



## PROGRAM

### Tuesday, June 14

09:00 Welcome coffee and Registration

10:00 **Opening Ceremony**

#### 10h15 **Plenary 1 : A. Minelli**

Department of Chemistry, University of Oxford (United Kingdom)

**Charge density waves studied through total scattering methods**

#### 11:00 **Session 1 - CHEMISTRY 1**

**001 Novel Zintl phases based on group 15 elements with and late d-metals and lathanides**

S. Bobev - University of Delaware, Newark (USA)

**002 Ternary AELiAu (AE = Ca, Sr, Ba, Eu, Yb) phases with TiNiSi type structure**

P. Höhn - Max Planck Institute for Chemical Physics of Solids, Dresden (Germany)

**003 New intermetallics observed in Friction Stir Welding**

M. Martinez Celis – Université de Caen Normandie, ENSICAEN, CNRS (France) and Charles University, Prague (Czech Republic)

**004 Synthesis, crystal structure and chemical bonding of RE–Pd–Ge compounds related to the AlB<sub>2</sub> aristotype (RE = rare earth metal)**

R. Freccero - Università degli Studi di Genova (Italy)

**005 New transition metal pyrochlore fluorides: Structure and magnetic properties of the NaCdM<sub>2</sub>F<sub>7</sub> family**

R. Colman - Charles University, Prague (Czech Republic)

12:40 Lunch on site

#### 14:00 **Plenary 2 : B. Verrecht**

Senior Program Manager Battery Recycling at Umicore

**Towards sustainable battery recycling**

#### 14:45 **Plenary 3 : E. Svanidze**

Max-Planck-Institut für Chemische Physik fester Stoffe, Dresden (Germany)

**Superconductivity and magnetism in complex mercury-based compounds**

15:30 Coffee break

#### 16:00 **SESSION 2A – CORRELATED MATTER 1**

**006 Unconventionnal superconductivity and Kondo lattice effects in La<sub>1-x</sub>Ce<sub>x</sub>FeSiH**

J. Sourd – Université de Bordeaux, CNRS, Bordeaux INP (France)

**007 Electron correlations and magnetism in pure and alloyed uranium hydrides**

L. Havela - Charles University, Prague (Czech R.)

#### 16:00 **SESSION 2B - THERMOELECTRICITY**

**012 Carrier concentration adjustment and texturation processing on thermoelectric silicide – CrSi<sub>2</sub> and Higher Manganese Silicide (HMS)**

D. Berthebaud - CNRS-Saint Gobain-NIMS, LINK Laboratory, Tsukuba (Japan)

- O08 Heavy-fermion superconductivity in  $\text{Ce}_2\text{PdIn}_8$  tuned by crystal growth conditions**  
G. Chajewski - Institute of Low Temperature and Structure Research, Polish Academy of Sciences, Wrocław (Poland)
- O09 Weak antilocalization effect and triply degenerate state in Cu-doped  $\text{CaAuAs}$**   
S. Malik - Indian Institute of Technology Kanpur (India)
- O10 Copper based quaternary chalcogenide : A composite quantum material**  
B. Sahni - Indian Institute of Technology Bombay (India)
- O11 Magnetic and magnetotransport properties of  $\text{UFe}_{0.5}\text{Sb}_2$**   
P. Gonçalves - Instituto Superior Técnico, Universidade de Lisboa (Portugal)
- O13 Structural analysis and thermoelectric properties of  $\text{Cr}_2\text{Sn}_3\text{S}_7$**   
F. Guiot - Université de Rennes, CNRS (France)
- O14 Scrutinizing the phonon Kondo effect in thermoelectric clathrates**  
F. Mazza - Vienna University of Technology (Austria)
- O15 Violation of translational symmetry and thermoelectric properties of materials**  
Y. Grin - Max-Planck-Institut für Chemische Physik fester Stoffe, Dresden (Germany)
- O16 Relationship between the deposition conditions and the memory effect in electrochromic sputtered  $\text{WO}_3$  films**  
B. Faceira - Université de Bordeaux, CNRS, Bordeaux INP (France)

**18:00 Poster session and cocktail « Wine and cheese »**

## Wednesday, June 15

### 09:00 **Plenary 4 : S. Sartori**

Department of Technology Systems at the University of Oslo (Norway)

**Hydrogen storage in intermetallic alloys – where are we now and future perspective**

### 09:45 **Session 3 - HYDROGEN**

#### **O17 Towards a better comprehension of the hydrogen absorption mechanism of different high entropy multicomponent alloys**

M. Moussa – Université de Bordeaux, CNRS, Bordeaux INP (France) et Université du Québec Trois-Rivières (Canada)

#### **O18 Fe-based high entropy alloys for hydrogen storage**

K. Marcus - Université de Grenoble Alpes, CNRS, Grenoble INP (France)

#### **O19 Microstructure and hydrogen storage properties of High Entropy Alloy $\text{TiHfZrNb}_{1-x}\text{V}_{1+x}$ , $x=0, 0.1, 0.2, 0.4, 0.6$ and $1$ .**

J. Huot - Hydrogen Research Institute, Université du Québec à Trois-Rivières (Canada)

**10:45 Coffee break**

### 11:00 **Session 4 - BATTERIES**

#### **O20 Novel organic-inorganic hybrid material through cation intercalation in layered van der Waals $\text{NiPS}_3$ - a mechanistic study via operando X-ray diffraction and X-ray absorption spectroscopy**

S. Pazek - IFW Dresden (Germany)

#### **O21 *In-situ* XRD and PDF investigation of battery fluoride materials $\text{MF}_{3.3}\cdot\text{H}_2\text{O}$ ( $M = \text{Fe}, \text{Cr}$ ) in controlled atmosphere: accessing new phases with controlled chemistry**

G. Nénert - Malvern Panalytical B. V., Almelo (The Netherlands)

#### **O22 Mixed-ion conduction ( $\text{Na}^+/\text{O}^{2-}$ ) in Nb-based perovskites**

G. Gouget - Université de Bordeaux, CNRS and Solvay, Research and Innovation Center Paris, (France)

**O23 Compositional influence onto electrochemical performance of cubic anti-perovskites in Li-batteries**  
M. Gorbunov - Leibniz Institute for Solid State and Materials Research, Dresden (Germany)

**O24 Modulating the properties of KVPO<sub>4</sub>F high voltage positive electrode through anionic substitution**  
R. Wernert - Université de Bordeaux, CNRS, Bordeaux INP and Univ. Montpellier, and RS2E (France)

12:40 *Lunch on site*

14:00 **Plenary 6 : M. Kitano**  
Materials Research Center for Element Strategy, Tokyo Institute of Technology (Japan)  
**Novel Solid Catalysts with Functional Anion Sites for Ammonia Synthesis**

14:45 **Plenary 5 : B. Dam**  
Department of Chemical Engineering, Delft University of Technology (The Netherlands)  
**Photochromism in Rare-Earth Oxyhydride thin films**

15:30 *Coffee break*

16:00 **Session 5a - CORRELATED MATTER 2**

16:00 **Session 5b - CATALYSIS/ENERGY**

**O25 Dirac states in Pd-Bi superconductors: on the hunt for Majorana modes**  
D. Kaczorowski - Institute of Low Temperature and Structure Research, Polish Academy of Sciences, Wrocław (Poland)

**O26 U<sub>2</sub>Ni<sub>2</sub>Sn-U<sub>2</sub>Fe<sub>2</sub>Sn system – where is QCP?**  
O. Koloskova - Charles University, Prague (Czech Republic)

**O27 YbPt<sub>5</sub>B<sub>2</sub>: a new ternary boride Kondo lattice compound with complex magnetic order**  
E. Bauer - Institute of Solid State Physics, TU Wien (Austria)

**O28 Crystal field excitations in A<sub>2</sub>Ir<sub>2</sub>O<sub>7</sub> (A = Er and Tm) pyrochlore iridates**  
M. Klicpera - Charles University, Prague (Czech Republic)

**O29 MnPO<sub>4</sub>: A Composite Quantum Compound**  
C. Sreeparvathy - Indian Institute of Technology - Bombay (India)

**O30** *Cancelled*

**O31 Intermetallic electrides with exotic electronic Properties as catalysts for the synthesis of ammonia**  
K. Alabd - Université de Bordeaux, CNRS, Bordeaux INP (France)

**O32 Al-Pt intermetallic compounds as OER electrocatalysts**  
I. Antonyshyn - Max-Planck-Institut für Chemische Physik fester Stoffe, Dresden (Germany)

**O33 Study of magnesium “super-structures” as materials for hydrogen generation via water hydrolysis**  
M. Legrée – Université de Bordeaux, CNRS, Bordeaux INP (France)

**O34** *Cancelled*

**O35 Revisiting the BaFeO<sub>3-δ</sub> system at the nanoscale**  
D. Gutierrez-Martin - Universidad Complutense de Madrid (Spain)

**O36 New promising p-type thermoelectric sphalerite derivative phases in the Cu<sub>2+x</sub>Sn<sub>1-x</sub>S<sub>3</sub> system: Cu<sub>5</sub>Sn<sub>2</sub>S<sub>7</sub> and Cu<sub>22</sub>Sn<sub>10</sub>S<sub>32</sub>**  
P. Lemoine - Université de Rennes, CNRS (France)

18:00 **Poster session and cocktail « Beer and Tapas »**

## Thursday, June 16

### 09:00 **Plenary 7 : J-M. Joubert**

ICMPE, CNRS, Thiais (France)

**Thermodynamic modeling of transition metal-hydrogen systems**

### 09:45 **Session 6 - THERMODYNAMICS**

#### **O37 Critical behavior of elastic constants in UIrSi<sub>3</sub> intermetallic**

T. Haidamak - Charles University, Prague (Czech Republic)

**O38** *Cancelled*

#### **O39 Pressure-temperature (p,T) magnetostructural phase diagrams of slowly cooled Co<sub>1-x</sub>Cu<sub>x</sub>MnGe (0.05 ≤ x ≤ 0.35)**

S. Baran - Jagiellonian University, Kraków (Poland)

10:45 *Coffee break*

### 11:00 **Session 7a - CHEMISTRY 2**

#### **O40 On the Compounds TZnSb, T = Ti, V, Cr**

P. Rogl - Universität Wien (Austria)

#### **O41 Characterization of boundaries of the chiral phase CoSi**

U. Burkhardt - Max-Planck-Institute for Chemical Physics of Solids, Dresden (Germany)

#### **O42 Influence of Nd/Zr substitution on the formation of ThMn<sub>12</sub>-type phase in (Zr,Ce)Fe<sub>10</sub>Si<sub>2</sub> alloys**

M. Kolodziej - Institute of Molecular Physics, Polish Academy of Sciences and NanoBioMedical Centre of Adam Mickiewicz University, Poznań (Poland)

#### **O43 A structural and magnetic study of the YCo<sub>12-x</sub>Fe<sub>x</sub>B<sub>6</sub> series of compounds**

B. Vallet-Simond - Université Grenoble Alpes, CNRS (France)

#### **O44 Polar multiatomic bonding in closest-packing-like atomic arrangement of Be<sub>3</sub>Ru**

L. Agnarelli - Max-Planck-Institut for Chemical Physics of Solids, Dresden (Germany)

### 11:00 **Session 7b - THEORY**

#### **O45 Cation Order in the Ternary and Quaternary Phosphides M<sup>II</sup>M<sup>I</sup><sub>2</sub>P<sub>8</sub>**

U. Wedig - Max Planck Institute for Solid State Research, Stuttgart (Germany)

#### **O46 Cluster-Based Molybdenum Chalcogenide Compounds for Thermoelectricity. Dream or Reality? A (Partial) Answer from Theory**

R. Gautier - Université de Rennes, ENSC Rennes, CNRS (France)

#### **O47 Anti-Th<sub>3</sub>P<sub>4</sub> Antimonides for Thermoelectric Applications: Experimental & Theoretical Investigations**

V. Pelletier - Université de Rennes, ENSC Rennes, CNRS (France)

#### **O48 Electronic Structure of Monolayer FeSe Superconductor on Si(001) from First Principles**

K. Carva - Charles University, Prague (Czech Republic)

#### **O49 Utilizing defects to enhance thermoelectric properties**

T. Mori - International Center for Materials Nanoarchitectonics (WPI-MANA), NIMS and University of Tsukuba (Japan)

12:40 *Lunch box*

**FREE AFTERNOON**

18:00 Departure by bus to « Château de Seguin » (Lignan-de-Bordeaux)

**20:00 GALA DINNER**

## Friday, June 17

### 09:00 **Plenary 8 : M.G. Vergniory**

Max Planck for the Chemical Physics of Solids, Dresden (Germany) and Donostia International Physics Center, Donostia-San Sebastian (Spain)  
**Topological Materials Database**

### 09:45 **Session 8 - MAGNETOCALORICS**

**O50 Unusual Magnetism, including Magnetocaloric Behaviour, of Materials containing Chains of edge-linked ferromagnetic  $\text{MnO}_6$  Octahedra**

C. Greaves - University of Birmingham (United Kingdom)

**O51 Magnetism, structure and magnetocaloric properties of  $\text{Mn}_3\text{Sn}_{1-x}\text{Zn}_x\text{C}$  antiperovskite carbides**

A. Kiecana - Delft University of Technology (The Netherlands)

**O52 Nonlinear influence of excess Mn on the magnetoelastic transition in  $(\text{Mn,Cr})_2\text{Sb}$**

Q. Shen - Delft University of Technology (The Netherlands)

10:45 *Coffee break*

### 11:00 **Session 9 - MAGNETISM**

**O53 Transition-metal van der Waals trihalides: Old materials, new approaches**

M. Kratochvilova - Charles University, Prague (Czech Republic)

**O54 Magnetic properties of polymorphic  $\text{A}_2\text{Ni}_7$ -type compounds**

V. Paul-Boncour - Université Paris Est, CNRS-UPEC, Thiais (France)

**O55 Magnetism of the Co-Cr-Fe-Mn-Ni high-entropy alloy – a concentrated solid solution composed of five types of magnetic moments**

P. Kozelj - Jožef Stefan Institute and University of Ljubljana (Slovenia)

**O56 Structural and magnetic properties of High Entropy Oxides**

J. Cieslak - AGH University of Science and Technology, Cracow (Poland)

12:40 *Lunch on site*

### 14:00 **Plenary 9 : E. Canadell**

Institut de Ciència de Materials de Barcelona (ICMAB-CSIC) (Spain)  
**Charge Density Waves in Transition Metal Chalcogenides**

### 14:45 **Session 10 - CORRELATED MATTER**

**O57 Magnetic reshuffling and feedback on superconductivity in  $\text{UTe}_2$  under pressure**

M. Valiska - Univ. Grenoble Alpes, CEA, Grenoble INP (France) and Charles University, Prague (Czech Republic)

**O58 Structure, magnetism and spin dynamics of van der Waals ferromagnet  $\text{VI}_3$**

D. Hovancik - Charles University, Prague (Czech Republic)