

# EUROPEAN CONFERENCE ON SOLID STATE CHEMISTRY 2023

## FINAL PROGRAMME

SUNDAY, JULY 9, 2023

13:00 - 19:00 **Registration**

*chairperson: David Sedmidubský*

16:00 - 16:20	<b>Opening Session</b> Tomas Wagner, Barbara Albert, Paul Attfield, David Sedmidubský
16:20 - 17:00 <b>PL 01</b>	<b>Metal-organic frameworks for sustainable separations and reactions: A computational perspective</b> J. Jiang
17:00 - 17:30 <b>InvL 01</b>	<b>Designer's metal-organic materials and interfaces through ALD/MLD</b> M. Karppinen
17:30 - 18:00 <b>InvL 02</b>	<b>Exploring model catalysts through the integration of in-situ near-ambient pressure XPS and STM</b> P. Matvijia, M. Vorokhta, F. Pchálek, S. Oveysipoor, L. Piliai, T.N. Dinhová, B. Šmíd, I. Matolínová

18:00 - 18:30 **Welcome Drink**

*chairperson: Tomas Wagner*

18:30 - 18:50 <b>L 01</b>	<b>Negative linear compressibility of the hybrid perovskite <math>[C(NH_2)_3]Er(HCO_2)_2(C_2O_4)</math></b> T. J. Hitchings, A. B. Cairns, D. Allen, P. J. Saines
18:50 - 19:10 <b>L 02</b>	<b>Complex modulations of the crystal structure of functional oxides with perovskite-related structure</b> S. García-Martín, R. Marín-Gamero, E. Urones-Garrote, X. Martínez de Irujo-Labelde
19:10 - 19:30 <b>L 03</b>	<b>Perovskite-type <math>RbNbO_3</math> as a high-pressure polymorphism</b> A. Yamamoto, K. Murase, K. Sugiyama, T. Kawamata
19:30 - 19:50 <b>L 04</b>	<b>Chemical and physical pressure effects on structural and magnetic properties of <math>R_2CuTiO_6</math> perovskite series with R ranging from La to Lu</b> L. Sederholm, A. Yamamoto, M. Karppinen

MONDAY, JULY 10, 2023

8:00 - 12:00 **Registration**

*chairperson: Barbara Albert*

9:00 - 9:40 <b>PL 02</b>	<b>Solid-state batteries – at the edge between Solid State Chemistry and Materials Science</b> J. Janek
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### SESSION I

*chairperson: Duncan H. Gregory*

9:40 - 10:10 <b>InvL 03</b>	<b>Prediction of electrical conductivity of porous composites using 3D equivalent electronic circuit network model. Solid oxides fuel cell electrode case study</b> D. Budáč, V. Miloš, M. Carda, M. Paidar, K. Bouzek
10:10 - 10:30 <b>L 05</b>	<b>Critical current density of <math>Li_6PS_5Cl</math> powder pellets and processed films</b> A. Tron, A. Beutl

### SESSION II

*chairperson: Ivan Khalakhan*

9:40 - 10:10 <b>InvL 04</b>	<b>Synthesis-dependent structure-property relationships of quantum materials</b> L. Clark, J. N. Graham, J. R. Stewart, J. A. Cooley, M. Songvilay, G. Confalonieri, D. Fortes, P. Manuel, A. R. Wildes
10:10 - 10:30 <b>L 06</b>	<b>Quantum spin liquids in cation ordered perovskites</b> M. J. Milton, P. Manuel, J. P. Attfield

10:30 - 11:00 Coffee Break

## SESSION I

chairperson: Maarit Karppinen

11:00 - 11:20 <b>L 07</b>	<b>Lithium transport mechanisms characterised by ssNMR and ToF-SIMS in hybrid electrolytes for solid-state batteries</b> <a href="#">T. Meyer</a> , T. Gutel, M. Bardet, H. Manzanarez, E. De Vito
11:20 - 11:40 <b>L 08</b>	<b>Packings of sphere packings - a new path to solid state ionic conductors?</b> <a href="#">M. Petrik</a> , W. Hornfeck
11:40 - 12:00 <b>L 09</b>	<b>Growth of metal oxide film electrodes for electrochemical capacitor by electrospray deposition</b> <a href="#">M. P. Chavhan</a>
12:00 - 12:20 <b>L 10</b>	<b>New tungsten bronzes via electrochemical intercalation</b> <a href="#">B. Rasche</a> , I. Neumann, Y. Chen, M. Yang
12:20 - 12:40 <b>L 11</b>	<b>Composition-activity-stability relationship in Pt-Au alloys for oxygen reduction reaction</b> <a href="#">X.X. Xie</a> , V. Briega-Martos, R. Farris, M. Vorokhta, T. Skála, I. Matolínová, K. M. Neyman, S. Cherevko, I. Khalakhan

## SESSION II

chairperson: Lucy Clark

11:00 - 11:20 <b>L 12</b>	<b>Metal-insulator transitions in hollandite vanadate and chromate</b> <a href="#">M. Isobe</a> , P. Puphal, H. Takagi
11:20 - 11:40 <b>L 13</b>	<b>Fluoridoargentates(II) as potential analogues to superconducting cuprates</b> <a href="#">M. Dragomir</a> , M. Belak Vivod, M. Lozinšek, Z. Jagličić, G. King
11:40 - 12:00 <b>L 14</b>	<b>FeMn<sub>3</sub>Ge<sub>2</sub>Sn<sub>7</sub>O<sub>16</sub>: a "partial" spin-liquid candidate with a perfectly isotropic 2-D Kagomé Lattice</b> <a href="#">C. D. Ling</a> , M. C. Allison, S. Wurmehl, B. Büchner, J. L. Vella, T. Söhnel, S. A. Bräuninger, H.-H. Klauss
12:00 - 12:20 <b>L 15</b>	<b>Hidden orders in 2D van der Waals materials: The example of magnetic crossover in the mixed-anion compound CrSBr</b> <a href="#">S. A. López-Paz</a> , Z. Guguchia, V. Y. Pomjakushin, C. Witteveen, A. Cervellino, H. Luetkens, N. Casati, A. F. Morpurgo, F. O. von Rohr
12:20 - 12:40 <b>L 16</b>	<b>Solid-state synthesis of carbon-coated lithium vanadate Li<sub>3</sub>VO<sub>4</sub>- as anodes for High-Performance Li-ion Capacitors</b> <a href="#">S. Lonkar</a> , C. Busa

12:40 - 13:40 Lunch

chairperson: Jürgen Janek

13:40 - 14:20 <b>PL 03</b>	<b>Fast cation conductivity in complex metal halides &amp; hydrides; Prospects for solid state electrolytes</b> <a href="#">D. H. Gregory</a>
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## SESSION I

chairperson: Peter Matvija

14:20 - 14:50 <b>InvL 05</b>	<b>Probing fuel cell catalysts degradation under simulated operational environment by advanced in situ techniques</b> <a href="#">I. Khalakhan</a>
14:50 - 15:10 <b>L 17</b>	<b>Elucidating catalytic performance of a family of low-valent metal nitrides for the hydrogen evolution reaction from water</b> <a href="#">A. Y. Ganin</a> , Y. Sun, O. Guseynikova, Y. Zhou, N. López
15:10 - 15:30 <b>L 18</b>	<b>Understanding the performance of high power niobium oxide based Li ion battery materials</b> A. Green, E. Driscoll, <a href="#">P. Slater</a>

## SESSION II

chairperson: Karel Bouzek

14:20 - 14:50 <b>InvL 06</b>	<b>Discovery of quantum materials by combining chemical and physical design principles</b> <a href="#">F. O. von Rohr</a>
14:50 - 15:10 <b>L 19</b>	<b>Supraparticles as identifiers or temperature indicators with spectral magnetic readout</b> <a href="#">S. Müssig</a> , J. Reichstein, S. Wintzheimer, K. Mandel
15:10 - 15:30 <b>L 20</b>	<b>Crystal and electronic structure of the lanthanide dibismuthides REBi<sub>2</sub> (RE = La, Ce, Pr, Nd, Sm)</b> <a href="#">A. Ovchinnikov</a> , M. Ruck

15:30 - 16:00 Coffee Break

## SESSION I

*chairperson: Fabian von Rohr*

16:00 - 16:20	<b>New nickel-based lithium rich layered/disordered rock salt cathode materials for lithium ion batteries</b>
<b>L 21</b>	<u>B. Dong</u> , J. Castells-Gil, P. Zhu, L. Driscoll, P. Allan, E. Kendrick, P. Slater
16:20 - 16:40	<b>Operando investigation of Ir-Ru-based catalyst for Proton Exchange Membrane Water Electrolysis</b>
<b>L 22</b>	<u>T. Hrbek</u> , P. Kúš, M. G. Rodriguez, H. Nedumkulam, M. Mirolo, J. Drnec, V. Matolín, I. Matolínová
16:40 - 17:00	<b>The influence of Al and Ga doping on the chemical and electrochemical cycling of T-LiFeO<sub>2</sub></b>
<b>L 23</b>	<u>S. Mahato</u> , X. M. De Irujo Labalde, S. Booth, M. Hayward
17:00 - 17:20	<b>Designing new lithium layered oxides from sodium layered oxides to stabilize oxygen redox</b>
<b>L 24</b>	<u>M. Guignard</u> , V. Saïbi, L. Castro, I. Sugiyama, C. Delmas
17:20 - 17:40	<b>Sodium insertion into TiO<sub>2</sub> hollandite: structural and electrochemical study</b>
<b>L 25</b>	<u>F. García-Alvarado</u> , A. Duarte, P. Díaz-Carrasco, A. Kuhn, A. Basa
17:40 - 18:00	<b>F. García-Alvarado, A. Duarte, P. Díaz-Carrasco, A. Kuhn, A. Basa</b>
<b>L 26</b>	<u>A. Kuhn</u> , J. C. Pérez-Flores, M. Hoelzel, V. Díez-Gómez, I. Sobrados, J. Sanz, F. García-Alvarado

## SESSION II

*chairperson: Jianwen Jiang*

16:00 - 16:20	<b>Evidence for a disorder-induced spin liquid in the tuneable spin ladder-chain system Ba<sub>2</sub>CuTe<sub>1-x</sub>W<sub>x</sub>O<sub>6</sub> (0 ≤ x ≤ 0.3)</b>
<b>L 27</b>	<u>O. Mustonen</u> , C. Pughe, A. Gibbs, A. Yaresko, P. Baker, L. Mangin-Thro, H. C. Walker, E.J. Cussen
16:20 - 16:40	<b>Structural variations of the magnetic topological insulators Mn<sub>1+x</sub>Sb<sub>2-2x</sub>/3Te<sub>4</sub></b>
<b>L 28</b>	<u>E. Kochetkova</u> , O. Renier, A. Isaeva, M. Sahoo, L.T. Corredor
16:40 - 17:00	<b>2D-Metals with locked charge density wave, in the novel layered monophosphate tungsten bronzes [Ba(PO<sub>4</sub>)<sub>2</sub>]<sub>W</sub>mO<sub>3m-3</sub></b>
<b>L 29</b>	<u>H. Nimoh</u> , R. Glaum, A. Cano, A. M. Arévalo-López, O. Mentré
17:00 - 17:20	<b>Experimental investigation of magnetic dilution effect on the frustrated quantum antiferromagnet SrCu<sub>2</sub>(BO<sub>3</sub>)<sub>2</sub></b>
<b>L 30</b>	<u>L. Šibav</u> , G. King, Z. Jagličić, M. Koblar, M. Otoničar, D. Arčon, M. Dragomir
17:20 - 17:40	<b>Magnetic structures of Dirac nodal-line semimetals LnSbTe</b>
<b>L 31</b>	<u>I. Plokhikh</u>

18:00 - 20:00	<b>POSTER SESSION I</b>
<b>P 01</b>	<b>Nitridooxorhenate and -technetate anions [MO<sub>3</sub>N]<sub>2</sub><sup>-</sup> (M = Tc, Re) from reactions in highly alkaline media</b> <u>D. Badea</u> , E. Strub, J. Bruns
<b>P 02</b>	<b>Ternary Alkali metal Thallides ATI (A=K/Rb, Cs/Rb)</b> <u>V. F. Schwinghammer</u> , S. Gärtner
<b>P 03</b>	<b>Solution combustion synthesis of thermodynamically metastable oxide-phosphates with rutile- and anatase-related structures</b> <u>S. Früchtnicht</u> , M. Weber, R. Glaum
<b>P 04</b>	<b>Ferroelectric Properties on Ba<sub>0.975</sub>Ln<sub>0.017</sub> (Zr<sub>x</sub>Ti<sub>0.95-x</sub>) Sn<sub>0.05</sub>O<sub>3</sub> Materials</b> <u>K. Taïbi</u> , S. Zemouri-Smail, A. Lahmar
<b>P 05</b>	<b>Electrocrystallisation of Ternary Amalgams</b> <u>D. Kraut</u> , C. Hoch
<b>P 06</b>	<b>Cs<sub>2</sub>O as a strong oxidiser - A new synthetic route towards oxometalates</b> <u>I. Zaytseva</u> , C. Hoch
<b>P 07</b>	<b>Novel representatives of the structure type Na<sub>7</sub>RbTi<sub>4</sub> with the lighter homologue Indium</b> <u>M. Janesch</u> , S. Gärtner
<b>P 08</b>	<b>High-pressure Synthesis of Alkaline Metal Niobates with Tetragonal Tungsten Bronze-type Structure</b> <u>K. Murase</u> , T. Sato, A. Yamamoto, K. Sugiyama
<b>P 09</b>	<b>Anion Redox in Lithium Main-group Metal Oxides</b> <u>Z. Chen</u> , S. Mahato, X. M. De Irujo Labalde, M. Hayward
<b>P 10</b>	<b>Synthesis and characterisation of lanthanum zirconate as a candidate filler material for polymer derived ceramic coatings</b> <u>P. N. Moghaddam</u> , M. Parchovianský, I. Parchovianská, A. Pakseresht
<b>P 11</b>	<b>Investigation of structure and luminescence properties of bismuth-based coordination polymers with N-donor ligands</b> <u>K. V. Borysova</u> , J. R. Sorg, E. A. Mikhalyova, K. Müller-Buschbaum

<b>P 12</b>	<b>Tin-Boroxines-Based Inorganic-Organic Macrocycles: Synthesis, Characterization and Hydrophobicity</b> <u>M. Novák</u> , M. Bouška, Š. Podzimek, R. Jambor
<b>P 13</b>	<b>High-Pressure Synthesis of SmSi<sub>3</sub></b> <u>T. Neziraj</u> , S. Wirth, Y. Grin, U. Schwarz
<b>P 14</b>	<b>Mixed-metal monophosphate tungsten bronzes containing divalent transition metal ions (MII: Fe, Co, Ni) and tungsten(VI)</b> <u>L. K. Aymans</u> , R. Glaum
<b>P 15</b>	<b>Amino acid crystals as high-performance, eco-friendly structural health monitors</b> <u>K. Hari</u> , S. Bhattacharya, S. Guerin
<b>P 16</b>	<b>High temperature magnetic ordering in new quadruple perovskites Sr<sub>4</sub>NaM<sub>3</sub>O<sub>12</sub> (M = Ru and Os)</b> <u>G. S. Thakur</u> , T. Doert, T. Hansen, E. Osmic, W. Schnelle, T. Herrmannsdörfer, M. Ruck
<b>P 17</b>	<b>Effect of concentration of conductive polymers in zinc-pigmented epoxy-ester based anticorrosive coatings</b> <u>Y. Raycha</u> , M. Kohl, A. Kalendová
<b>P 18</b>	<b>Oligothiophene Dendron-Modified CdS Nanoparticles and Their Optical Properties</b> <u>A. Yoshida</u> , R. Nozawa, Y. Sakagami, M. Matsubara, A. Mori, A. Muramatsu, K. Kanie
<b>P 19</b>	<b>Synthesis and characterization of glass and crystalline compositions in the (Na<sub>2</sub>Se)<sub>x</sub>(As<sub>2</sub>Se<sub>3</sub>)<sub>1-x</sub> chalcogenide system</b> <u>A. Sammoury</u> , M. Kassem, M. Bokova, T. Hamieh, J. Toufaily, E. Bychkov
<b>P 20</b>	<b>Influence of twill fabric topography on bloodstain pattern shape</b> <u>S. Brnada</u> , A. Kalazic
<b>P 21</b>	<b>Assessing the local structure and quantifying defects in Ca<sub>4</sub>Fe<sub>9</sub>O<sub>17</sub> combining STEM and FAULTS</b> <u>J. Oró-Solé</u> , J. Serrano-Sevillano, J. Gázquez, C. Frontera, A. P. Black, M. Casas-Cabanas, M. Rosa Palacín
<b>P 22</b>	<b>Resonant Properties of Polycrystalline Biomolecular Assemblies</b> <u>T. E. Ryan</u> , S. Guerin
<b>P 23</b>	<b>Polysulfide in-situ characterization with 3D electron diffraction for Lithium-Sulfur batteries</b> <u>S. Rahimi</u> , A. Hajizadeh, J. Hadermann
<b>P 24</b>	<b>In-situ 3D ED to study the structural transformation of NMC during electrochemical reactions</b> <u>A. Hajizadeh</u> , S. Rahimi, J. Hadermann
<b>P 25</b>	<b>Bloodstain pattern analysis using shape descriptors</b> <u>A. Kalazic</u> , S. Brnada
<b>P 26</b>	<b>The effects of alkali metal intercalation on the structure and superconductivity of Niobium Selenide.</b> <u>K. Steele</u> , S. J. Clarke
<b>P 27</b>	<b>Discovery of superconductivity in Nb<sub>4</sub>SiSb<sub>2</sub> with a V<sub>4</sub>SiSb<sub>2</sub>-type structure and implications of interstitial doping on its physical properties</b> <u>M. D. Balestra</u> , O. Atanov, O. Blacque, R. Lefèvre, Y. H. Ng, R. Lortz, F. O. von Rohr

## TUESDAY, JULY 11, 2023

*chairperson: Spyros Yannopoulos*

9:00 - 9:40	<b>Phase change optical memory materials: Why are alloys of Ge, Sb, and Te almost the only materials of choice?</b> <u>R. O. Jones</u>
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### SESSION I

*chairperson: Jiří Orava*

9:40 - 10:10	<b>Chalcogenide glasses and fibers for photonic applications in the infrared</b> <u>J.-L. Adam</u> , J. Trolès, C. Boussard-Plédel, X.H. Zhang
10:10 - 10:30	<b>Light-induced surface microstructures on Ge-As-S glasses</b> <u>E. Samsonova</u> , P. Kutálek, E. Černošková, P. Knotek, J. Schwarz

### SESSION II

*chairperson: Joke Hadermann*

9:40 - 10:10	<b>Polymorphism and magnetic properties in high pressure A-site manganites</b> <u>E. Solana-Madruga</u>
10:10 - 10:30	<b>Locking any magnetization by freezing of magnetic domains in a transient soft to super-hard magnet</b> <u>O. Mentré</u> , B. Leclercq, A. Pautrat, A.M. Arevalo-Lopez, S. petit, V. Stolyarov

10:30 - 11:00 Coffee Break

## SESSION I

chairperson: Miroslav Vlček

11:00 - 11:20	<b>Er<sup>3+</sup>-doped TeO<sub>2</sub>-ZnO-La<sub>2</sub>O<sub>3</sub> optical glasses</b> <b>L 34</b>	<a href="#">J. Suský</a> , <a href="#">S. Šlang</a> , <a href="#">L. Beneš</a> , <a href="#">B. Frumarová</a> , <a href="#">R. Svoboda</a> , <a href="#">T. Wágner</a> , <a href="#">L. Střížík</a>
11:20 - 11:40	<b>Structural analyses and properties of complex sulphides in the Cr-Sn-S system</b> <b>L 35</b>	<a href="#">F. Guiot</a> , <a href="#">V. Dorcet</a> , <a href="#">E. Guilmeau</a> , <a href="#">B. Malaman</a> , <a href="#">T. Schweitzer</a> , <a href="#">P. Lemoine</a> , <a href="#">C. Prestipino</a>
11:40 - 12:00	<b>Holmium-doped TeO<sub>2</sub>-ZnO-La<sub>2</sub>O<sub>3</sub> tellurite glasses for photonics applications and fibre optics</b> <b>L 36</b>	<a href="#">J. Hrabovsky</a> , <a href="#">F. Desevedavy</a> , <a href="#">L. Strizik</a> , <a href="#">J. Oswald</a> , <a href="#">L. Nowak</a> , <a href="#">T. Wagner</a> , <a href="#">F. Smektala</a> , <a href="#">M. Veis</a>
12:00 - 12:20	<b>Gold(I)-thiolate coordination polymers as transparent glasses and cyclic phase-changing materials</b> <b>L 37</b>	<a href="#">S. Vaidya</a> , <a href="#">O. Veselska</a> , <a href="#">Z. Fan</a> , <a href="#">A. Zhadan</a> , <a href="#">A. Fateeva</a> , <a href="#">P. Bordet</a> , <a href="#">S. Horike</a> , <a href="#">A. Demessence</a>
12:20 - 12:40	<b>Tuning the metallic glasses properties via ultrafast heating/cooling</b> <b>L 38</b>	<a href="#">J. Orava</a> , <a href="#">Y. H. Sun</a> , <a href="#">I. Kaban</a>

## SESSION II

chairperson: Elena Solana-Madruga

11:00 - 11:20	<b>Cation ordered doping of ferrite perovskites: influence on redox behaviour, magnetism, and mixed ionic electronic conductivity</b> <b>L 39</b>	<a href="#">A. J. Brown</a> , <a href="#">O. Wagstaff</a> , <a href="#">A. Manjón-Sanz</a> , <a href="#">H. Brand</a> , <a href="#">M. Avdeev</a> , <a href="#">I. Evans</a> , <a href="#">C. D. Ling</a>
11:20 - 11:40	<b>Understanding the texture degree on zinc aluminate Nd, Ce sub-micrometer films by screen printing for NIR emitting applications</b> <b>L 40</b>	<a href="#">R. E. Rojas-Hernandez</a> , <a href="#">F. Rubio-Marcos</a> , <a href="#">J. F. Fernandez</a> , <a href="#">I. Hussainova</a>
11:40 - 12:00	<b>Many body localisation in CeMnAsO<sub>1-x</sub>F<sub>x</sub>?</b> <b>L 41</b>	<a href="#">A. C. McLaughlin</a> , <a href="#">G. Lawrence</a> , <a href="#">S. Simpson</a> , <a href="#">E. J. Wildman</a>
12:00 - 12:20	<b>V-V dimerization in MnVO<sub>3</sub> ilmenite low-pressure polymorph: Crystal and magnetic structures and properties</b> <b>L 42</b>	<a href="#">A. M. Arévalo-López</a> , <a href="#">D. Khalyavin</a> , <a href="#">O. Mentré</a>
12:20 - 12:40	<b>Multifunctional coordination polymers for fluorescent sensing of VOCs and hazardous ions from contaminated water</b> <b>L 43</b>	<a href="#">K. A. Siddiqui</a>

12:40 - 13:40 Lunch

chairperson: Paul Attfield

13:40 - 14:20	<b>New possibilities in in situ and ex situ crystal structure determination based upon 3D ED</b> <b>PL 05</b>	<a href="#">R. Poppe</a> , <a href="#">D. Vandemeulebroucke</a> , <a href="#">M. Quintelier</a> , <a href="#">A. Hazijadeh</a> , <a href="#">S. Rahimi</a> , <a href="#">S. Gholam</a> , <a href="#">M. Batuk</a> , <a href="#">J. Hadermann</a>
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## SESSION I

chairperson: Olivier Mentré

14:20 - 14:50	<b>In-situ characterization of gas-solid interfaces by near-ambient pressure X-ray photoelectron spectroscopy</b> <b>InvL 09</b>	<a href="#">M. Vorokhta</a> , <a href="#">L. Piliai</a> , <a href="#">T.N. Dinhová</a> , <a href="#">P. Matvija</a> , <a href="#">I. Matolinová</a>
14:50 - 15:20	<b>Bias-free graphene-based in situ TEM observation of electrode materials for batteries</b> <b>InvL 10</b>	<a href="#">J. Y. Cheong</a> , <a href="#">J. H. Chang</a>
15:20 - 15:40	<b>Structural investigation of new Li ion containing oxides using combined diffraction and NMR and EXAFS spectroscopy</b> <b>L 44</b>	<a href="#">F. N. Sayed</a> , <a href="#">Q. Jacquet</a> , <a href="#">P. Groszewicz</a> , <a href="#">S. P. Emge</a> , <a href="#">P. C. M. M. Magusin</a> , <a href="#">C. O'Keefe</a> , <a href="#">S. Dey</a> , <a href="#">C. Kocer</a> , <a href="#">A. Morris</a> , <a href="#">C. P. Grey</a>

## SESSION II

chairperson: Martin Sahlberg

14:20 - 14:50	<b>Investigating the catalytic potential of iron-doped calcium titanate: a study of oxide vacancy structures and microstructures</b> <b>InvL 11</b>	<a href="#">M. Amano Patino</a> , <a href="#">M. Ibrahim</a> , <a href="#">N. Frederich</a> , <a href="#">H. Kaper</a> , <a href="#">M. Ceretti</a> , <a href="#">W. Paulus</a>
14:50 - 15:10	<b>Theoretical insights into the monolayer adsorption and characterization of HB238 merocyanine on Ag(100) surface</b> <b>L 45</b>	<a href="#">R. Tomar</a> , <a href="#">A. Kny</a> , <a href="#">M. Sokolowski</a> , <a href="#">T. Bredow</a>
15:10 - 15:30	<b>Understanding the synthetic reliability of Na<sub>x</sub>MnO<sub>2</sub> and similar layered phases</b> <b>L 46</b>	<a href="#">J. Beecham-Lonsdale</a> , <a href="#">D. C. Arnold</a> , <a href="#">S. Ramos-Perez</a>

15:30 - 16:00 Coffee Break

## SESSION I

chairperson: Claus Feldmann

16:00 - 16:20	<b>X-ray photoelectron spectroscopy: a key tool for assessment of 2D molybdenum dichalcogenides synthesized by ALD</b> L 47 J. Rodriguez-Pereira, R. Zazpe, J. Charvot, F. Bures, J.M. Macak
16:20 - 16:40	<b>Charge density refinement on inorganic crystals using electron diffraction</b> L 48 E. Yörük, A. Suresh, P. Brázda, M. K. Cabaj L. Palatinus
16:40 - 17:00	<b>Chemistry at the nanoscale: AFM meets IR spectroscopy</b> L 49 J. Horák
17:00 - 17:20	<b>CeScSi-type intermetallics: Modulation of magnetic properties through light elements insertion and catalysis of ammonia</b> L 50 E. Gaudin, K. Alabd, C. Croisé, F. Can, X. Courtois, N. Bion, A. Villesuzanne, S. Tencé
17:20 - 17:40	<b>Analysis of ground particle behavior in wet ball milling by DEM-CFD simulation</b> L 51 K. Kushimoto, J. Kano

## SESSION II

chairperson: Helmer Fjellvag

16:00 - 16:20	<b>Optomagnetic composites by combination of strong magnetic and luminescent components</b> L 52 K. Müller-Buschbaum, M. Seuffert, T. Wehner
16:20 - 16:40	<b>Exploring structure-property correlations in the frustrated layered material, Mn<sub>2</sub>Mo<sub>3</sub>O<sub>8</sub></b> L 53 D. C. Arnold, H. L. McPhillips, S. Ramos
16:40 - 17:00	<b>Developments in high-pressure growth of rare earth nickelates single crystals</b> L 54 D. J. Gawryluk
17:00 - 17:20	<b>Tuning physicochemical properties in TbMgNi<sub>4-x</sub>Cox-(H,D)<sub>2</sub> system</b> L 55 V. Shtender
17:20 - 17:40	<b>Magnetic properties controlled by short-range structural and spin order in layered materials</b> L 56 J. D. Bocarsly, S. E. Dutton, C. P. Grey

18:00 - 20:00	<b>POSTER SESSION II</b>
P 28	<b>Selective ion transport of catalytic hybrid aerofilm Li-S batteries</b> C. Senthil, S.S. Kim, H.S. Kim, J.W. Hong, H.Y. Jung
P 29	<b>Solid-state electrolytes for Na-ion batteries: exploring the synergy between metal-organic frameworks and ionic liquids</b> A. Mirandona-Olaeta, E. Goikolea, S. Lanceros-Mendez, A. Fidalgo-Marijuan, I. Ruiz de Larramendi
P 30	<b>Understanding Fe-cation migration in LiFe<sub>2-x</sub>In<sub>x</sub>SbO<sub>6</sub> Cathode Materials</b> X. Martinez de Irujo-Labalde, S. Mahato, M. Hayward
P 31	<b>Synthesis of Low-Pt-Based Electrocatalyst Derived from Porous MOF-808(Zr)-NH<sub>2</sub> Nanoparticles Towards Oxygen Reduction Reaction</b> T. M. Pham, J. Kim
P 32	<b>Upcycling Lithium Titanate (LTO) Anodes into the Next Generation of High Power Ti Doped Nb<sub>2</sub>O<sub>5</sub> Anodes (TNO).</b> A. J. Green, E. H. Driscoll, P. R. Slater
P 33	<b>Investigation of electrochemical properties of Zn-ion batteries based on ZnMo<sub>6</sub>S<sub>8</sub> cathodes</b> Y. Wang, A. Y. Ganin
P 34	<b>Crystal chemistry of Argyrodite type Li-ion conductors</b> D. Shanbhag, J. Auvergniot, V. Viallet, C. Masquelier
P 35	<b>Boosting the electrochemical performance of TNO anode material through structural and compositional modifications</b> E. García-González, A. Solana-Bello, F. García-Alvarado
P 36	<b>Fe-substituted LiTi<sub>2</sub>O<sub>4</sub> ramsdellite as electrode material in lithium batteries</b> P. Díaz-Carrasco, A. Kuhn, N. Menéndez, F. García-Alvarado
P 37	<b>Fabrication and characterization of Cu, Zn-doped Li<sub>4</sub>Ti<sub>5</sub>O<sub>12</sub> anode nanomaterials for energy conversion applications</b> J. Dhairat, B. A. Albiss, A. Bozeyya
P 38	<b>Alloy Nanowire Arrays With Controlled Compositions Templated by Block Copolymers</b> O. Burg, R. Shenhar
P 39	<b>Local Structure Insight into Hydrogen Evolution Reaction with Bimetal Nanocatalysts</b> Q. Li, X. Xing

<b>P 40</b>	<b>Impact of Surfactant-Assisted Downsizing to Luminescent nanoMOFs on Morphological and Photophysical Properties</b> M. Maxeiner, L. Wittig, A. Sedykh, T. Kasper, K. Müller-Buschbaum
<b>P 41</b>	<b>Hydrophobic materials based on heteroboroxines</b> R. Jambor, M. Srb, M. Novák
<b>P 42</b>	<b>Preparation of GeTe nanoparticles by low temperature synthetic method</b> M. Bouška, Y. Milasheuskaya, R. Jambor, P. Němec
<b>P 43</b>	<b>High-spin vs low-spin Ni<sup>2+</sup> ions in highly distended octahedral environments: Sr<sub>2</sub>NiO<sub>2</sub>Cu<sub>2</sub>Se<sub>2</sub>, Sr<sub>2</sub>NiO<sub>2</sub>Cu<sub>2</sub>S<sub>2</sub> and the solid solution Sr<sub>2</sub>NiO<sub>2</sub>Cu<sub>2</sub>(Se<sub>1-x</sub>S<sub>x</sub>)<sub>2</sub></b> R. D. Smyth, J. N. Blandy, Z. Yu, S. Liu, C. V. Topping, S. J. Cassidy, C. F. Smura, D. N. Woodruff, P. Manuel, C. L. Bull, N. P. Funnell, J. E. McGrady, S. J. Clarke
<b>P 44</b>	<b>Complex magnetic ordering of the mixed-valent layered oxychalcogenides Ca<sub>2</sub>Fe<sub>2.6</sub>O<sub>3</sub>S(2-x)Se(x) (x=0, 0.5, 1, 1.5)</b> A. Gillette, B. Sheath, S. J. Clarke
<b>P 45</b>	<b>Tuning magnetism and superconductivity in transition metal chalcogenides as a function of composition</b> L. Taskesen, S. J. Clarke
<b>P 46</b>	<b>Lattice Dynamics of Cs<sub>2</sub>[Mo<sub>2</sub>O<sub>7</sub>]*CsX (X = Cl, Br, I)</b> A. K. Weber, K. Denisova, P. Lemmens, A. Möller
<b>P 47</b>	<b>Novel Oxochloridoselenites(IV) with Cuban-derived Structural Motives</b> M. A. Bonnin, C. Feldmann
<b>P 48</b>	<b>Wurtzite-Type Be<sub>2</sub>PN<sub>3</sub> - a new and hard-type material</b> G. Krach, M. Pointner, K. Witthaut, W. Schnick
<b>P 49</b>	<b>Ionic-liquid-based synthesis of Ge<sub>3</sub>N<sub>4</sub> nanoparticles</b> F. Jung, C. Feldmann
<b>P 50</b>	<b>Structural Influence of Lone Pairs in GeP<sub>2</sub>N<sub>4</sub>, a Germanium(II) Nitridophosphate</b> S. J. Ambach, C. Somers, T. de Boer, L. Eisenburger, A. Moewes, W. Schnick
<b>P 51</b>	<b>Ca<sub>5</sub>AsSb(NH)<sub>2</sub> – a cation-deficient Antiperovskite with A-site ordering</b> T. Chau, S. Rudel, D. Han, F. Wolf, T. Bein, H. Ebert, W. Schnick
<b>P 52</b>	<b>Morin transition in beta-Fe<sub>2</sub>SeO</b> N. Qureshi, R. Morrow, S. Eltokhy, V. Grinenko, Y. A. Onykienko, D. S. Inosov, M. Valldor
<b>P 53</b>	<b>Electron-Electron and Electron-Phonon Interactions in van-der-Waals compounds: MOX, M = Sc, Ti, V, Fe and X=Cl, Br</b> F. Predelli, F. Büscher, P. Lemmens, V. P. Gnezdilov, Yu. G. Pashkevich, T. N. Shevtsova, S. Berinskat, A. Möller
<b>P 54</b>	<b>Intercalation chemistry of excitonic insulator candidate Ta<sub>2</sub>NiSe<sub>5</sub></b> P. A. Hyde, J. Cen, S. J. Cassidy, N. H. Rees, P. Holdship, R. I. Smit, D. O. Scanlo, S. J. Clarke
<b>P 55</b>	<b>Functionalisation of CaAl<sub>2</sub>O<sub>4</sub>:Eu<sup>2+</sup>, Nd<sup>3+</sup> phosphors with Fe<sub>3</sub>O<sub>4</sub> magnetic nanoparticles</b> S. T. Tsantis, G. Kastrinaki, V. Zaspalis, C. Sarafidis, C. Chatzidoukas, S. N. Yannopoulos
<b>P 56</b>	<b>Transition metal doping strategy for the reversible anion redox process</b> A. Wang, Z. Chen, M. Hayward

## WEDNESDAY, JULY 12, 2023

*chairperson: Robert Jones*

9:00 - 9:40	<b>Exploring new transition metal nitride materials</b>
<b>PL 06</b>	A. Fuertes

### SESSION I

*chairperson: Midori Amano Patino*

9:40 - 10:10	<b>Compositionally complex alloys for the hydrogen society</b>
<b>InvL 12</b>	M. Sahlberg
10:10 - 10:30	<b>Crystal growth of new uranium and transuranic phases via high temperature solution and mild hydrothermal methods: Exploration of new materials as potential nuclear waste forms</b>
<b>L 57</b>	H.-C. zur Loye, T. K. Deason, A. T. Hines, H. Tisdale, T. M. Besmann, J. Amoroso, D. P. DiPrete

### SESSION II

*chairperson: Jean-Luc Adam*

9:40 - 10:10	<b>Mineral-inspired sulphides for thermoelectric energy harvesting</b>
<b>InvL 13</b>	A.V. Powell

10:10 - 10:30 <b>L 58</b>	<b>In-situ XRD and PDF investigation of battery fluoride materials MF<sub>3</sub>.3H<sub>2</sub>O (M = Fe, Cr) in controlled atmosphere: accessing new phases with controlled chemistry</b> G. Nénert, L. Ding, K. Forsberg, C. V. Colin
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10:30 - 11:00 Coffee Break

## SESSION I

*chairperson: Amparo Fuertes*

11:00 - 11:20 <b>L 59</b>	<b>A facile preparation of Y<sub>2</sub>O<sub>3</sub>S nanoparticles through sulfidation under a CS<sub>2</sub> atmosphere</b> Y. Kanazawa, M. Matsubara, R. Ohsuga, A. Muramatsu, K. Domen, K. Kanie
11:20 - 11:40 <b>L 60</b>	<b>Mechanochemical process to prepare amorphous oxides precursor with isomorphous substitution of Si(IV) by heteroatoms and successive hydrothermal synthesis to crystalize zeolites</b> A. Muramatsu, H. Kobayashi, G. Tanaka, M. Yabushita, R. Osuga, K. Ninomiya, M. Matsubara, S. Maki, M. Nishibori, K. Kanie
11:40 - 12:00 <b>L 61</b>	<b>Alkali shuffling in honeycomb layered oxides</b> E. Mumba-Mpanga, R. Berthelot
12:00 - 12:20 <b>L 62</b>	<b>Inorganic materials synthesis in ultra-alkaline hydroflux</b> H. He, Y. Li, R. Albrecht, M. Ruck
12:20 - 12:40 <b>L 63</b>	<b>Anion redox as a means to derive layered manganese oxychalcogenides with exotic intergrowth structures</b> S. Giri, S. Sasaki, S. Cassidy, S. Dey, G. Cibin, C. Grey, S. Clarke

## SESSION II

*chairperson: Flaviano Garcia-Alvarado*

11:00 - 11:20 <b>L 64</b>	<b>Quadrature frequency resolved spectroscopy on green upconversion photoluminescence in GeGa(As)S:Er<sup>3+</sup> CHALCOGENIDE GLASSES</b> L. Strizik, T. Aoki, V. Prokop, J. Hrabovsky, T. Wagner
11:20 - 11:40 <b>L 65</b>	<b>TESCAN's Analytical Solutions for Lithium-Ion Battery Research</b> J. Honč, T. Šamořil, J. Dluhoř, T. Sui, X. Yao
11:40 - 12:00 <b>L 66</b>	<b>Local structure and high performance catalysts</b> X. Xing, Q. Li
12:00 - 12:20 <b>L 67</b>	<b>Defect engineering: Eu<sup>3+</sup> emission enhancement via induced local distortion</b> S. C. S. Lemos, M. Assis, L. Gracia, L. K. Ribeiro, A. F. Gouveia, Y. G. Galvão, E. Cordocillo, R. C. Lima, E. Longo, J. Andrés
12:20 - 12:40 <b>L 68</b>	<b>Urinary oxidative stress sensor based on zinc oxide nanorods</b> A. Ejaz, D. Gibson, C. Garcia Nuñez

12:40 - 13:40 Lunch

## SESSION I

*chairperson: Anthony V. Powell*

13:40 - 14:10 <b>InvL 14</b>	<b>Reaction mechanisms in molten salts for the design of solid-state materials at the nanoscale</b> D. Portehault, F. Igoa Saldaña, E. de Rolland Dalon, M. Baron, A. Ghoridi, A. Séné, E. Defoy, Y. Song, P.-O. Autran, D. Thiaudière
14:10 - 14:30 <b>L 69</b>	<b>Tecto-borosulfates—syntheses, structures and properties</b> E. Turgunbajew, P. Netzsch, M. Hämmer, G. Buchner, H. A. Höpfe
14:30 - 14:50 <b>L 70</b>	<b>Crystal structures of new phosphidosilicates and its homologues</b> D. Johrendt, A. Haffner, V. Weippert, J. Aicher, K. Witthaut
14:50 - 15:10 <b>L 71</b>	<b>Exploring trirutile materials as a platform for energy storage</b> E. Djafri, D. Arnold, O. Mentré
15:10 - 15:30 <b>L 72</b>	<b>Understanding the formation mechanism of intermetallic nanoparticles in polyol processes</b> M. Smuda, J. Ströh, N. Pienack, A. Khadiev, H. Terraschke, M. Ruck, T. Doert

## SESSION II

*chairperson: Mirela Dragomir*

13:40 - 14:10 <b>InvL 15</b>	<b>Nanostructured thin-film catalysts for hydrogen production via PEM water electrolysis</b> P. Kúř, T. Hrbek, H. Nedumkulam, M. Mirolo, I. Martens, J. Drnec, I. Matolínová
14:10 - 14:30 <b>L 73</b>	<b>Structural trends and ion diffusion mechanisms in the postspinel-type NaFe<sub>1+x</sub>Ru<sub>1-x</sub>O<sub>4</sub> system</b> L. Benincasa, M. Duttine, M. Suchomel, M. Guignard
14:30 - 14:50 <b>L 74</b>	<b>Base-metal nanoparticles as reactants at room temperature</b> C. Feldmann



14:50 - 15:10	<b>Functionalization of chalcogenide IR photonic sensor by polymer membrane for the purpose of detecting aromatic hydrocarbon pollutants in water</b>
<b>L 75</b>	<u>M. Vrazel</u> , R. K. Ismail, M. Baillieul, P. Nemeč, P. Loulergue, A. Szymczyk, K. Boukerma, R. Courson, A. Hammouti, L. Bodiou, J. Charrier, T. Halenkovic, M. Bouska, V. Nazabal
15:10 - 15:30	<b>Soft chemistry of layered titanium and vanadium oxytellurides</b>
<b>L 76</b>	<u>N. D. Kelly</u> , S. J. Clarke

15:30 - 16:00 Coffee Break

## SESSION I

*chairperson: Peter Kúš*

16:00 - 16:20	<b>Thermal transformations and cation redistribution on A<sub>2</sub>B<sub>2</sub>O<sub>6</sub> oxides</b>
<b>L 77</b>	<u>K. Ji</u> , E. Solana-Madruga, M. A. Patino, Y. Shimakawa, J. P. Attfield
16:20 - 16:40	<b>Photoluminescence properties of nanocrystalline multicomponent garnet Gd<sub>3</sub>Sc<sub>x</sub>Ga<sub>5-x</sub>O<sub>12</sub> doped with Er<sup>3+</sup></b>
<b>L 78</b>	<u>T. Netolicky</u> , L. Benes, S. Slang, B. Frumarova, J. Oswald, T. Wagner
16:40 - 17:00	<b>Borosulfates – silicate analogue anions with the potential to stabilize polycations</b>
<b>L 79</b>	<u>J. Bruns</u>
17:00 - 17:20	<b>Characterisation of Rh<sup>4+</sup> oxides, an unusual case of pyrochlore stabilisation under high pressure, high temperature synthesis conditions</b>
<b>L 80</b>	<u>S. D. Injac</u> , B. Mullens, F. Denis Romero, M. Avdeev, C. Barnett, A. K. L. Yuen, B. J. Kennedy, Y. Shimakawa
17:20 - 17:40	<b>Alkali metal oxide mercurides with isolated mercuride anions</b>
<b>L 81</b>	L. Nusser, S. Feldl, <u>C. Hoch</u>

## SESSION II

*chairperson: Jun Young Cheong*

16:00 - 16:20	<b>Synthesis and characterization of a novel oxychloride, SrTe<sub>2</sub>FeO<sub>6</sub>Cl</b>
<b>L 82</b>	<u>J. A. Sannes</u> , B. Gonano, Ø. S. Fjellvåg, S. Kumar, O. Nilsen, M. Valldor
16:20 - 16:40	<b>The absence of expected paramagnetic behavior in Ba<sub>6</sub>Fe<sub>2</sub>Te<sub>3</sub>S<sub>7</sub></b>
<b>L 83</b>	<u>E. H. Frøen</u> , P. Adler, M. Valldor
16:40 - 17:00	<b>Oxides as Pt catchment materials in the ammonia oxidation process - methodology and mechanistic insight</b>
<b>L 84</b>	<u>J. Hessevik</u> , A. S. Fjellvåg, O. Iveland, C. S. Carlsen, H. Sønsteby, T. By, J. Skjelstad, D. Waller, H. Fjellvåg, A. O. Sjøstad
17:00 - 17:20	<b>Probing for dynamics in a strongly frustrated magnet</b>
<b>L 85</b>	<u>L. Kubíčková</u> , A. K. Weber, M. Panthöfer, A. Möller
17:20 - 17:40	<b>Chemical pressure driving phase transition and morphology in Eu<sup>3+</sup>-doped KY<sub>3</sub>F<sub>10</sub>: An experimental and theoretical insight</b>
<b>L 86</b>	<u>P. Serna-Gallén</u> , S. C. S. Lemos, L. Gracia, E. O. Gomes, H. Beltrán-Mir, E. Cordoncillo, J. Andrés
17:40 - 18:00	<b>Closing Ceremony</b>
	Tomas Wagner