

Dalton Discussion 7: Ionic and Electronic Properties of Solids

University of St Andrews, UK

5-7 July 2004

PROGRAMME

Monday 5 July 2004

Session 1

Keynote 1

Schizophrenic electrons in ruthenium-based oxides

R J Cava

Princeton University, USA

Spin dimer and classical spin analyses of the ordered magnetic structures of alkali iron pyrophosphates NaFeP_2O_7 and LiFeP_2O_7

M-H Whangbo*, D Dai and H-J Koo

North Carolina State University, USA

Phase separation in manganites induced by orbital-ordering strains

J P Attfield, J P Chapman* L M Rodriguez-Martinex, L Lezama and T Rojo

University of Edinburgh, UK

The pyrochlore family – a potential panacea for the perovskite chemist

M T Weller*, R W Hughes, J Rooke, C S Knee and J Reading

University of Southampton, UK

Session 2

Li^+ ion conductivity in rock salt-structured nickel-doped Li_3NbO_4

V L McLaren, C A Kirk, M Poisot, M Castellanos and A R West*

University of Sheffield, UK

Structure and inter-phase stability in low dimensional polymer electrolytes with high lithium conductivity

J Liu, Y Zheng, L-P Liao, G Ungar and P V Wright*

University of Sheffield, UK

Solid state NMR study of the anionic conductor Ca-doped $\text{Y}_2\text{Ti}_2\text{O}_7$

C P Grey and N Kim

State University of New York at Stony Brook, USA

Tuesday 6 July 2004

Session 3

Keynote 2

Various strategies to tune the ionic/electronic properties of electrode materials for better storage devices

J M Tarascon

Universite de Picardie Jules Verne, France

Doping and defect association in $AZrO_3$ (A= Ca, Ba) and $LaMO_3$ (M= Sc, Ga) perovskite-type ionic conductors

M S Islam* and R A Davies

University of Surrey, UK

What variable-pressure variable-temperature measurements are telling us about ion transport in glass

M D Ingram*, C T Imrie and I Konidakis

University of Aberdeen, UK

Session 4

Simulating surface diffusion and surface growth in ceramics

D J Harris, M Lavrentiev, J H Harding*, N L Allan and J A Purton

University College London, UK

The interdependence of defects, electronic structure and surface chemistry

P Lindan*, E Duplock, C Zhang, M Thomas, R Chatten, and A Chadwick

University of Kent, UK

Phosphorus carbides: theory and experiment

N L Allan*, F Claeysens, G M Fuge, P W May, S R J Pearce and M N R Ashfold

University of Bristol, UK

Session 5

Keynote 3

Intrinsic performance limits in metals and metallic materials

P P Edwards

University of Oxford, UK

Evolution of structure, transport properties and magnetism in ternarylithium nitridometalates $Li_{3-x-y}M_xN$, M = Co, Ni, Cu

Z Stoeva*, R Gomez, D H Gregory, G B Hix and J J Titman

University of Nottingham, UK

Computer modelling of mixed metal fluorides for optical applications

R A Jackson*, M E G Valerio and M A Coutos dos Santos *Keele University, UK*

Hydrogen in oxides

T Norby*, M Widerøe, R Gløckner and Y Larring

University of Oslo, Norway

Session 6

Oxide ion transport in optimised LAMOX materials

S J Skinner*, S Georges, P Lacorre and M C Steil
Imperial College London, UK

Doping strategies to optimise the oxide ion conductivity in apatite-type ionic conductors

P R Slater*, J E H Sansom, J R Tolchard, A Najib, and M S Islam
University of Surrey, UK

Influence of synthesis route on the properties of doped-lanthanum cobaltite and its performance as an electrochemical reactor for the partial oxidation of natural gas

R M Ormerod*, R A Richardson and J W Cotton
Keele University, UK

Wednesday 7 July 2004

Session 7

Keynote 4

Electronic phase separation in transition metal oxide

C N R Rao*, A K Kundu, M M Seikh and L Sudheendra
Nehru Centre for Advanced Scientific Research, Bangalore, India

Structure and reactivity of V₂O₅: bulk solid, nanosized clusters, species supported on silica and alumina, cluster cations and anions

J Sauer* and J Döbler *Humboldt University, Germany*

Rubidium doped zeolite rho: structure and microwave conductivity of a metallic zeolite

P A Anderson*, A R Armstrong, P D Barker, M J Edmondson, P P Edwards and A Porch
University of Birmingham, UK

structural and electrical characterisation of Li₂O : TiO₂: SnO₂: P₂O₅ electrolyte glass

I Abrahams*, E Hadzifejzovic and J R Dygas
Queen Mary, University of London, UK

Session 8

Expanded fullerides and electron localisation – lithium-rich ammoniated C₆₀ phases

M J Rosseinsky*, P Durand, Y Dubitsky and A Zaopo *University of Liverpool, UK*

Temperature-induced valence transition and associated lattice collapse in samarium fulleride

K Prassides*, J Arvanitidis, K Pagagelis and S Margadonna
University of Sussex, UK

Transport numbers from hydrogen concentration cells over different oxides under oxidising and reducing conditions

M Widerøe*, N Kochetova and T Norby
University of Oslo, Norway