

TM
S70/5L

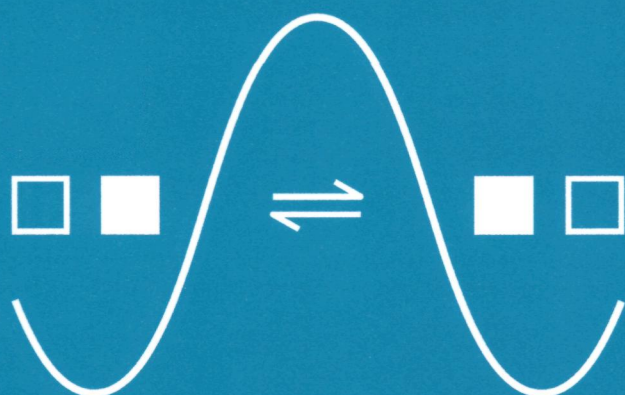
VOLUME 252, 1 December 2013

ISSN 0167-2738



SOLID STATE IONICS

DIFFUSION & REACTIONS



SSPC-16 Conference Proceedings SSI Special Issue

Guest Editors

S. Lyonnard, Grenoble, France

S. Mossa, Grenoble, France

F. Lefebvre-Joud, Grenoble, France

Principal Editor

Joachim Maier, Stuttgart, Germany

Regional Editor Europe

John Kilner, London, UK

Regional Editor Asia

Koichi Eguchi, Kyoto, Japan

Hong Li, Beijing, China

Regional Editor USA

Arumugam Manthiram, Austin, TX, USA

Editors

Klaus Funke, Münster, Germany

Truls Norby, Oslo, Norway

Josh Thomas, Uppsala, Sweden

Founding Editor

M. Stanley Whittingham, Binghamton, NY, USA

Editorial Assistant

Rotraut Merkle, Stuttgart, Germany

Abstracted / Indexed in: Chemical Abstracts / Aluminium Industry Abstracts / ISMEC / METADEX / PASCAL / PIRA / Engineered Materials Abstracts / Analytical Abstracts / Chemical Engineering and Biotechnology Abstracts / CAB Abstracts / GeoRef / Energy Science and Technology. Also covered in the abstract and citation database Scopus®. Full text available on ScienceDirect®.

CONTENTS

Special Issue

SSPC-16 Conference Proceedings SSI Special Issue

Guest Editors: S. Lyonnard, S. Mossa and F. Lefebvre-Joud

Editorial

SSPC-16 Conference Proceedings SSI Special Issue

S. Lyonnard, S. Mossa and F. Lefebvre-Joud

1

Proton Transport at the Nanoscale

Proton diffusivity in spark plasma sintered $\text{BaCe}_{0.8}\text{Y}_{0.2}\text{O}_{3-\delta}$: *In-situ* combination of quasi-elastic neutron scattering and impedance spectroscopy

Q. Chen, J. Banyte, X. Zhang, J.P. Embs and A. Braun

2

Bulk protons in anhydrous perovskites—neutron scattering studies

A. Slodczyk, P. Colomban, N. Malikova, O. Zaafrani, S. Longeville, J.-M. Zanotti, O. Lacroix and B. Sala

7

Proton dynamics in $\text{La}_{0.8}\text{Ba}_{1.2}\text{GaO}_{3.9}\cdot n\text{H}_2\text{O}$ studied by quasielastic incoherent neutron scattering

N. Jalarvo, L. Stingaciu, D. Gout, Z. Bi, M.P. Paranthaman and M. Ohl

12

Hydronium dynamics in the perchloric acid clathrate hydrate

A. Desmedt, R.E. Lechner, J.-C. Lassegues, F. Guillaume, D. Cavagnat and J. Grondin

19

The nanosecond proton dynamics of phosphoric acid – from the solid to the melt – investigated by neutron backscattering

B. Frick, L. Vilčiauskas, P.P. Deen and S. Lyonnard

26

First principles molecular dynamics study of proton dynamics and transport in phosphoric acid/imidazole (2: 1) system

L. Vilčiauskas, M.E. Tuckerman, J.P. Melchior, G. Bester and K.-D. Kreuer

34

Protons in Al doped BaZrO_3 escape dopant traps to access long range proton conduction highways

M.A. Gomez and F.-J. Liu

40

Kinetic Monte Carlo study of protonic diffusion and conduction in Gd-doped BaCeO_3

J. Hermet, F. Bottin, G. Dezanneau and G. Geneste

48

Structure-Function Interplay

Water management in proton exchange membrane fuel cell at sub-zero temperatures: An in operando SANS-EIS coupled study

A. Morin, Z. Peng, J. Jestin, M. Detrez and G. Gebel

56

Microstructure, state of water and proton conductivity of sulfonated poly(ether ether ketone)

G. Portale, A. Carbone, A. Martinelli and E. Passalacqua

62

Contents continued on last page of this issue



Contents continued

Structural and transport properties of Nafion in hydrobromic-acid solutions A. Kusoglu, K.T. Cho, R.A. Prato and A.Z. Weber	68
Sulfonated poly(pentafluorostyrene): Synthesis & characterization V. Atanasov, M. Bürger, S. Lyonard, L. Porcar and J. Kerres	75
The influence of the cationic form and degree of hydration on the structure of Nafion™ E. Negro, M. Vittadello, K. Vezzù, S.J. Paddison and V. Di Noto	84
The role of <i>internal pressure</i> for the hydration and transport properties of ionomers and polyelectrolytes K.-D. Kreuer	93
Effect of ethylene carbonate on proton conducting polymer electrolyte based on poly(ϵ -caprolactone) (PCL) H.J. Woo, S.R. Majid and A.K. Arof	102
Structural and electrochemical properties of hydrogen titanium oxides K. Kataoka, N. Kijima and J. Akimoto	109
Superprotonic conductivity of $(\text{NH}_4)_3\text{H}(\text{SO}_4)_2$ in the high-temperature phase Y.J. Sohn, K.M. Sparta, M. Meven, G. Roth and G. Heger	116
Theoretical modeling of defect segregation and space-charge formation in the BaZrO_3 (210)[001] tilt grain boundary A. Lindman, E.E. Helgee and G. Wahnström	121
High activation energy for proton migration at $\Sigma 3(111)/[1\bar{1}0]$ tilt grain boundary in barium zirconate J.-H. Yang, D.-H. Kim, B.-K. Kim and Y.-C. Kim	126
Two-fold -to-single-fold transition of the conductivity relaxation patterns of proton-conducting oxides upon hydration/dehydration E. Kim and H.-I. Yoo	132
Degradation and Systems	
Degradation studies on acid–base blends for both LT and intermediate T fuel cells A. Chromik and J.A. Kerres	140
BaCeO_3 – $\text{BaCe}_{0.8}\text{Sm}_{0.2}\text{O}_{3-\delta}$ bi-layer electrolyte-based protonic ceramic fuel cell I. Park, J. Kim, H. Lee, J. Park and D. Shin	152
Electrolysis of CO_2 in a proton conducting membrane E. Ruiz-Trejo and J.T.S. Irvine	157
Calendar	165