

Water splitting performance of selenium based Chevrel phase: CoW_6Se_8

Gencer, A.* (1), Surucu, G. (2), Ozel, F. (3).

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* lead presenter

The energy requirement of the world is constantly increasing and the studies for the alternative energy sources are ongoing. The hydrogen energy is one of the promising solutions for these alternative energy sources due to the high abundance of the hydrogen on the earth. However, the hydrogen must be produced and the photocatalytic hydrogen production is one of the methods to generate hydrogen from water using sun light. For photocatalytic hydrogen production, the photocatalysis must have a suitable band gap and appropriate valence and conduction bands potentials to reduction and oxidations reactions [1]. In this study, the selenium based chevrel phase CoW_6Se_8 has been considered for the water splitting performance. The Chevrel phases that are discovered by Chevrel and Sergent have superior properties composing with three refractory metals [2]. The Chevrel phases have $\text{M}_x\text{Mo}_y\text{Ch}_8$ formula where M is a metal and Ch is a chalcogen with y as 3 or 6 and x as 0, 1, 2, 3, or 4 values in a Chevrel phase [3]. In literature, the sulphur based Chevrel phases have been investigated for the superconductivity, cathode material properties, hydrogen production properties, etc. [4-6]. However, there is a lack of interest for selenium based Chevrel phases in the literature. In addition, the Chevrel phases are considered with molybdenum atoms where tungsten atoms could be used instead of molybdenum atoms. In this study, CoW_6Se_8 have been examined using the Density Functional Theory (DFT) [7,8] to reveal its structural and electronic properties. The DFT is a powerful theory to get the materials properties without any input from experimental values. To get detailed water splitting performance, the hybrid functional [9] calculations have been performed and the results have been analyzed. The selenium based chevrel phase CoW_6Se_8 is a potential candidate material for water splitting applications. This work is supported by TUBITAK under project number 120F305.

References

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European Materials Research Society

Spring Meeting 2022

May 30 | June 3
Virtual Conference

SYMPOSIUM I

Sustainable approaches for renewable energy conversion
to fuels and chemicals

Symposium Organizers :

Ann MAGNUSON, Department of Chemistry - Ångström Laboratory

Bert M. WECKHUYSEN, Utrecht University

Francisco FABREGAT-SANTIAGO, Institute of Advanced Materials
(INAM) Universitat Jaume I

Frédéric CHANDEZON, IRIG Dir



**XOP
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Monday may 30

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

Artificial Photosynthesis I : MW

09:00 **INV Kinetic challenges for solar driven fuel synthesis - matching photoexcited state and catalysis timescales** I 1.1
James Durrant
Department of Chemistry, Centre for Processable Electronics, Imperial College London, London W12 0BZ, U.K. and SPECIFIC IKC, College of Engineering, University of Swansea, Swansea, U.K. E-mail: j.durrant@imperial.ac.uk

09:30 **INV Molecular Mechanisms of Artificial Photosynthesis** I 1.2
Leif Hammarström
Department of Chemistry – Ångström Laboratory, Uppsala University, Box 523, S75120 Uppsala, Sweden

10:00 **Oligoethylene glycol side chains increase charge generation in organic semiconductor nanoparticles photocatalyst** I 1.3
Kosco, J. (1), Gonzalez-Carrero, S.* (2), Howells, C. T. (1), Zhang, W. (1), Moser, M. (3), Sheelamanthula, R. (1), Zhao, L. (1), Willner, B. (3), Hidalgo, T. C. (1), Faber, H. (1), Purushothaman, B. (1), Sachs, M. (2), Cha, H. (2), Sougrat, R. (1), Anthopoulos, T. D. (1), Inal, S. (1), Durrant, J. R. (2), McCulloch, I. (1,3)
(1) King Abdullah University of Science and Technology (KAUST), Thuwal, Kingdom of Saudi Arabia (2) Department of Chemistry and Centre for Processable Electronics, Imperial College London, London, UK* (3) Department of Chemistry University of Oxford, Oxford, UK

10:15 **Periodic micropillar patterned FTO covered with hematite nanorod arrays for efficient photoelectrochemical water splitting** I 1.4
Nak Hyun Kim*(1), Sucheol Ju(1), Jaemin Park(1).
(1) Korea University, South Korea *lead presenter

10:30 **Discussion**

10:45 **Coffee**

Artificial Photosynthesis II : LH

11:00 **INV Molecular approaches to artificial photosynthesis and solar fuel production** I 2.1
Murielle Chavarot-Kerlidou
LCBM, Université Grenoble Alpes/CNRS/CEA Grenoble, France

11:30 **Photosynthesis re-wired on the pico-second timescale** I 2.2
Laura T. Wey2+, Tomi K. Baikie1+, Hitesh Medipally3, Erwin Reisner4, Marc M. Nowaczyk3, Richard H. Friend1, Christopher J. Howe2*, Christoph Schnedermann1*, Akshay Rao1*, Jenny Z. Zhang4*
1 - Cavendish Laboratory, University of Cambridge, J. J. Thomson Avenue, Cambridge, CB3 0HE, UK 2 - Department of Biochemistry, University of Cambridge, Tennis Court Road, Cambridge, CB2 1QW, UK 3 - Plant Biochemistry, Ruhr-Universität Bochum, Universitätsstrasse 150, 44780 Bochum, Germany 4 - Department of Chemistry, University of Cambridge, Lensfield Road, Cambridge, CB1 2EW, UK

11:45 **Organic Polymer Dots for Photocatalysis** I 2.3
Haining Tian
Department of Chemistry - Ångström Lab., Uppsala University, Box 523, 75120 Uppsala, Sweden

12:00 **Discussion**

12:15 **Lunch**

Water decontamination and new catalysts : SM

15:00 **Engineering solar-driven photocatalysts based on g-C3N4 for the removal of water pollutants** I 3.1
María Bernechea1,2,3,4*, María Aguirre1,2, M. Pilar Lobera1,2,3
1 Instituto de Nanociencia y Materiales de Aragón (INMA) CSIC-Universidad de Zaragoza, Zaragoza, Spain 2 Departamento de Ingeniería Química y Tecnologías del Medio Ambiente, Universidad de Zaragoza, Zaragoza, Spain 3 Networking Biomedical Research Centre of Bioengineering, Biomaterials and Nanomedicine (CIBER-BBN), Madrid, Spain 4 ARAID, Zaragoza, Spain * mbernechea@unizar.es

15:15 **Perovskite-Type Oxynitride Nanofibers Performing Photocatalytic Oxygen and Hydrogen Generation** I 3.2
Hofmann, A.*, Weiss, M., Timm, J., Marschall, R.
University of Bayreuth, Universitätsstr. 30, 95447 Bayreuth, Germany * lead presenter

15:30 **Mesoporous High-Entropy Oxide Thin Film Electrodes: Electrocatalytic Water Oxidation on High-Surface Area Spinel** I 3.3
Marcus Einert*, Maximilian Mellin, Niloufar Bahadorani, Christian Dietz, Stefan Lauterbach, and Jan P. Hofmann*
Surface Science Laboratory, Department of Materials and Earth Sciences, Technical University of Darmstadt, Otto-Berndt-Strasse 3, 64287 Darmstadt, Germany Institute of Materials Science, Physics of Surfaces, Technical University of Darmstadt, Alarich-Weiss-Strasse 2, 64287 Darmstadt, Germany Institute for Applied Geosciences, Geomaterial Science, Technical University of Darmstadt, Schnittpahnnstrasse 9, 64287 Darmstadt, Germany

15:45 **Metallochaperone-like effect of a hydrophobic ligand in FeOx/BiVO4 nano hybrid formation for photoelectrochemical water oxidation** I 3.4
Timea Benkó (1), Shaohua Shen (2), Miklós Németh (1), Akos Szamosvölgyi (3), András Sápi (3), György Sáfrán (4), Sahir M. Al-Zurajji (1), József Sándor Pap (1) (1) Centre for Energy Research, Surface Chemistry and Catalysis Department, 29-33 Konkoly-Thege Street, H-1121 Budapest, Hungary, (2) International Research Center for Renewable Energy (IRCRES), State Key Laboratory of Multiphase Flow in Power Engineering (MFPE), Xi'an Jiaotong University, Xi'an, Shaanxi 710049, China, (3) University of Szeged, Interdisciplinary Excellence Centre, Department of Applied and Environmental Chemistry, H-6720, Rerrich Béla tér 1, Szeged, Hungary, (4) Centre for Energy Research, Institute of Technical Physics and Materials Science, Thin Film Physics Department, Konkoly-Thege street 29-33, 1121 Budapest, Hungary

16:00 **Role of anion etching and heteroatom incorporation in cobalt silicate precatalyst for improved OER** I 3.5
Dr. Debashrita Sarkar1,2 ,Dr. Sagar Ganguli1,3 ,Ayan Mondal1 ,Prof. Venkataramanan Mahalingam1
1- Indian Institute of Science Education and Research Kolkata, India 2- Université de Paris, France 3- Uppsala University, Sweden

16:15 **Discussion**

16:30 **Coffee**

I : Francisco Fabregat-Santiago & Ann Magnusson

16:45 **Energy Generation From Active Heteroatom (N and P) Based Porous Carbon: Hydrazine Oxidation Reaction** I P1.1
Nisha Dhiman, Kumud Malika Tripathi, Paritosh Mohanty
Nisha Dhiman: Indian Institute of Technology, Roorkee and Indian Institute of Petroleum and Energy, Visakhapatnam Paritosh Mohanty: Indian Institute of Technology, Roorkee Kumud Malika Tripathi: Indian Institute of Petroleum and Energy, Visakhapatnam

16:45 **Enhanced elastocaloric cooling performances in gradient nanograined NiTi shape memory alloy** I P1.2
Junyu Chen
State Key Laboratory of Tribology, Department of Mechanical Engineering, Tsinghua University, Beijing 100084, China

16:45 **A polyphenolic interface layered Al-fluorinated organic compounds for improved combustion properties for energetic applications** I P1.3
Virendrakumar G. Deonikar, Hern Kim* Lead presenter: Virendrakumar G. Deonikar, Email: virendradeonikar@gmail.com *Corresponding author: Prof. Hern Kim, Email: hernkim@mju.ac.kr Environmental Waste Recycle Institute, Department of Energy Science and Technology, Myongji University, Yongin, Gyeonggi-do 17058, Republic of Korea

16:45 **Catalytic performance of ionic liquid on the carboxylation of glycerol to glycerol carbonate with carbon dioxide** I P1.4
Atul A. Pawar, Hern Kim*
Myongji University Yongin, Republic of Korea.

16:45 **Transition metal-carbon composites as an efficient electrocatalyst for nitrogen reduction to ammonia** I P1.5
Rajendra B. Mujmule, Hern Kim*
Department of Energy Science and Technology / Environmental Waste Recycle Institute, Myongji University

16:45	Tuning the properties of MnO₂ OER electrocatalysts: influence of the substrate and of surface functionalization Alberto Gasparotto,* ^{a,b} Lorenzo Bigiani, ^a Chiara Maccato, ^{a,b} Cinzia Sada, ^c Johan Verbeeck, ^d Teresa Andreu, ^{e,f} Juan Ramón Morante, ^{e,f} Davide Barreca. ^b a. Department of Chemical Sciences, Padova University and INSTM, 35131 Padova, Italy b. CNR-ICMATE and INSTM, Department of Chemical Sciences, Padova University, 35131 Padova, Italy c. Department of Physics and Astronomy, Padova University and INSTM, 35131 Padova, Italy d. EMAT and NANOLab Center of Excellence, University of Antwerp, 2020 Antwerpen, Belgium e. Universitat de Barcelona (UB), 08028 Barcelona, Spain f. Catalonia Institute for Energy Research - IREC, Sant Adrià de Besòs, 08930 Barcelona, Spain	I P1.6
16:45	Synthesis of metal@carbon nanostructured model electrodes and studies of their electrochemical response at the nanoscale Brazel, L. (1),* Brunet Cabré, M.(1), Schroeder, C.(1), Nolan, H.(1), McKelvey, K.(1) (2), Colavita, P.E.(1) (1) School of Chemistry, Trinity College Dublin, College Green, Dublin 2, Ireland, (2) School of Chemical and Physical Sciences, Victoria University of Wellington, Wellington 6012, New Zealand	I P1.7
16:45	Improving the heat-electricity conversion performance of thermoelectric generators based on evaporative cooling technology Liang Jun Zheng, Dong Hee Kang, Min Liang Wang, Hyun Wook Kang * Department of Mechanical Engineering, Chonnam National University, Korea	I P1.8
16:45	Electrochemical study of copper oxides heterostructures as photocatalysts for CO₂ conversion to formic acid Bălan, A.E. (1), Stamatina, S.N. (1), Iacob, M.T. (1,2), Diac, C.*(1), Mitrea, B.C. (1,2), Esmail Jalali Lavasani (1,2), Stamatina, I. (1) (1) 3Nano-SAE Research Centre, PO Box MG-38, Bucharest – Magurele, Romania (2) University of Bucharest, Faculty of Physics, PO Box MG-38, Bucharest – Magurele, Romania	I P1.9
16:45	The Influence of Cu, Ag, and TiO₂ Nanoparticles on Plants Photosynthesis Process Mitrea B. C. (1,2), Nichita C. (1,2), Diac C. (1), Dobrica B.(1), Stamatina I. (1) (1) 3Nano-SAE Research Centre, PO Box MG-38, Bucharest – Magurele, Romania (2) University of Bucharest, Faculty of Physics, ICUB, PO Box MG-38, Bucharest – Romania	I P1.10
16:45	Effect of Noble Metal Dope into 2D Layered Perovskites for Photocatalytic CO₂ Reduction Yilmaz, B.*(1), Unal, U.(1) (1)Koc Univesity, Turkey	I P1.11
16:45	Graphene/TiO₂ Photocatalysts Synthesis By Laser Pyrolysis For Ethylene Production Juliette Karpel ^{1,2} , Pierre Lonchambon ¹ , Frédéric Dappozze ² , Nathalie Herlin ¹ , Chantal Guillard ² (1) University of Paris-Saclay, CEA,CNRS, NIMBE, Gif-sur-Yvette Cedex, France. (2) University of Lyon 1, IRCELYON, CNRS, Villeurbanne, France.	I P1.12

Tuesday may 31

CO₂ reduction I : MR

09:00	INV Unveiling the Dynamic Behavior of CO₂ Electrocatalysts through in situ Microscopy and Operando Spectroscopy Beatriz Roldan Cuenya Department of Interface Science, Fritz-Haber-Institute of the Max Planck Society, Berlin	I 4.1
09:30	INV Probing CO₂ reduction dynamics with time-resolved Raman spectroscopy Ward van der Stam Inorganic Chemistry and Catalysis, Utrecht University, The Netherlands. Email: w.vanderstam@uu.nl	I 4.2
10:00	Shaping of mesoporous CeO₂ powder into mm-sized catalyst supports for CO₂ methanation Elena Martín Morales, Andreína Alarcón, Elena Xuriguera, Jordi Guilera Catalonia Institute for Energy Research (IREC), Jardins de les Dones de Negre 1, 08930 Sant Adrià de Besòs, Spain, Escuela Superior Politécnica del Litoral, ESPOL, Facultad de Ingeniería en Ciencias de la Tierra, Campus Gustavo Galindo Km.30.5 Vía Perimetral, P.O. Box 09-01-5863, Guayaquil, Ecuador, DIOPMA, Departament de Ciència de Materials i Química Física, Facultat de Química, Universitat de Barcelona, Martí i Franquès 1-11, 08028, Barcelona, Spain, Chemical Engineering and Analytical Chemistry Department, University of Barcelona, Martí i Franquès 1-11, 08028 Barcelona, Spain	I 4.3
10:15	Nanoscale properties of colloidal CeO₂: Synthesis, lanthanide doping and applications Hervés-Carrete, C. (1)*, Bastús, N.G. (1), Puentes, V.F. (1, 2, 3) (1) Catalan Institute of Nanoscience and Nanotechnology (ICN2), Spain (2) Vall d'Hebron Institut de Recerca (VHIR), Spain (3) Institució Catalana de Recerca i Estudis Avançats (ICREA), Spain	I 4.4
10:30	Discussion	
10:45	Coffee	

CO₂ reduction II : CF

11:00	INV Hybridization of molecular and conductive/semi-conductive porous materials for CO₂ catalytic reduction Marc Robert Université de Paris, Laboratoire d'Electrochimie Moléculaire, CNRS, F-75006 Paris, France	I 5.1
11:30	Direct-synthesis of Ag_xCu_{100-x} bimetallic nanoparticles on p-Si supports for the photoelectrochemical reduction of CO₂ Harsh Chaliyawala ¹ , Stephane Bastide ¹ , Diane Muller-Bouvet ¹ , Tarik Bourouina ² , Frédéric Marty ² , Abir Rezgui ² , S. Le Gall ³ , Encarnacion Torralba ¹ * (1) Univ Paris Est Creteil, CNRS, Institut de Chimie et des Matériaux Paris-Est (ICMPE), UMR 7182, 2 rue Henri Dunant, 94320 Thiais, France (2) ESYCOM - Electronique, Systèmes de communication et Microsystèmes (Université de Paris-Est - Marne-la-Vallée) Cité Descartes, 77454 Marne-la-Vallée Cedex 2, France (3) Group of electrical engineering Paris, UMR CNRS 8507, Centrale Supélec, (Univ. Paris Sud) 91192 Gif sur Yvette CEDEX, France	I 5.2
11:45	Electrochemical CO₂ conversion to nanocarbons in Li-K-Na molten salt electrolyte: tuning the nanocarbon morphology Giannakopoulou T.*, Todorova N., Vagenas M., Plakantonaki N., Papailias I., Trapalis C. Institute of Nanoscience and Nanotechnology, National Centre for Scientific Research "Demokritos", Greece	I 5.3
12:15	Discussion	
12:30	Lunch and Plenary	

CO₂ reduction III : JK

15:00	INV Alternative fuels and chemicals – with materials science from renewable electricity, CO₂ and water up to the final product Dr. Carina Faber, Dr. Hélène Lepaumier, Jim Griepkoven, Dr. Jan Mertens ENGIE Laborelec, Linkebeek, Belgium, ENGIE Laborelec, Linkebeek, Belgium, ENGIE Laborelec, Linkebeek, Belgium, ENGIE S.A., Paris, France,	I 6.1
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15:30	High-rate CO₂ electrocatalytic reduction to formate with InP colloidal quantum dots derived catalysts Ivan Grigioni, Edward H. Sargent, Elena Sellia Dipartimento di Chimica, Università degli Studi di Milano, Via Golgi 19, 20133 Milano, Italy Department of Electrical and Computer Engineering, University of Toronto, Ontario, Canada, Department of Electrical and Computer Engineering, University of Toronto, Ontario, Canada, Dipartimento di Chimica, Università degli Studi di Milano, Via Golgi 19, 20133 Milano, Italy	I 6.2
15:45	CO₂ reduction using nanostructured metal oxide/catalyst hybrid layers assembled at photoelectrodes Julian Guerrero[1][2], Nathanaelle Schneider[2], Daniel Lincot[2], Negar Naghavi[2], Marc Robert[1][3] [1] J. Guerrero, Prof. M. Robert Laboratoire d'Electrochimie Moléculaire, Université de Paris, CNRS, F-75006 Paris, France [2] J. Guerrero, N. Schneider, N. Naghavi, Prof. D. Lincot Institut Photovoltaïque d'Île-de-France (IPVF), CNRS, UMR 9006, 91120 Palaiseau, France [c] Prof. M. Robert Institut Universitaire de France (IUF), F-75005, Paris, France	I 6.3
16:00	Effect of noble metal doping on Layered CsCa₂Ta₃O₁₀ for photocatalytic conversion of CO₂ into valuable fuels Tugba Yalcin (1,2), Ugur Unal (1) (1) Koc University, Materials Science and Engineering Dept. Rumelifeneri yolu Saryer Istanbul Turkey , (2) Arçelik, Turkey	I 6.4
16:15	Discussion	
16:30	Coffee	
	Characterization and Modeling I : SH	
16:45	Recent Insights on Photoelectrochemical Interfaces from XPS Studies Roel van de Krol 1. Institute for Solar Fuels, Helmholtz-Zentrum Berlin für Materialien und Energie, 14109 Berlin, Germany. Email: roel.vandekrol@helmholtz-berlin.de 2. Institut für Chemie, Technische Universität Berlin, Berlin, Germany	I 7.1
17:15	Bifunctional earth-abundant catalysts combined with solar cells for solar to hydrogen fuel production M.G. Méndez-Medrano,1 Nicolas Loones,1 Frederique Donsanti,1 Alexandre Blaizot,1 Negar Naghavi,1,2 1 IPVF Institut Photovoltaïque d'Île-de France, 91128 Palaiseau, France. 2 CNRS- Institut Photovoltaïque d'Île-de France, UMR 9006 , 91128 Palaiseau, France,	I 7.2
17:30	Superior overall water splitting performances of electroless deposited Ni-P films Sergio Battiato, Luca Bruno, Antonio Terrasi, Salvo Mirabella Dipartimento di Fisica e Astronomia "Ettore Majorana" and IMM-CNR, via S. Sofia 64, 95123, Catania, Italy	I 7.3
17:45	Hydrogen Evolution Reaction catalysed by low-cost synthesized WO₃ nanorods G. Mineo1-2, M. Scuderi3, E. Bruno1-2, S. Mirabella1-2 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,	I 7.4
18:00	Discussion	

Wednesday June 1

Bioconversion & Synthesis of added value products I : AM

09:00	Rational design of bio-organic interfaces for improved efficiency of photosystem I-based solar converting nanodevices Joanna Kargul Solar Fuels Laboratory, Centre of New Technologies, University of Warsaw, Banacha 2C, 02-097 Warsaw, Poland	I 8.1
09:30	Bioinspired nonadiabatic principles for artificial photosynthesis with high yield Huub de Groot Leiden Institute of Chemistry, Leiden University, The Netherlands	I 8.2
10:15	Development of Ru-Carbon Electrocatalysts for the Electrochemical Nitrogen Reduction Reaction Dario Formenti (1),* Yannik Kohlhaas (2), Zhenglin Zhuang (1), Xin Wei (1), Maria Meledina (3), Matthias Wessling (2), Robert Keller (2), Joachim Mayer (3), Ulrich Simon (1) (1) Institute of Inorganic Chemistry – RWTH Aachen University, Germany, (2) Chemical Process Engineering – RWTH Aachen University, Germany, (3) Central Facility for Electron Microscopy – RWTH Aachen University, Germany	I 8.3
10:30	What makes lithium unique in its ability to reduce nitrogen to ammonia? Ifan E. L. Stephens Department of Materials, Imperial College London	I 8.4
10:45	Discussion	

Bioconversion & Synthesis of added value products II : MS

11:00	Electrosynthesis with molecular catalysts immobilized on conducting surfaces via host-guest interactions David Tilley University of Zurich	I 9.1
11:30	Alternative generation of ammonia via nitrate and N₂ reduction through electrochemical routes Sebastian Murcia-Lopez,1 Marcelo E. Chavez,1 Juan R. Morante 1,2 1. Catalonia Institute for Energy Research (IREC), Jardins de les Dones de Negre 1, Sant Adrià de Besòs, 08930, Spain 2. University of Barcelona (UB), Martí i Franquès 1, Barcelona, 08020, Spain	I 9.2
11:45	Reforming of Soluble Biomass and Plastic Derived Waste using a Bias-Free Cu₃₀Pd₇₀perovskite/Pt Photoelectrochemical Device Subhajt Bhattacharjee, Virgil Andrei, Chanon Pornrunroj, Motiar Rahaman, Christian M. Pichler and Erwin Reisner* Yusuf Hamied Department of Chemistry, University of Cambridge, Lensfield Road, Cambridge CB2 1EW, United Kingdom.	I 9.3
12:00	Discussion	
12:15	Lunch and Plenary	

Bioconversion & Synthesis of added value products III : DT

15:00	Photo- and electro-catalyst development: carbon nitride and NiFe-oxide for catalytic oxidation of organic molecules to value-add Menny Shalom Department of Chemistry, Ben-Gurion University of the Negev, Beer-Sheva, Israel	I 10.1
15:30	Co-based bimetallic catalysts for the production of hydrocarbons (C₂-C₄) via the direct hydrogenation of CO₂ and CO. A. Alarcón 1, O. Palma1, E. Martínez1, M. Biset1, T. Andreu2, J. Guilera1 1. Catalonia Institute for Energy Research (IREC), Jardins de les Dones de Negre 1, 08930 Sant Adrià de Besòs, Spain 2. Departament de Ciència de Materials i Química Física, Universitat de Barcelona, Martí i Franquès, 1, Barcelona 08028, Spain	I 10.2
15:45	Study of the electrochemical hydrogenation of nitrobenzene in Cu and CuPd electrodes Carvajal, D* (1), Arcas, R (1), Mesa, C (1), Giménez, S (1), Fabregat-Santiago, F (1), Mas-Marzá, E (1). (1) Group of Advances Materials and Energy, Institute of Advanced Materials, Universitat Jaume I, Spain.	I 10.3

16:00	Optimization of electrochemical conditions for Hydrogen storage in the GO lattice Nina M. Carretero*, S. Murcia*, J. R. Morante*+ * IREC, Catalonia Institute for Energy Research, Sant Adrià del Besòs, 08930, Spain, + Dept. Enginyeries: Electronica, Universitat de Barcelona, Barcelona, 08028, Spain	I 10.4	16:45	Investigation of the photoelectrochemical hydrogen evolution reaction on exfoliated SnSe electrodes Qianqian Ba, Péter S Tóth, Csaba Janáky Department of Physical Chemistry and Materials Science, Interdisciplinary Excellence Center, University of Szeged, Rerrich Sq. 1, Szeged, 6720, Hungary	I P2.11
16:15	Discussion		16:45	Effect of Noble Metal Doping to Layered KCa₂NaNb₄O₁₃ on Hydrogen Evolution Reaction Demir, A.B.*(1), Unal, U(2) (1) Koc University, Turkey	I P2.12
16:30	Coffee		16:45	Cobalt iron oxyhydroxide electrocatalyst for water oxidation obtained by in-situ transformation of phosphides María Isabel Díez García, Guillem Montaña, Marc Botifoll, Andreu Cabot, Jordi Arbiol, Mohammad Qamar, Joan Ramon Morante María Isabel Díez-García,1 Guillem Montaña,1 Marc Botifoll,2 Andreu Cabot,1,3 Jordi Arbiol,2,3 Mohammad Qamar,4 Joan Ramon Morante1 1 Catalonia Institute for Energy Research (IREC) Jardins de les Dones de Negre 1, Sant Adrià de Besòs, Spain 2 Catalan Institute of Nanoscience and Nanotechnology (ICN2), CSIC and BIST, Campus UAB, Bellaterra, 08193 Barcelona, Catalonia, Spain 3 ICREA, Pg. Lluís Companys 23, 08010 Barcelona, Catalonia, Spain 4 Interdisciplinary Research Center for Hydrogen and Energy Storage, King Fahd University of Petroleum and Minerals, Dhahran, 31261, Saudi Arabia	I P2.14
	II : Bert Weckhuysen & Frederic Chandezon		18:00	E-MRS EU-40 Materials Prize & MRS Mid-Career Researcher Award Presentations	
16:45	NiO nanoparticles obtained by pulsed laser ablation in liquid for oxygen evolution reaction V. Iacono (1,2), L. Bruno (1,2), E. Bruno (1,2), F. Ruffino (1,2), S. Mirabella (1,2) (1) Dipartimento di Fisica e Astronomia "Ettore Majorana", Università di Catania, via S. Sofia 64, 95123 Catania, Italy, (2) CNR-IMM (Catania Università), via S. Sofia 64, 95123 Catania, Italy,	I P2.1			
16:45	Tuning oxygen evolution performance via A-site Ag+ doping in SrCo_{0.75}Fe_{0.25}O₃ perovskite Ziwei Huo.*(1) , Dongsheng Geng.*(1). (1)Beijing Advanced Innovation Center for Materials Genome Engineering, School of Materials Science and Engineering, University of Science and Technology Beijing, Beijing 100083, China * lead presenter	I P2.2			
16:45	Plasma-assisted fabrication of Mn₂O₃-based electrocatalysts on Ni foam substrates for the oxygen evolution reaction Davide Barreca,a,* Chiara Maccato,a,b Lorenzo Bigiani,b Teresa Andreu,c,d Alberto Gasparotto,a,b Cinzia Sada,e Evgeny Modin,f Oleg I. Lebedev,g Juan Ramon Morante.c,d a. CNR-ICMATE and INSTM, Department of Chemical Sciences, Padova University, 35131 Padova, Italy b. Department of Chemical Sciences, Padova University and INSTM, 35131 Padova, Italy c. IREC, Catalonia Institute for Energy Research, 08930 Sant Adrià de Besòs, Barcelona, Catalonia, Spain d. Universitat de Barcelona (UB), 08028 Barcelona, Spain e. Department of Physics and Astronomy, Padova University and INSTM, 35131 Padova, Italy f. CIC nanoGUNE BRTA, 20018 Donostia - San Sebastian, Spain g. Laboratoire CRISMAT, ENSICAEN UMR6508, 14050 Caen Cedex 4, France	I P2.3			
16:45	Enhanced Electrocatalytic Intrinsic Activity of NiO Microflowers on Graphene Paper for Oxygen Evolution Reaction Bruno, L.*(1,2), Scuderi, M.(3), Priolo, F.(1,2), Falcicola, L. (4) & Mirabella, S.(1,2) (1) Dipartimento di Fisica e Astronomia "Ettore Majorana", Università di Catania, via S. Sofia 64, 95123 Catania, Italy, (2) CNR-IMM, via S. Sofia 64, 95123 Catania, Italy, (3) CNR-IMM, VIII strada 5, 95121 Catania, Italy, (4) Dipartimento di Scienze Chimiche, Università degli Studi di Catania, viale Andrea Doria 8, 95123, Catania, Italy.	I P2.4			
16:45	Modifying the Electron-Trapping Process at the BiVO₄ Surface States via the TiO₂ Overlayer for Enhanced Water Oxidation Usman, E.*(1),(2), Barzgar Vishlaghi, M.(1),(2), Kahrman, A.(1),(2), Solati, N.(1),(2), Kaya, S.(1),(2),(3) (1) Materials Science and Engineering, Koc University, Turkey, (2) Koc University Tupras Energy Center (KUTEM), Turkey, (3) Department of Chemistry, Koc University, Turkey, * lead presenter	I P2.5			
16:45	Plasma-Assisted Synthesis of Co₃O₄-Based Electrocatalysts on Ni Foam Substrates for the Oxygen Evolution Reaction Chiara Maccato, Lorenzo Bigiani, Leonardo Girardi, Alberto Gasparotto, Oleg I. Lebedev, Evgeny Modin, Davide Barreca, Gian Andrea Rizzi L. Bigiani, L. Girardi, Department of Chemical Sciences, Padova University and INSTM, Padova 35131, Italy, Chiara Maccato, Alberto Gasparotto, Gian Andrea Rizzi, Department of Chemical Sciences, Padova University, CNR-ICMATE and INSTM, Padova 35131, Italy, Davide Barreca, CNR-ICMATE, INSTM and Department of Chemical Sciences, Padova University, 35131, Padova, Italy, Oleg I. Lebedev, Laboratoire CRISMAT UMR 6508 CNRS/ENSICAEN/UCBN, Caen Cedex 4 14050, France, Evgeny Modin, CIC nanoGUNE BRTA, Donostia, San Sebastian 20018, Spain	I P2.6			
16:45	Kinetics of Active Oxide Species Derived from Metallic Nickel Surface for Efficient Electrocatalytic Water Oxidation Yimeng Ma College of Chemistry and Chemical Engineering, Donghua University, Shanghai, 201620, China	I P2.7			
16:45	Synthesis and Development of Thin-film Catalyst Materials for Electrolysis Muhammad Sadaf Hussain, Faria Rafique, Dr Imran Din Institute of Chemistry, University of the Punjab Lahore, Pakistan	I P2.10			

Thursday June 2

Water Splitting I : MC

- 09:00 **INV (Photo)electrochemical Water Splitting Catalyzed by Materials with Well Defined Active Site Structures** I 11.1
Licheng Sun
1 Center of Artificial Photosynthesis for Solar Fuels, School of Science, Westlake University, 310024 Hangzhou, China 2 Department of Chemistry, KTH Royal Institute of Technology, 10044 Stockholm, Sweden
- 09:30 **INV Molecular anodes for green and sustainable energy applications** I 11.2
Antoni Llobet
Institute of Chemical Research of Catalonia (ICIQ), Barcelona Institute of Science and Technology (BIST), Av. Paisos Catalans 16, E-43007 Tarragona, Spain and Departament de Química Universitària Autònoma de Barcelona, Cerdanyola del Vallès, E-08193 Barcelona, Spain. E-mail: allobet@iciq.cat
- 10:00 **Core shell nanoparticles: a catalyst for the oxygen evolution reaction** Lisa Royer, Antoine Bonenfant, Benoit Pichon, Elena Savinova I 11.3
Lisa Royer: Institut de Chimie et Procédés pour l'Energie, l'Environnement et la Santé, UMR 7515, CNRS-University of Strasbourg, 67087 Strasbourg Cedex 2, France, Benoit Pichon: Institut de Physique et de Chimie des Matériaux de Strasbourg, UMR 7504, CNRS-University of Strasbourg, 67034 Strasbourg Cedex 2, France, Bonenfant Antoine, Institut de Chimie de Strasbourg, UMR 7177 CNRS-University of Strasbourg, 67070, Strasbourg, France, Elena Savinova: Institut de Chimie et Procédés pour l'Energie, l'Environnement et la Santé, UMR 7515, CNRS-University of Strasbourg, 67087 Strasbourg Cedex 2, France
- 10:15 **Development of Highly Efficient Self-Supported Transition Metal Based Catalysts for Water Splitting** I 11.4
Faria Rafique, Dr Habib ur Rehman, Dr. Joe Briscoe
Syed Babar Ali School of Science and Engineering, LUMS - Lahore University of Management Sciences School of Engineering and Materials Science, Queen Mary University of London
- 10:30 **Discussion**
- 10:45 **Coffee**

Water Splitting II : TL

- 11:00 **INV Water splitting using wired perovskite tandem solar cells and molecular catalysts.** I 12.1
Yuanyuan Shi 1, Tsung-Yu Hsieh 1, Md Asmaul Hoque 1, Werther Cambarau 1, Stéphanie Narbey 2, Carolina Gimbert-Suriñach 1, Emilio Palomares 1 3, Mario Lanza 4, Antoni Llobet 1 5
1 Institute of Chemical Research of Catalonia (ICIQ), Barcelona Institute of Science and Technology (BIST), Avinguda Paisos Catalans, 16, 43007 Tarragona, Spain. 2 Solaronix S.A., Rue de l'Ouriette 129, CH-1170 Aubonne, Switzerland. 3 ICREA, Passeig Lluís Companys 23, 08010 Barcelona, Spain. 4 Physical Sciences and Engineering Division, King Abdullah University of Science and Technology (KAUST), 23955-6900 Thuwal, Saudi Arabia. 5 Departament de Química, Universitat Autònoma de Barcelona (UAB), 08193 Cerdanyola del Vallès, Barcelona, Spain.
- 11:30 **Water splitting performance of selenium based Chevrel phase: CoW6Se8** I 12.2
Gencer, A.* (1), Surucu, G. (2), Ozel, F. (3).
(1) Karamanoglu Mehmetbey University, Department of Physics, Karaman, Turkey, (2) Ahi Evran University, Department of Electric and Energy, Kirsehir, Turkey, (3) Karamanoglu Mehmetbey University, Department of Metallurgy and Materials Engineering, Karaman, Turkey,
- 11:45 **Ferroelectric BiFeO3-PbTiO3 films for photoelectrochemical water splitting** I 12.3
Haozhen Yuan, Joe Briscoe
School of Engineering and Material Science and Materials Research Institute, Queen Mary University of London, London, E1 4NS
- 12:00 **Discussion**
- 12:15 **Lunch and Plenary**

Applications to industry : RV

- 15:00 **INV Scalable photoelectrochemical hydrogen production and storage in a liquid silicon hydride carrier** I 13.1
Hannah Johnson
Toyota Europe

- 15:30 **TRIBOCHEMICAL DECOMPOSITION OF SODIUM ALANATE (NaAlH₄)** Muñoz-Cortés, E.*(1), Ibryayeva O. L.,(2) Manso, M.,(3) Zabala, B.,(4) Flores. E.,(5) Ares, J.R.(1) & Nevshupa, R (6). I 13.2
(1) Department of Physics of Materials, Autonoma University of Madrid, Spain, (2) Department of System Programming, South Ural State University, Chelyabinsk, Russia, (3) Department of Applied Physics, Nicolás Cabrera Institute and Centre for Microanalysis of Materials, Autonoma University of Madrid, Spain, (4) Tribology unit, Fundación Tekniler, Eibar, Spain, (5) Departamento de Física Aplicada, Centro de Investigación y de Estudios Avanzados, Unidad Mérida, 97310, Mérida, Yucatan, México, (6) Spanish National Research Council, Eduardo Torroja Institute of Construction Sciences (IETCC-CSIC), Madrid, Spain, *esmeralda.munnoz@estudiante.uam.es
- 15:45 **Towards high productivity cathodes for hydrogen evolution reaction based on metal phosphides** I 13.3
María Isabel Díez García, Sebastian Murcia, Joan Ramon Morante
María Isabel Díez García, Sebastian Murcia, Joan Ramon Morante Catalonia Institute for Energy Research (IREC) Jardins de les Dones de Negre 1, Sant Adrià de Besòs, Spain
- 16:00 **Exploring the Advanced Tailor-made Catalyst materials and Systems for the Up-scaled Electroconversion of CO₂** I 13.4
Tandava. V.S.R.K., Andrés Alberto García, Sebastián Murcia-López, Joan Ramón Morante*
Catalonia Institute for Energy Research (IREC), Jardins de les Dones de Negre 1, 08930, Sant Adrià de Besòs, Spain.
- 16:15 **Discussion**
- 16:30 **Coffee**

Water Splitting III : JC

- 16:45 **INV Development upscaling of an electrochemical technology for the conversion of CO₂** I 14.1
Annelie Jongerius
Avantium Chemicals
- 17:15 **Copper Vanadate Nanobelts as Anodes for PEC Water Splitting: Influence of CoO_x Overlayers on Functional Performances** I 14.2
Leonardo Girardi, Gian Andrea Rizzi*, Lorenzo Bigiani, Davide Barreca, Chiara Maccato, Carla Marega, Gaetano Granozzi
Leonardo Girardi – Department of Chemical Sciences, Padova University and INSTM, Padova 35131, Italy, Gian Andrea Rizzi* – Department of Chemical Sciences, Padova University, CNR-ICMATE and INSTM, Padova 35131, Italy, Lorenzo Bigiani – Department of Chemical Sciences, Padova University and INSTM, Padova 35131, Italy, Davide Barreca – CNR-ICMATE, INSTM and Department of Chemical Sciences, Padova University, Padova 35131, Italy, Chiara Maccato – Department of Chemical Sciences, Padova University, CNR-ICMATE and INSTM, Padova 35131, Italy, Carla Marega – Department of Chemical Sciences, Padova University and INSTM, Padova 35131, Italy, Gaetano Granozzi – Department of Chemical Sciences, Padova University and INSTM, Padova 35131, Italy
- 17:30 **Recent advances in lanthanide-doped TiO₂ thin films for green hydrogen strategies** Katarzyna Zakrzewska, Marta Radecka I 14.3
AGH-University of Science and Technology, al. Mickiewicza 30, 30-059 Kraków, Poland
- 17:45 **(Cu_{3-x}Nix)Co₂-Layered Double Hydroxide Nanosheets for Enhanced Electrocatalytic Activity Towards Water Splitting** I 14.4
Sakshi Kansal, Debabrata Mandal, Surbhi Priya, Satvik Anshu, Trilok Singh, Amreesh Chandra Research Scholar, Research Scholar: Research Scholar, Research Scholar, Professor, Professor
- 18:00 **Discussion**

Friday June 3

Characterization and Modeling II : HG

- 09:00 **INV Multi-scale modelling for photoelectrochemical water and CO₂ splitting** I 15.1
Sophia Haussener
Laboratory of Renewable Energy Science and Engineering, Institute of Mechanical Engineering, École Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland.
- 09:30 **INV Charge-carrier dynamics in hybrid materials based on colloidal semiconductor nanocrystals for light-driven catalysis** Maria Wächter I 15.2
Leibniz Institute of Photonic Technology
- 10:00 **Oxygen electrocatalysis at transition metal oxides: correlating activity with orbital occupancy under operational conditions** I 15.3
Mohammed A. Alkhalifah, Benjamin Howchen, Joseph Staddon, Veronica Celorrio, Devendra Tiwari, David J. Fermin
School of Chemistry, University of Bristol, Cantocks Close, Bristol BS8 1TS, UK
- 10:15 **Probing the optoelectronic structure of (Ir, Al)-codoped SrTiO₃ for enhanced photocatalytic activity** I 15.4
Namitha Anna Koshi, † Dharmapura H K Murthy, ‡ Sudip Chakraborty, ¶ Seung-Cheol Lee, § and Satadeep Bhattacharjee †
†Indo-Korea Science and Technology Center (IKST), Jakkur, Bengaluru 560065, India ‡Materials Science and Catalysis Division, Poornaprajna Institute of Scientific Research, Devanahalli, Bengaluru 562164, India ¶Materials Theory for Energy Scavenging (MATES) Lab, Harish-Chandra Research Institute (HRI) Allahabad, HBNL, Chhatnag Road, Jhansi, Prayagraj (Allahabad) 211019 India §Electronic Materials Research Center, KIST, Seoul 136-791, South Korea
- 10:30 **Discussion**
- 10:45 **Coffee**

Water Splitting IV : EP

- 11:00 **INV Coupling of enzymes and sulphides to achieve water splitting and CO₂ reduction** I 16.1
Conesa, J.C.*(1), Osgouei, M.(1), Faraldos, M.(1), Coito, A.M.(2), Pereira, I. A. C.(2), Shleev, S.(3), Rana, M.(4), Vilatela, J.J.(4), Pita, M.(1), De Lacey, M.(1)
(1) Instituto de Catálisis y Petroleoquímica, CSIC, Spain, (2) ITQB, Universidade Nova de Lisboa, Oeiras, Portugal, (3) Biomedical Science, Faculty of Health and Society, Malmö University, Malmö, Sweden, (4) Instituto IMDEA Materiales, Madrid, Spain. *lead presenter
- 11:30 **The role of spin degrees of freedom in manipulating the reactivity of a metal surface containing 3d transition metals** I 16.2
Satadeep Bhattacharjee and Seung Cheol Lee
Indo Korea Science and Technology Center, Bangalore, India. Center for Electronic Materials, Korea Institute of Science and Technology (KIST)
- 11:45 **Catalyst Surfaces for Energy Conversion – In-situ Studies of Electrochemical driven Nanoparticle Exsolution** I 16.3
R. Rameshan, L. Lindenthal, F. Schrenk, T. Ruh, A. Nanning, A.K. Opitz, C. Rameshan
Institute of Materials Chemistry, TU Wien, Austria, Institute of Chemical Technologies and Analytics, TU Wien, Austria
- 12:00 **Discussion**
- 12:15 **Closing**