Jiamei Liu, Xin Jia, Yingbo Zhang,Decai Zhu, Yuzhao Ouyang, Xiaowei Gao, Jie Yu, Chengjun Zhu*
Key Laboratory of Semiconductor Photovoltaic Technology of Inner Mongolia Autonomous Region, School of Physical Science and Technology, Inner Mongolia University, 235 West Daxue Street, Hohhot, 010021, China

17:00 **Performance evaluation of Ca2.9-xBi0.1PrxCo4O9−δ cathode for anode-supported intermediate temperature solid oxide fuel cells** **G P1.23**
Xin Jia, Jiamei Liu, Yingbo Zhang, Decai Zhu, Xinfang Li, Yuzhao Ouyang, Xiaowei Gao, Jie Yu, Chengjun Zhu*
Key Laboratory of Semiconductor Photovoltaic Technology of Inner Mongolia Autonomous Region, School of Physical Science and Technology, Inner Mongolia University, 235 West Daxue Street, Hohhot, 010021, China

17:00 **Azaadamantane derivatives enable improved thermal and photochemical stability of multication lead halide perovskites** **G P1.24**
Victoria V. Ozerova (1,2), Nikita A. Emelianov (1), Alexey Yu. Sukhorukov (3), Lyubov A. Frolova (1), and Pavel A. Troshin (1)
(1) The Institute for Problems of Chemical Physics of the Russian Academy of Sciences (IPCP RAS), Semenov Prospect 1, Chernogolovka, 141432, Russia, (2) D. I. Mendeleev University of Chemical Technology of Russia, Miusskaya sq. 9, 125947, Moscow, Russia, (3) N. D. Zelinsky Institute of Organic Chemistry of Russian Academy of Sciences, Leninsky Prospect, 47, Moscow

17:00 **Molecular Engineering of Polytriarylamine-Based Hole-Transport Materials for p-i-n Perovskite Solar Cells: Methyl Groups Matter** **G P1.25**
Mohamed M. Elnaggar,a,b,c,* Lavrenty G. Gutsev,a,d Nikita A. Emelianov,a Petr M. Kuznetsov,a Lyubov A. Frolova,a Sergey M. Aldoshina and Pavel A. Troshine,a
a The Institute for Problems of Chemical Physics of the Russian Academy of Sciences, Semenov Prospect 1, Chernogolovka 141432, Russia b Moscow Institute of Physics and Technology, Dolgoprudny 141700, Moscow, Russia c Department of Physics, Faculty of Science, Tanta University, Tanta 31527, Egypt d Institute for Micromanufacturing, Louisiana Tech University, Ruston LA 71272, United States e Silesian University of Technology, Akademicka 2A, Gliwice 44-100, Poland

Tuesday may 31

Thermoelectrics I : Emanuel Guilmeau, Romain Viennois

09:00 INV **Superior thermoelectric performance of SiGe nanowires epitaxially integrated into thermal micro-harvesters** — G TH.1
Jose Manuel Sojo Gordillo (a), Carolina Duque Sierra (a), Gerard Gadea Diez (e), Jaime Segura (b), Valentina Bonino (b), Marc Nuñez Eroles (a), Juan Carlos Gonzalez-Rosillo (a), Denise Estrada-Wiese (c), Marc Salleras (c), Marc Chaigneau (f), Luis Fonseca (c), Alex Morata (a), Albert Tarancón (a,d).
(a) Catalonia Institute for Energy Research (IREC), Jardins de Les Dones de Negre 1, 08930, Sant Adrià de Besòs, Barcelona, Spain (b) The European Synchrotron Radiation Facility (ESRF), 71, Avenue des Martyr, 38043, Grenoble, France (c) Institute of Microelectronics of Barcelona, IMB-CNM (CSIC), C/Til□lers s/n (Campus UAB), 08193, Bellaterra, Barcelona, Spain (d) Catalan Institution for Research and Advanced Studies (ICREA), Passeig Lluís Companys 23, 08010, Barcelona, Spain (e) University of Basel, Physics Department, Klingelbergstrasse 82, 4056, Basel (f) HORIBA, France Jobin Yvon S.A.S., CS 45002, Palaiseau, France

09:30 **Electrical and thermal transport in type-I clathrate nanowires** — G TH.2
Luznik, M.*(1), Lientschnig, G. (1), Taupin, M. (1), Steiger-Thirsfeld, A. (2), and Paschen, S. (1)
(1) Institute of Solid State Physics, TU Wien, Wiedner Hauptstr. 8-10, 1040 Vienna, Austria (2) USTEM, TU Wien, Wiedner Hauptstr. 8-10, 1040 Vienna, Austria * lead presenter

09:45 **Thermoelectric properties of co-doped Tetrahedrite with Se and Ni** — G TH.3
Moço, D. *(1), Lopes, E.(1), Santos, L.(2), & Gonçalves , A.P.(1).
(1) C2TN, DECN, Instituto Superior Técnico, Univ. Lisboa, Campus Tecnológico e Nuclear (2) CQE, Instituto Superior Técnico, Univ. Lisboa, Portugal

10:00 **Strong renormalization of Ba vibrations in thermoelectric type IX clathrate Ba24Ge100** — G TH.4
R. Viennois *, M. Beaudhuin *, M. M. Koza
#* ICGM, Univ Montpellier, CNRS, ENSCM, Montpellier, France # Institut Laue Langevin, 71 Avenue des Martyrs, CS 20156, F-38042 Grenoble, France

10:15 **ELECTRICAL CONTACTS CHARACTERIZATION OF TETRAHEDRITE BASED DEVICES** — G TH.5
Rodrigo Coelho*(1), Yassine De Abreu (2), Francisco Carvalho (3) , Elsa Branco Lopes (1), António Pereira Gonçalves (1),
(1) C2TN, DECN, Instituto Superior Técnico, Universidade de Lisboa, Campus Tecnológico e Nuclear, 2695-066 Bobadela LRS, Portugal, (2) CESI, Campus d'enseignement supérieur et de formation professionnelle, 15C Av. Albert Einstein, 69100 Villeurbanne, France (3) DEEC, Instituto Superior Técnico, Universidade de Lisboa, 1049-001 Lisboa, Portugal

10:30 **Discussion Thermoelectrics I.I**

10:45 **Violating translational symmetry in thermoelectric materials** — G TH.6
Yuri Grin
Max-Planck-Institut für Chemische Physik fester Stoffe

11:00 **Seebeck coefficient of porous Silicon and graphenized porous Silicon** — G TH.7
S. Nar1-2*, A. Stolz1, D. Machon2, A. Boucherif2, N. Semmar1
1. GREMI, UMR 7344, Université d'Orléans, CNRS, Orléans, France 2. Laboratoire Nanotechnologies Nanosystèmes (LN2) - CNRS UMI-3463, Institut Interdisciplinaire d'Innovation Technologique (3IT), Université de Sherbrooke, Canada Corresponding author's E-mails: *sibel.nar@univ-orleans.fr and sibel.nar@usherbrooke.ca

11:15 **High Power Density Thermoelectric Generators with Skutterudites** — G TH.8
Soufiane El Oualid1, Iurii Kogut1, Mohamed Benyahia3, Eugen Geczi2, Uwe Kruck2,†, Francis Kosior1, Philippe Masschelein1, Christophe Candolfi1, Anne Dauscher1, Jan Dieter Koenig2, Alexandre Jacquot2, Thierry Caillat4, Eric Alleno3, Bertrand Lenoir1,
1 Institut Jean Lamour, UMR 7198 CNRS – Université de Lorraine, Campus ARTEM, 2 allée André Guinier, BP 50840, 54011 Nancy, France 2 Fraunhofer Institute for Physical Measurement Techniques IPM, 79110 Freiburg, Germany 3 Univ Paris Est Creteil, CNRS, ICMPE, UMR 7182, 2 rue Henri Dunant, 94320 Thiais, France 4 Jet Propulsion Laboratory, California Institute of Technology, Pasadena, CA 91109, USA

11:30 INV **Recent advances and progress in thermoelectric sulfides** — G TH.9
Emmanuel Guilmeau
Normandie Univ, ENSICAEN, UNICAEN, CNRS, CRISMAT, 14000 Caen, France

12:00 **Discussion Thermoelectrics I.II**

12:15 **Lunch and Plenary**

Catalysis : Sebatien Fontana, Pierre Ruterana

15:00 INV **Development of three-dimensional nitrogen-doped graphenic materials: towards PEMFC catalysts without platinum** — G C.1
Sébastien Fontana (1), Lilian Moumaneix(1, 2), Franvois Lapicque (2), Claire Hérold (1)
(1) IJL CNRS UMR 7198, Université de Lorraine, 2 allée André Guinier 54000 Nancy (2) LRGP CNRS UMR 7274, 1 rue Grandville 54001 Nancy

15:30 **Evaluation of CO2 Absorption by a New Barium Nickel Oxycarbonate** — G C.2
D. Gutiérrez-Martín 1, M. Hernando 1, A. Torres-Pardo 1,2, J.M. González-Calbet 1,2, A. Varela 1 and M. Parras 1
1. Inorganic Chemistry Department, Universidad Complutense de Madrid, Spain,
2. ICTS National Center for Electronic Microscopy, Universidad Complutense de Madrid, Spain

15:45 **Second harmonic generation (SHG) from semiconductors nanopowders: a polarization and an intensity profile studies** — G C.3
Faheem Ahmed (1), Mohammed Benali Kanoun (1), Christophe Moulin (1), Christian Jonin (2), Pierre-Francois Brevet (2), Chawki Awada*(1)
(1) Department of Physics, College of Science, King Faisal University, P.O. Box 400, Al-Ahsa 31982, Saudi Arabia (2) Institut Lumière Matière, Université de Lyon, UMR 5306 CNRS and Université Claude Bernard Lyon 1, France

16:00 **Tailoring the morphology of cost-effective vanadium diboride through cobalt substitution for highly efficient alkaline water** — G C.4
Ebrahim Sadeghi1,2,*, Naeimeh Sadat Peighambardoust1, and Umut Aydemir1,3
1 Koç University Boron and Advanced Materials Application and Research Center (KUBAM), Sariyer, Istanbul, 34450, Turkey 2 Graduate School of Sciences and Engineering, Koç University, Sariyer, Istanbul, 34450, Turkey. 3 Department of Chemistry, Koç University, Sariyer, Istanbul, 34450, Turkey

16:15 **Computational investigation of Fe-doped NiOOH electrocatalysts** — G C.5
Zheng-Da He, Rebekka Tesch, Mohammad J. Eslamibigoli, Michael Eikerling, Piotr Kowalski
Institute of Energy and Climate Research (IEK-13), Forschungszentrum Jülich, Wilhelm-Johnen-Straße, 52425 Jülich, Germany, Institute of Energy and Climate Research (IEK-13), Forschungszentrum Jülich, Wilhelm-Johnen-Straße, 52425 Jülich, Germany, Institute of Energy and Climate Research (IEK-13), Forschungszentrum Jülich, Wilhelm-Johnen-Straße, 52425 Jülich, Germany, Institute of Energy and Climate Research (IEK-13), Forschungszentrum Jülich, Wilhelm-Johnen-Straße, 52425 Jülich, Germany, Institute of Energy and Climate Research (IEK-13), Forschungszentrum Jülich, Wilhelm-Johnen-Straße, 52425 Jülich, Germany, Jülich Aachen Research Alliance, JARA Energy & Center for Simulation and Data Science (CSD), Jülich, Germany

16:30 INV **Boosting heterogeneous catalyst discovery by structurally constrained Machine Learning models** — G C.6
Alexey Korovin, Innokentiy Humonen, Artem Samtsevich, Roman Eremin, Artem Vasilyev, Vladimir Lazarev, Semeon Budennyy
AIRI, Moscow, Russia

17:00 **Discussion Catalysis**

Fuel Cells : Adam Lee, Jianbing Huang

09:00 INV **Ultrafine and Highly Dispersed PtRu Alloy on Polyacrylic Acid Grafted Carbon Nanotube@Tin Oxide Core/shell Composite for Direct** — G PH.1
Yaqin Sang, Renyan Zhang, Jian Yang, Chunyan Zhao, and Hui Xu*
Institute of Advanced Synthesis, School of Chemistry and Molecular Engineering, Nanjing Tech University, Nanjing 211816, China.

09:30 **Goal oriented materials optimisation using deep reinforcement learning** — G PH.2
Felix Bennemann
Prof. Nicholas M Harrison, Imperial College London

09:45 **Cubic silicon carbide/zinc oxide heterostructure fuel cells** — G PH.3
Yueming Xing, Enyi Hu, Faze Wang, Naveed Muhammad, Baoyuan Wang, Jun Wang, Ammara Maryam, Muhammad Naveed Rasheed, Muhammad Asghar, Chen Xia, Sining Yun, and Bin Zhu
Engineering Research Center of Nano-Geo Materials of Ministry of Education, Faculty of Materials Science and Chemistry, China University of Geosciences, No. 388 Lumo Road, Wuhan 430074, China

10:00 **Standardized Procedures Important for Improving Low-Temperature Ceramic Fuel Cell Technology** — G PH.4
Xinlei Yang, Fan Yang, Bin Zhu, Jingjing Liu, Yifei Zhang, Wanli Sun
Jiangsu Provincial Key Laboratory of Solar Energy Science and Technology, School of Energy & Environment, Southeast University

10:15 **Self-assembled SrCo0.8Fe0.2O3–δ/Fe3O4 heterostructure proton membrane for advanced semiconductor ionic fuel cell** — G PH.5
Nabeela Akbar1, Sara Paydar1, Wu Yan1, Bin Zhu1,2
1. Engineering Research Center of Nano-Geo Materials of Ministry of Education, Faculty of Materials Science and Chemistry, China University of Geosciences, 388 Lumo Road, Wuhan 430074, China 2. Jiangsu Provincial Key Laboratory of Solar Energy Science and Technology/ Energy Storage Joint Research Center, School of Energy and Environment, Southeast University, No.2 Si Pai Lou, Nanjing 210096, China.

10:30 **Discussion Fuel Cells I**

11:00 **Tailoring transition metal elements to improve the stability of the semiconductor membrane fuel cell** — G FC.7
Sun Wanli, Yang Fan, Zhu Bin, Liu Jingjing, Zhang Yifei, Yang Xinlei
Jiangsu Provincial Key Laboratory of Solar Energy Science and Technology
School of Energy & Environment Southeast University

11:15 **Surface-Engineered Homostructure for Enhancing Proton Transport** — G FC.8
Enyi Hu1, Faze Wang1, Jun Wang1, Bin Zhu1, Peter Lund2
1Jiangsu Provincial Key Laboratory of Solar Energy Science and Technology, School of Energy & Environment, Southeast University, Nanjing, 210096, China.
2Department of Engineering Physics/Advanced Energy Systems, School of Science, Aalto University, 00076 Aalto, Espoo, Finland.

11:30 **WO3-LSCF composite electrolyte with high ionic conductivity for low temperature solid oxide fuel cell** — G FC.9
Xiaoqian Jin , Wenjing Dong , Chen Xia , Baoyuan Wang , Xunying Wang
Hydrogen, as a secondary energy, can be produced by electrolyzing water using surplus renewable energy (eg. solar or wind energy), and its combustion product is only water. Solid oxide fuel cell (SOFC) can transform hydrogen into electricity efficiently. What's more, compared with proton exchange membrane fuel cell, SOFC possesses the advantage of needless of precious metal catalyst and low requirement for hydrogen purity. However, high work temperature limits its commercialization. Increase ionic conductivity of electrolyte can effectively decrease the SOFC work temperature. Recently, constructing heterointerface has been an emerging approach for increasing electrolyte materials conductivity. [1-6]. The most typical example is YSZ-SrTiO3 (STO) 2D heterostructure which was reported by Garcia Barriocanal et al [1, 2]. The O2- conductivity of heterointerface between YSZ film and SrTiO3 film was nearly 8 orders of magnitude enhancement than that of bulk YSZ. Besides, other 2D heterostructure materials (eg. YSZ-MgO and Ce0.8Sm0.2O2-δ-Al2O3) also showed excellent ionic conductivity [3, 4]. Recently, 3D heterostructure materials were constructed extensively, and they displayed enhanced ionic conductivity compared with pure phase material under low temperature. The O2- conductivity of SrTiO3 semiconductor was enhanced about 5 orders of magnitude by being covered with an amorphous core-shell heterostructure [5]. Large number of oxygen vacancies were detected in the shell layer, which was considered as the main reason for the excellent O2- conductivity. CeO2/CeO2−δ core-shell heterostructure electrolyte exhibited the proton conductivity of 0.16 S cm-1 under 520 °C [6]. It was considered that oxygen vacancies and charged layers at the interface mainly contributed to the excellent proton conductivity. Recently, we constructed 3D YSZ-LaNiO3 heterostructure electrolyte, and the power density of corresponding SOFC achieved 1045 mW cm-2 at 600 °C [7]. Study results indicated that the heterointerface between YSZ and LaNiO3 provided a large number of oxygen vacancies which are beneficial to enhance O2- conductivity. It has been reported that constructing built-in electric field can effectively prevent electrons transport across electrolyte and accelerate ion conduction. Here we adopted n-type WO3 and p-type LSCF to constructing p-n heterojunction and studied the effect of heterostructure on the SOFC performance.

11:45 **How ternary Li-oxide coatings affect the interfacial dynamics between LiCoO2 and Li7La3Zr2O12 in thin-film solid-state cells** — G FC.10
André Müller, Abdessalem Aribia, Moritz H. Futscher, and Yaroslav E. Romanyuk
Laboratory for Thin Films and Photovoltaics Empa-Swiss Federal Laboratories for Materials Science and Technology, Überlandstrasse 129, Dübendorf CH-8600, Switzerland

12:00 INV **Low temperature ceramic fuel cell with NASICON Na5YSi4O12 and semiconductor Ni0.8Co0.15Al0.05LiO2 composite electrolyte** — G FC.11
Yong Yu1, Jianbing Huang1,*, Bin Zhu1,2,*
1.State Key Laboratory of Multiphase Flow in Power Engineering, Xi'an Jiaotong University, Xi'an 710049, Shaanxi, China, 2.Jiangsu Provincial Key Laboratory of Solar Energy Science and Technology/Energy Storage Joint Research Center, School of Energy & Environment, Southeast University, Nanjing 210096, Jiangsu, China

12:30 **Discussion Fuel Cells II**

12:45 **Lunch and Plenary**

Photovoltaics : Pierre Ruterana, Song Yi Park

15:00 INV **Organic bilayer-heterojunctions for efficient indoor photovoltaic applications** — G PH.1
Song Yi Park, Chiara Labanti, Joel Luke, Yi-Chun Chin, Ji-Seon Kim
Imperial College London

15:30 **Investigation of Electronic Properties of Grains and Grain Boundaries of CsPbBr3 Halide Perovskite Thin Films** — G PH.2
Chandra Shakher Pathak and Eran Edri
Department of Chemical Engineering and Ilse Katz Institute for Nano-scale Science and Technology, Ben-Gurion University of the Negev, Israel

15:45 **Effect of microstructure on hydrogenation pathways illustrated by correlative high-resolution SIMS, TEM, and optical microscopy** — G PH.3
Andersen, D.* (1), Chen, H. (2), Cressa, L. (1), Wirtz, T. (1), Schmitz, G. (2), & Eswara, S. (1)
(1) Advanced Instrumentation for Nano-Analytics (AINA), Materials Research and Technology Department, Luxembourg Institute of Science and Technology (LIST), Luxembourg, (2) Institute for Materials Science (IMW), Department for Materials Physics, University of Stuttgart, Germany * lead presenter

16:00 **Asymmetrical supercapacitor based on WO3 nanorods grown by one-step hydrothermal synthesis** **G PH.4**
G. Mineo1-2, M. Scuderi3, S. Mirabella1-2, E. Bruno1-2
1 Dipartimento di Fisica e Astronomia “Ettore Majorana”, Università degli Studi di Catania, via S. Sofia 64, 95123 Catania, Italy, 2 CNR-IMM (Università di Catania), via S. Sofia 64, 95123 Catania, Italy, 3 IMM-CNR, VIII strada 5, 95121 Catania, Italy,

16:15 **Contribution of ion beam analysis in multilayer Si1-xCx:H/W solar selective absorber materials characterization** **G PH.5**
Babacar DIALLO 1, Aïssatou DIOP 2,4, Danielle NGOUE 2,3, Aurélien BELLAMY 1, Olivier WENDLING 1, Paul SIGOT 1, Sebastien. QUOIZOLA 2, Antoine GOULLET 5, Audrey SOUM-GLAUDE 2, Eric TOMASELLA 4, Laurent THOMAS 2,3, Thierry SAUVAGE 1
1 CEMHTI (Conditions Extrêmes et Matériaux), Orléans, France 2 PROMES-CNRS (Laboratory of PROcess, Materials, Solar Energy) -Perpignan/Font-Romeu- Odeillo-Via, France 3 Université de Perpignan, Perpignan, France 4 ICCF (Institut de Chimie de Clermont-Ferrand), Aubière, France 5 IMN (Institut des Matériaux Jean Rouxel), Nantes, France

16:30 **Photoelectron Spectroscopy provides insights in perovskite solar cells from single layers to buried interfaces of a full device** **G PH.6**
Maheu, C.* (1), Hellmann, T. (1), Baretzky, C. (2), Sirtl, M. T. (3), Bein, T. (3), Würfel, U. (2), Mayer, T. (1), Hofmann, J. P. (1).
(1) Surface Science Laboratory, Department of Materials and Earth Sciences, Technical University of Darmstadt, 64287 Darmstadt, Germany (2) Freiburg Materials Research Center (FMF), University of Freiburg, Stefan-Meier-Str. 21, 79104, Freiburg, Germany (3) Department of Chemistry and Center for NanoScience (CeNS), University of Munich (LMU), Butenandtstr. 11, 81377 Munich, Germany * lead presenter

16:45 INV **Zr-doped Indium Oxide as transparent electrodes for photovoltaics** **G PH.7**
Melanie Micali (1,2), Marco Leonardi (1,3), Salvatore Lombardo (3), Giuseppe Bengasi (4), Claudio Colletti (4), Virginia Boldrini (5), Esther Alarcón Lladó (6), Antonio Terrasi (1,2)
1) Dipartimento di Fisica, Università di Catania, via S. Sofia 64, I-95123, Catania, Italy , 2) IMM-CNR, Sede Catania (Università), via S. Sofia 64, 95123 Catania, Italy, 3) Istituto per la Microelettronica e Microsistemi- Consiglio Nazionale delle Ricerche, Zona Industriale, Ottava Strada n.5, 95121 Catania, Italy, 4) ENEL Green Power, Contrada Blocco Torrazze sn- Z.I., 95121 Catania, Italy, 5) CNR-IMM Bologna via Gobetti 101, 40129 Bologna (Italy) , 6) AMOLF physics of functional matter, Science Park 104, NL1098XG, Amsterdam, The Netherland,

17:15 **Discussion Photovoltaics**

18:00 **E-MRS EU-40 Materials Prize & MRS Mid-Career Researcher Award Presentations**

Thursday june 2

Batteries I : Adam Lee, Guanjie He

09:00 INV **Cathode materials for Zn-ion batteries** **G B1.1**
Guanjie He
School of Engineering and Materials Science, Queen Mary University of London

09:30 **Hydroxysulfates as cathode materials for rechargeable batteries** **G B1.2**
Shashwat Singh1*, Valérie Pralong2, and Prabeer Barpanda1
1. Faraday Materials Laboratory, Materials Research Centre, Indian Institute of Science, Bangalore – 560012, India 2. Normandie University, Ensicaen, Unicaen, CNRS, Crismat, 14000 Caen, France

09:45 **Electronic Self-Passivating Behavior of Li-LIPON Solid-Electrolyte Interphases from Defect Calculations** **G B1.3**
Yuheng Li, Pieremanuele Canepa, Prashun Gorai
National University of Singapore, National University of Singapore, Colorado School of Mines

10:00 **A 3-D tunnel type Intercalation Cathode Material for Lithium-Ion Battery** **G B1.4**
Sai Pranav Vanam*, Prabeer Barpanda
Faraday Materials Laboratory, Materials Research Centre, Indian Institute of Science, Bangalore- 560012, India

10:15 **Conductor:Insulator Interfaces – Conductivity Enhancement in LiBH4:Oxide Nanocomposites** **G B1.5**
Thomas Scheiber, H. Martin R. Wilkening
Institute of Chemistry and Technology of Materials, Graz University of Technology (NAWI Graz), Stremayrgasse 9, 8010 Graz, Austria

10:30 **Discussion Batteries I.I**

10:45 **Anionic redox activity in lithium metal bisulfate cathodes: A first-principles investigation** **G B1.6**
Pawan Kumar Jha(1)*, Shashwat Singh(1), Mayank Srivastava(1), Prabeer Barpanda(1), Gopalakrishnan Sai Gautam(1).
1. Indian Institute of Science, Bangalore 560012, India

11:00 **Lithiated Mn and Fe based nitrides as competitive negative materials for Li-ion battery** **G B1.7**
Y. Zhou, N. Emery, J.P. Pereira-Ramos, O. Nguyen, R. Baddour-Hadjean
Institut de Chimie et des Matériaux Paris Est (ICMPE), UMR 7182 CNRS-Université Paris-Est, Technocentre Renault, Institut de Chimie et des Matériaux Paris Est (ICMPE), UMR 7182 CNRS-Université Paris-Est, Institut de Chimie et des Matériaux Paris Est (ICMPE), UMR 7182 CNRS-Université Paris-Est, Technocentre Renault, Institut de Chimie et des Matériaux Paris Est (ICMPE), UMR 7182 CNRS-Université Paris-Est

11:15 **The impact of coating material on advanced SnO2 nanowire-based lithium-ion battery anodes** **G B1.8**
Jasmin-Clara Bürger [1], Serin Lee [2], Sebastian Gutsch [1], Frances M. Ross [2], Margit Zacharias [1]
[1] Laboratory for Nanotechnology, Department of Microsystems Engineering (IMTEK), University of Freiburg, Georges-Koehler-Allee 103, 79110 Freiburg, Germany, [2] Department of Materials Science and Engineering, Massachusetts Institute of Technology (MIT), 77 Massachusetts Avenue, Cambridge, MA 02139, USA

11:30 INV **Exploration of Li-P/B-S-O/Cl system for discovery of new solid electrolyte** **G B1.9**
Audric Neveu1, Vincent Pelé3, Christian Jordy3 and Valerie Pralong1,2*
1-Normandie Univ, Ensicaen, Unicaen, CNRS, Crismat, 14000 Caen, France
2-Réseau sur le Stockage Electrochimique de l’Energie (RS2E), FR CNRS 3459, France 3-SAFT, 111-113 Bd Alfred Daney 33074 Bordeaux, France

12:00 **Discussion Batteries I.II**

12:15 **Lunch and Plenary**

Batteries II : Valerie Pralong, Arumugam Manthiram

15:00 INV **Spray-Drying Synthesis of Na2+2xFe2-x(SO4)3: Electrochemistry, Thermodynamic stability and humidity induced phase transition** — G B2.1
Pubali Barman* (1), Debasmita Dwibedi (1,2), K Jayanti (3), Sher Singh Meena (4), Supreeth Nagendran (5,6), Alexandra Navrotsky (3), & Prabeer Barpanda (1)
(1) Indian Institute of Science, India, (2) The University of Tokyo, Japan, (3) Arizona State University, United State, (4) Bhabha Atomic Research Centre, India, (5) Bangalore University, India, (6) University of Cambridge, United Kingdom

15:30 **Structure-Phase Transformations in LiF Crystals Initiated by Nuclear Reactions** — G B2.2
Ibragimova E.M., Buzrikov Sh.N., Iskandarov N.E., Mussaeva M.A., Nazarov Kh.T.
Ibragimova E.M.1,2, Buzrikov Sh.N.1, Iskandarov N.E.2, Mussaeva M.A.1, Nazarov Kh.T.2. 1 Institute of nuclear physics, Academy of sciences, Tashkent, Uzbekistan, 2 Center for advanced technologies, Ministry of innovative development, Tashkent, Uzbekistan

15:45 **The batteries' new clothes - Li and H dynamics in Li2OHCl as seen by spin-lattice relaxation NMR** — G B2.3
Jonas Spychala,* H. Martin R. Wilkening
Institute for Chemistry and Technology of Materials, Graz University of Technology (NAWIGraz), Stremayrgasse 9, 8010 Graz, Austria

16:00 **Regulating anode self-discharge for boosting energy density of aqueous Mg batteries** — G B2.4
Min Deng, Linqian Wang, Bahram Vaghefinazari, Darya Snihirova, Sviatlana V. Lamaka, Daniel Höche, Mikhail L. Zheludkevich
Institute of Surface Science, Helmholtz-Zentrum Hereon, 21502 Geesthacht, Germany, Institute of Materials Science, Faculty of Engineering, Kiel University, 24143 Kiel, Germany.

16:15 **How K metal governs electrochemical performance and SEI formation in half-cells** — G B2.5
Caracciolo, L.(1), Gachot, G.(2,3), Touja, J.(3,4), Stievano, L.(3,4), Monconduit, L.(3,4), Martinez, H.(1,3), Madec, L.*(1,3)
(1) Universite de Pau et des Pays de l'Adour, E2S UPPA, CNRS, IPREM, Pau, France, (2) LRCS, Université de Picardie Jules Verne, 80039 Amiens, France, (3) Réseau sur le Stockage Electrochimique de l'Energie, CNRS FR3459, Amiens, France, (4) ICGM, Université de Montpellier, CNRS, Montpellier, France

16:30 **Discussion Battery II**

Friday june 3

Batteries III : Adam Lee, Yuping Wu

09:00 INV **The Detrimental Impact of Local Disorder on Ion Transport: Case Study on Nanocrystalline and Amorphous Li10GeP2S12** — G B3.1
Katharina Hogrefe1*, Lukas Schweiger,1 Bernhard Gadermaier1, Jennifer L. M. Rupp2,3, and H. Martin R. Wilkening1
1 Institute for Chemistry and Technology of Materials, Christian Doppler Laboratory for Lithium Batteries, Graz University of Technology (NAWI Graz), 8010 Graz, Austria, 2 Electrochemical Materials, Department of Materials Science and Engineering, Massachusetts Institute of Technology, Cambridge, MA 02139, USA, 3 Electrochemical Materials, Department of Electrical Engineering & Computer Science, Massachusetts Institute of Technology, Cambridge, MA 02139, USA

09:30 **To tame polysulfides shuttling by modification of separators with three-dimensional interconnected graphene-like carbon and ruti** — G B3.2
Shuang Xia, Yusong Zhu, Lijun Fu, Yuping Wu
nanjing tech university

09:45 **Rational design of organic redox-active materials for high-capacity and high-rate potassium-ion batteries** — G B3.3
Pavel A. Troshin
(1) Faculty of Chemistry, Silesian University of Technology, Strzody 9, 44-100 Gliwice, Poland (2) Institute for Problems of Chemical Physics of RAS, Acad. Semenov str.1, Chernogolovka 142432 Russia.

10:00 **Analysis of Si surface/polymers interface for self-healed next generation Lithium ion batteries** — G B3.4
a. Rita Maji b. Michele Aparecida Salvador c. Elena Degoli d. Alice Ruini e. Rita Magri
a. Dipartimento di Scienze e Metodi dell'Ingegneria, Università di Modena e Reggio Emilia, Via Amendola 2 Padiglione Tamburini, I-42122 Reggio Emilia, Italy b. Dipartimento di Scienze Fisiche, Informatiche e Matematiche sede ex-Fisica, Università di Modena e Reggio Emilia,Via Campi 213/A, 41125 Modena c. Dipartimento di Scienze e Metodi dell'Ingegneria, Università di Modena e Reggio Emilia, Via Amendola 2 Padiglione Morselli, I-42122 Reggio Emilia, Italy Centro Interdipartimentale En&Tech, Via Amendola 2 Padiglione Morselli, I-42122 Reggio Emilia, Italy Centro S3, Istituto Nanoscienze-Consiglio Nazionale delle Ricerche (CNR-NANO), Via Campi 213/A, 41125 Modena, Italy d. Dipartimento di Scienze Fisiche, Informatiche e Matematiche sede ex-Fisica, Università di Modena e Reggio Emilia,Via Campi 213/A, 41125 Modena e. Dipartimento di Scienze Fisiche, Informatiche e Matematiche sede ex-Fisica, Università di Modena e Reggio Emilia,Via Campi 213/A, 41125 Modena

10:15 **Study the high voltage performance of Li-ion conducting Li3PO4 coated NMC811 cathode material for rechargeable Li polymer batter** — G B3.5
Himani Gupta
Faraday Materials Laboratory, Materials Research Centre, Indian Institute of Scien ce Bangalore-560012, India

10:30 **Discussion Battery III.I**

10:45 **High-Entropy Disordered Rock-Salt: Tailoring the Potential Window of Electrodes for Li-Ion Batteries** — G B3.6
Qingsong Wang, Ben Breitung, Horst Hahn, Robert Kruk, Abhishek Sarkar
Chair of Inorganic Active Materials for Electrochemical Energy Storage, University of Bayreuth, Universitaetsstr. 30, 95447 Bayreuth, Germany Bavarian Center for Battery Technology (BayBatt), Universitaetsstr. 30, 95447 Bayreuth, Germany Institute of Nanotechnology, Karlsruhe Institute of Technology, 76344 Eggenstein-Leopoldshafen, Germany Joint Research Laboratory Nanomaterials – Technische Universität Darmstadt and Karlsruhe Institute of Technology, 64287 Darmstadt, Germany

11:00 **Bio-based poly(hydroxyurethanes) networks as polymer electrolyte for solid-sate lithium batteries** — G B3.7
Ashish Raj, Dr. Satyannarayana Panchireddy, Dr. Bruno Grignard, Dr. Christophe Detrembleur, Prof. Jean-Francois Gohy
Institute of Condensed Matter and Nanoscience (IMCN), UCLouvain, Place L. Pasteur 1, 1348 Louvain-la-Neuve, Belgium., Center for Education and Research on Macromolecules (CERM), CESAM Research Unit, University of Liège, allée du 6 août, Building B6A, Agora Square, 4000 Liège, Belgium

11:15 **Tip-Enhanced Raman Spectroscopy of inorganic compounds in energy devices: a versatile approach for nanometric chemical insights** — G B3.8
Juan Carlos Gonzalez-Rosillo, Patrick Hsia, Marc Chaigneau, Alex Morata, Albert Tarancón
Catalonia Institute for Energy Research (IREC), Jardins de les Dones de Negre 1, Planta 2, 08930, Sant Adrià del Besòs, Barcelona, Spain , HORIBAFrance , Palaiseau, France, HORIBAFrance , Palaiseau, France, Catalonia Institute for Energy Research (IREC), Jardins de les Dones de Negre 1, Planta 2, 08930, Sant Adrià del Besòs, Barcelona, Spain, Catalonia Institute for Energy Research (IREC), Jardins de les Dones de Negre 1, Planta 2, 08930, Sant Adrià del Besòs, Barcelona, Spain

11:30 INV **Optimized electrode formulation for enhanced performance of graphite in K-ion batteries.** — G B3.9
Badre Larhrib (a), Lénaïc Madec (a,c), Laure Monconduit (b,c), Hervé Martinez (a,c)
a Université de Pau et des Pays de l'Adour, E2S UPPA, CNRS, IPREM, Pau, France b ICGM, Université de Montpellier, CNRS, Montpellier (France) c Réseau sur le Stockage Electrochimique de l'Energie, CNRS FR3459, Amiens, France

12:00 **Discussion Battery III.I and Closing , Symposium Chairs**