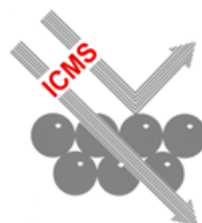


CPSSC 16

Challenges and Prospects for Solid State Chemistry



Book of
Abstracts

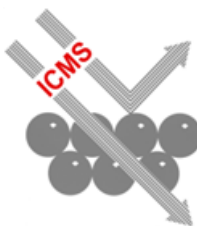


Book of Abstracts

CHALLENGES AND PROSPECTS FOR SOLID STATE CHEMISTRY

University of Sevilla, 9 and 10 September 2016

SUPPORTED BY



CHALLENGES AND PROSPECTS FOR SOLID STATE CHEMISTRY

This Discussion Meeting of the EuCheMS Division of Solid State and Materials Chemistry is focused on the latest developments in synthesis, properties, and structural investigations of solids. The meeting has been held just before the 6th EuCheMS Congress, 11-15 September (euchems-seville2016.eu/).

Topics included:

- Frontiers of solid materials synthesis - FSM
- Structural advances through new methodology – SAM
- Solid state chemistry and applications - SSC
- Rationales for functional materials synthesis - RFM

The conference includes plenary invited talks and poster presentations.

ORGANIZING COMMITTEE

Paul Attfield, University of Edinburgh

Alfonso Caballero, University of Seville and ICMS-CSIC

Martin Jansen, MPI Stuttgart

Antoine Maignan, University of Caen

Emilio Moran, Complutense University Madrid

Jose Antonio Odriozola, University of Seville and ICMS-CSIC

CHALLENGES AND PROSPECTS FOR SOLID STATE CHEMISTRY

University of Sevilla, 9 and 10 September 2016

Program

Friday, 9 September 2016

- 09:00 - 09:30 Registration
- 09:30 - 10:00 Opening Remarks
- Prof. José Antonio Odriozola, Organizing Committee
Prof. Pilar Malet Maenner, Dean of the Chemistry Department
Prof. Martin Jansen, Chair of Division
- Frontiers of solid materials synthesis***
- Chair: *Maria Gracia Francesconi*
- 10:00 - 10:50 Ullrich Haussermann, Stockholm University
"Hydrogen incorporation in Zintl phases and transition metal oxides– new environments for the lightest element in the solid state"
- 10:50 - 11:30 COFFEE BREAK
- Chair: *Alfonso Caballero Martínez*
- 11:30 - 12:20 Andrei Shevelkov, Moscow State University
"Back to the Iron Age: Structure and properties of iron compounds with strong electron correlations"
- 12:20 - 13:10 Amparo Fuertes, ICMAB Barcelona
"New developments in the chemistry of oxynitride materials"
- 13:10 - 15:00 LUNCH
- Structural advances through new methodology***
- Chair: *Paul Attfield*
- 15:00 - 15:50 Florence Babonneau, UMPC Paris
"Solid-state NMR characterization of organic-inorganic materials: some recent advances"
- 15:50 - 16:50 COFFEE BREAK AND POSTER SESSION
- Chair: *Wolfgang Bensch*
- 16:50 - 17:40 Thierry Epicier, INSA Lyon
"Life materials chemistry at the nano scale in environmental transmission electron microscopy"

17:40 - 18:30 Andrew Goodwin, Oxford University
"Local symmetry and hidden order"

Saturday, 10 September 2016

Solid state chemistry and applications

Chair: *Colin Greaves*

10:00 - 10:50 Barbara Albert, TU Darmstadt
"Complexity in borides: exotic solids or useful materials?"

10:50 - 11:40 Clare Grey, Cambridge University
"Challenges for rechargeable batteries - new characterisation approaches and new chemistries"

11:40 - 12:20 COFFEE BREAK

Chair: *Antoine Maignan*

12:20 - 13:10 Teofilo Rojo, CIC energiGUNE
"Towards all solid state batteries"

13:10 - 15:00 LUNCH

Rationales for functional materials synthesis

Chair: *Edmund Cussen*

15:00 - 15:50 Claudia Felser, MPI-CPS Dresden
"Topology – from the materials perspective"

15:50 - 16:40 Maarit Karpinnen, Aalto University
"Layer-engineering of novel functional oxide materials"

16:40 - 17:10 COFFEE BREAK

Chair: *Emilio Moran*

17:10 - 18:00 Joao Rocha, Aveiro University
"Microporous lanthanide silicates and coordination polymers for optical sensing and nanothermometry"

18:00 - 18:30 Quo vadimi?

Panel and audience: Concluding discussion

INDEX

- New Double Cation Ordering in High Pressure Double Perovskites** **FSM1**
A.M. Arévalo-López, E. Solana-Madruga, A.J. Dos Santos-García, R. Sáez-Puche, J.P. Attfield
- Uncommon morphological shapes of graphene: 3D graphenes** **FSM2**
A. Benítez de la Torre, C. Hernández Rentero
- Structural and orbital orders in Ga-V oxide spinels** **FSM3**
A.J. Browne, J.P. Attfield
- Hydrides of CrB-structure type Zintl phases – An in situ investigation** **FSM4**
H. Auer, H. Kohlmann
- Microcrystalline calcium phosphate synthesis in non-aqueous medium** **FSM5**
M. Kuzina, D. Larionov, V. Putlyaev
- Towards All Solid State Batteries** **FSM6**
T. Rojo
- Conversion reactions of binary of ternary chalcogenides** **FSM7**
S. Rommel, S. Haumann, F. Pielnhofer, A. S. Tragl, F. Bachhuber, J. Rothballer, W. Yan, P. Peter, A. Krach, A. Furtner, R. Wehrich
- The parent Li(OH)FeSe phase of lithium iron hydroxide selenide superconductors** **FSM8**
D.N. Woodruff, F. Schild, C.V. Topping, S.J. Cassidy, J.N. Blandy, S.J. Blundell, A.L. Thompson, S.J. Clarke
- Microstructural Flexibility and Magnetic Structure of $SbxV_{1-x}O_2$ ($0 < x < 0.5$) Solid Solution** **SAM1**
A.R. Landa-Cánovas, P. Vilanova-Martínez, F. Agulló-Rueda, J. Hernández-Velasco
- Functionalized Gold Nanoparticles as Platforms for Ligand-Receptor-Interactions** **SAM2**
F. Machka, E. Pouokam, M. Diener, M.S. Wickleder
- Synthesis and Characterization of Rare Earth doped ZrO_2 Nanoparticles** **SAM3**
A.S. Schulze, M.S. Wickleder
- Orbital Dinner model for Spin-Glass State in $Y_2Mo_2O_7$** **SAM4**
P.M.M. Thygesent, J.A.M. Paddison, R. Zhang, K.A. Beyer, K.W. Chapman, H.Y. Playford, M.G. Tucker, D.A. Keen, M.A. Hayward, A.L. Goodwin

Efficient UV-photocatalytic activity of ZnO and Ag/ZnO synthesized by a facile method	SSC28
C. Jaramillo-Páez, J.A. Navío*, M.C. Hidalgo, M. Macías	
Solid solutions of layered tetrel antimony chalcogenides	SSC29
R. Schlegel, S. Schwarzmüller, J. Barnes, H. Hölzig, O. Oeckler	
Disorder-phonon coupling in crystal-like aperiodic solids	SSC30
A. Overy, A. Cairns, M. Cliffe, A. Simonov, P. Chater, M. Tucker, A. Goodwin	
Perturbation of the Verwey structure of Fe₃O₄	SSC31
E. Pachoud, G. Perversi, J. Cumby, J.P. Wright, J.P. Attfield	
Mixed ionic-electronic conductors based on lanthanum molybdates	SSC32
J.M. Porras-Vázquez, L. dos Santos-Gómez, C. Frontera, J. Canales-Vázquez, D. Marrero-López, E. Ramírez-Losilla	
Magnesium secondary battery: New electrolytes and cathode materials	SSC33
E. Anger, I. Dez, A.C. Gaumont, V. Pralong	
Synthesis, Physico-chemical and Electrochemical Characterizations of Na₄VO(PO₄)₂ as Cathode Material for Na-ion Batteries	SSC34
W. Deriouche, M. Freire, N. Amdouni, A. Maignan, V. Pralong	
An active Li-Mn-O compound for high energy density Li-ion batteries	SSC35
M. Freire, N.V. Kosova, C. Jordy, D. Chateigner, O.I. Lebedev, A. Maignan, V. Pralong	
Fe[HO₃PCH(OH)CO₂]-2,5H₂O and doped metal derivatives: photocatalytic properties	SSC36
I.R. Salcedo, M. Bazaga-García, R.M.P. Colodrero, A.S. Albean, P.Olivera-Pastor, A. Cabeza	
Obtainment of polyethyleneimine modified ZnO nanoparticles for bioanalytical applications	SSC37
M. Shiriaev, J. Young Jeong, B. Hyun Chung, A. Baranov	
Insertion of diols into a layered niobate	SSC38
C.I. Thomas, M. Stenholm, M.J. Karppinen	
Effect of preparation pH on Bismuth Titanate materials with high visible light photocatalytic activity	SSC39
P. Zambrano, J.A. Navío, M.C.Hidalgo	
Synthesis and scale-up of non-active and active Belite-Alite-Ye'elinite Clinker (BAY)	SSC40
J.D. Zea-García, M.A.G. Aranda, A.G. De la Torre, I. Santacruz	
New representatives and physical properties of 3d-5d double perovskites	RFM1

Abstracts

Synthesis and scale-up of non-active and active Belite-Alite-Ye'elimite clinker (BAY)

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Research field: Solid state chemistry and applications.

Abstract:

Ordinary Portland cement (OPC) is an environmentally contentious material, as for every ton of OPC produced, ~0.97 tons of CO₂ are released. This opens the need of designing new formulations of cements formed by low calcite-demanding phases, such as ye'elimite, that release less CO₂ during their fabrication. Belite-Alite-Ye'elimite (BAY) cements are promising eco-friendly building materials as OPC substitutes at a large scale [1]. The reaction of alite and ye'elimite with water should develop cements with high mechanical strengths at early ages, while belite will contribute to later curing times. However, they develop lower mechanical strengths at early-medium ages than OPC [2]. It is known that the presence of different polymorphs of belite and ye'elimite affects the hydration due to the different reactivity of those phases [3].

The aim of this work is to process, characterize and scale-up a non-active BAY clinker (with coexisting alite, β -belite and ye'elimite) and an active-BAY clinker (with coexisting alite, α' -belite and ye'elimite) to develop, in a future step, comparable mechanical strengths to OPC. The parameters evolved in the preparation of the clinker have been optimized, such as the selection of raw materials (including mineralizers and activators), clinkering conditions and scale-up methodology. Finally, the clinker was characterized through laboratory X-ray powder diffraction in combination with the Rietveld methodology.

References:

- [1] Pérez-Bravo R, Álvarez-Pinazo G, Compañía J M, Santacruz I, Losilla E R, Bruque S and De la Torre A G, 2014, *Advances in Cement Research*, 26(1), 10–20.
- [2] Londono-Zuluaga D, Tobón J I, Aranda M A G, Santacruz I, De la Torre A G, 2016, Submitted to *Cement and Concrete Composites*.
- [3] Álvarez-Pinazo G, Santacruz I, León-Reina L, Aranda M A G and De la Torre A G, 2013, *Ind. Eng. Chem. Res.* 52, 16606–16614.



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