

# Curriculum Vitae

## Clare P. Grey

Department of Chemistry,  
University of Cambridge,  
Lensfield Road, Cambridge, CB2 1EW, UK  
E-mail: [cpg27@cam.ac.uk](mailto:cpg27@cam.ac.uk)  
Tel: +44(0)1223 336509  
FAX: +44(0)1223 336017  
<http://www.ch.cam.ac.uk/staff/cpg.html>

### EDUCATION:

D.Phil. in Chemistry, University of Oxford (1991)  
Thesis title: A  $^{199}\text{Sn}$  and  $^{89}\text{Y}$  MAS NMR study of Rare-Earth Pyrochlores. Thesis advisor:  
Prof. A. K. Cheetham  
B.A. in Chemistry, *First Class Honours*, University of Oxford, (1987)

### PROFESSIONAL EXPERIENCE:

Adjunct Professor, Department of Chemistry, State University of New York at Stony Brook  
(May 2015 - present)  
Fellow Pembroke College Cambridge (2011 – present)  
Head, Materials Research Interest Group (2010-2015) and Inorganic Sector (2009 –2010)  
Cambridge University  
Associate Director (2011-2015), Director and PI (2009-2011), Northeastern Chemical  
Energy Storage Center, a Department of Energy Frontier Center, Stony Brook University  
Geoffrey Moorhouse Gibson Professor in Materials Chemistry, University of Cambridge,  
UK, (July 2009-present)  
Visiting Professor, Université de Picardie Jules Vernes, Amiens, (2006-07; 2007-08)  
Associate Director, NSF Center for Environmental Molecular Sciences, (2002- 2009)  
Professor, Department of Chemistry, State University of New York at Stony Brook (Sept.  
2001-2015)  
Visiting Professor, Université Louis Pasteur, Strasbourg, (2000)  
Associate Professor, Department of Chemistry, State University of  
New York at Stony Brook (Sept. 1997-Aug. 2001)  
Assistant Professor, New York at Stony Brook (Jan. 1994-Aug. 1997)  
Visiting Scientist at DuPont CR&D (Feb. 1992-Jan. 1994)  
Royal Society Post-doctoral Fellow in the laboratory of Prof. W.S. Veeman, University of  
Nijmegen (Jan. 1991-Feb. 1992)  
Research Fellow, Balliol College, University of Oxford (Sept. 1990-Jan.1991).

### AWARDS:

Arfvedson-Schlenk-Preis from the German Chemical Society (2015)  
Davy Medal from the Royal Society (2014)  
Honorary Fellowship, Balliol College Oxford (2014)

Honorary PhD Degree from Lancaster University (2013)  
Laukien Award from the Experimental NMR Conference (2013)  
Research Award, International Battery Association (2013)  
Honorary PhD Degree “Docteur Honaris Causa” from the University of Orleans (2012)  
Royal Society Kavli Medal and Lecture (2011)  
Fellow of the Royal Society (2011)  
Fellow of the International Society of Magnetic Resonance (2011)  
RSC John Jeyes Award (2010)  
AMPERE Award (2010)  
Vaughan Lecturer (2008)  
NYSTAR Award (2007)  
Research Award of the Battery Division of the Electrochemical Society, (2007)  
NSF POWRE Award (2000)  
Camille and Henry Dreyfus Teacher-Scholar Award (1998)  
Alfred P. Sloan Foundation Research Fellow (1998)  
Cottrell Scholar (1997)  
DuPont Young Professor Award (1997)  
NSF National Young Investigator (1994)  
Royal Society European Post-doctoral Fellowship (1991)  
Junior Research Fellowship, Balliol College, University of Oxford (1990)  
S.E.R.C. Quota Award (1987-1990)  
Senior Scholarship, Christ Church, University of Oxford (1988)  
Dixon Scholarship, Christ Church, University of Oxford (1987)  
Open Scholarship, Christ Church, University of Oxford (1983)

#### **TEACHING:**

Stony Brook: Inorganic chemistry (for undergraduate majors + 1<sup>st</sup> semester graduate level); Designed and ran inorganic (and solid state) chemistry laboratory course for chemistry majors; Freshman (1st year) chemistry laboratory; Solid-State chemistry, crystallography, NMR and group theory (graduate level).

University of Picardie, Amiens: European Masters Course on Energy: Applications of NMR to Batteries and Fuel Cells.

Cambridge: 3<sup>rd</sup> year (Part II) “Characterization methods for inorganic chemistry” – ESR and magnetism. 4<sup>th</sup> year (Part III) “Inorganic Magnets” – magnetism, solid chemistry, crystallography.

#### **PROFESSIONAL SERVICES/ OTHER AWARDS AND HONOURS:**

Opened the New Chemistry Building at Lancaster University, October 2016

Presentation to an All-Party Parliamentary Climate Change Group event, ‘Energy storage and the transition to a low carbon economy’,

<http://www.policyconnect.org.uk/appccg/news/energy-storage-and-transition-low-carbon-economy-summary> Houses of Parliament, London, July 2016

“Putting Science to Work” Radio 4 Programme on Mitigating Air Pollution in Cities, Dec 2015

Panelist, BBC World Service, “The future of renewable energy” for the programme, “the Forum”, (<http://www.bbc.co.uk/programmes/p01g94yj>), September 2013.

Member of the Emerging Technologies Panel for the World Economic Forum (2012 – 2015). Helped write “Energy Harnessing: New Solutions for Sustainability and Growing Demand” (Oct 2013, <http://www.weforum.org/reports/energy-harnessing-new-solutions-sustainability-and-growing-demand>).

Royal Society of Chemistry Roadmap Champion for Energy Conversion and Storage (2011-2014)

Presentation to the Department of Energy and Climate Change (DECC) “Strategy Coffee Morning”: “Challenges in Using Lithium Ion Batteries in Road Transportation”, London, July

RSC Public Lecture, Burlington House, London, September: “Recharging the Planet: The Prospects and Chemical Challenges of using Batteries to Power a Low Carbon Economy” ([http://thereaction.net/events/y2011/Recharging\\_our\\_future.aspx](http://thereaction.net/events/y2011/Recharging_our_future.aspx))

Kavli Public Lecture, The Royal Society, London, October: “Following function in real time: Towards the Next Generation of Batteries for Supercapacitors for Transport and Grid Storage” (<http://royalsociety.org/events/Following-function-in-real-time/>)

Presentation to National Academy, Solid State Sciences Committee, "New Materials and Challenges for Lithium-Ion Battery Research", April 2008

Department of Energy, Basic Energy Sciences: "Basic Research Needs for Electrical Energy" Workshop, April 2007. Panel Lead and Writer. (Characterization)

US/Africa Workshop, "Frontiers in Materials Research and Education", Abuja, Nigeria, January 2007: Panel Lead, (Materials Chemistry)

National Science Foundation Workshop on "Sustainability and Chemistry," May-June 2006 Report "Chemistry for a Sustainable Future": Panel Lead (Energy) and Writer (Energy and Environmental Chemistry)

National Science Foundation Workshop, “The status of solid state chemistry and its impact in the physical sciences, May 2006, Workshop organizer

National Science Foundation Workshop, Approaches for Combating Terrorism, July 2005, Panel Lead and Writer, (Power Sources)

Editorial Board, Accounts of Chemical Research, 2015 - present

Editorial Board, Journal of the American Chemical Society, 2011-present

Editorial Board, Journal of Materials Chemistry, July 2009-2010

Editorial Board, Chemistry of Materials, Jan. 2005-Jan. 2010

Editorial Board, Solid State Sciences, Jan 2002-present

Editorial Board, Journal of Magnetic Resonance, Jan 1999-present

Program Chair, Alpine NMR Meeting, Chamonix, 2009

Session Organizer, MRS Meeting, December 2005, Battery Session

Chair, NMR symposium of the 43<sup>rd</sup> Rocky Mountain Conference on Analytical Chemistry [Vice-chair 1999; committee member 1994-1999; Session organizer 1996-1999];

Advisory Board, Winton Programme for the Physics of Sustainability, Cambridge University, 2011-present

Advisory Board, Max Planck Institute for Polymer Physics, 2009-2015

Advisory Board, Center for Functional Nanomaterials (CFN), Brookhaven National Laboratory, 2006-2012.

NY State Advanced Energy Center, Member, Research Committee (2006-2009)

Advisory Board, Penn. State, Center for Environmental Kinetics Analysis (NSF EMSI), Dec. 2005-2010

Member of the Stony Brook University "Status of Women Faculty" Taskforce (representative for the physical sciences) (1999-2009); Member of the Stony Brook Women in Science and Engineering (WISE) Advisory Working Group (1994 -2009)

ECS Biannual Meeting, Educational Division Talk, "XYZ for the Rest of Us" Los Angeles, October 2005

## **TALKS AT INSTITUTIONS, COMPANIES AND CONFERENCES**

**(since 1994)**

**1994** 34th Experimental NMR Conference, Asilomar, April  
Eastern Analytical Symposium, New Jersey, November  
Adelphi University, November

**1995** Nato Summer School, on the 'Characterization of Advanced Materials' Pisa, Italy, September  
DuPont Central Research, Wilmington DE, October  
Eastern Analytical Symposium, New Jersey, November  
Unilever Research, Port Sunlight, UK, December

**1996** ALCOA Technical Center, Pittsburgh, January  
SUNY Stony Brook, (Chemistry Department) March  
ACS Meeting, New Orleans, March  
MRS Meeting, San Francisco, March  
Georgetown University, April  
Collaborative Laboratories, April  
University of Connecticut, May  
Solid State Gordon Conference, July  
Chemagnetics Users Meeting, July  
Brookhaven National Laboratory, May  
McGill University, October  
SUNY Brockport, October  
Rutgers University, Camden, November  
Drexel University, Philadelphia, November  
University of Birmingham, UK, November  
Royal Society Anglo-Indian Meeting, Bangalore, December

**1997** Department of Earth and Space Sciences, SUNY Stony Brook, January  
University of Massachusetts, Amherst, January  
Washington Regional NMR Meeting, N.I.H., February

University of Utah, March  
37th Experimental NMR Conference, Orlando, March  
Chemistry Department, North Carolina State University, May  
Physics Department, University of Kent, May  
Inorganic Chemistry Laboratory, University of Oxford, May  
Air Products, May  
Zeolites Gordon Conference (short talk), June  
Denver, CO, July  
Tulane University, October 1997

**1998** ACS Dallas Meeting, March  
National Chemical Laboratory, Pune, India, May  
National Institute of Standards and Technology, June  
Duracell, Boston, June  
Air Products, August  
University of Illinois at Chicago, October  
6th NSF Materials Chemistry Workshop, October  
Recent Advances in Magnetic Resonance, Schlumberger-Doll Research Center, Connecticut,  
November  
University of South Carolina, November  
New York Technical College, December  
MRS Fall Meeting, Boston, December

**1999** University of West Virginia, January  
Pennsylvania State University, February  
Queens College, CUNY, March  
University of Waterloo, Toronto, Canada, March  
Florida Catalysis Conference, Palm Coast, FL, April  
Zeolite Gordon Research Conference, Plymouth, NH, June  
1<sup>st</sup> Alpine NMR Conference, Chamonix, France, September  
Northeastern Corridor Zeolite Association Meeting, Philadelphia, December

**2000** Institut des Materiaux Jean Rouxel, CRNS-Nantes, February  
Institut de Chimie de la Matière Condensée de Bordeaux, CRNS-Pessac, France, February  
Université Louis Pasteur, Strasbourg, France, March  
Duracell Worldwide Technology Center, Needham, MA, March  
British Zeolite Associate Meeting, London, April  
Inorganic Chemistry Laboratory, University of Oxford, April  
University of Cambridge, April  
CRNS-Orleans, April  
National Synchrotron Light Source Users Meeting, Brookhaven National Laboratory, May  
Catalysis Gordon Conference, New London, NH, June  
Inorganic Gordon Conference, Newport, R.I, July  
Chemagnetics Workshop, Estes Park, CO, August

Ampere meeting on “NMR of novel Materials”, Greece, September  
198<sup>th</sup> Meeting of the Electrochemical Society, Phoenix, Arizona, October  
Workshop on Interfaces, Phenomena, and Nanostructures in Lithium Batteries, Argonne  
National Laboratory, December

**2001** University of Munich (LMU), January  
Ohio State University, February  
American Chemical Society Meeting, San Diego, April  
Department of Energy, Separations and Analytical Chemistry Contractors Meeting, April  
Iowa State University, April  
American Ceramics Society, Indianapolis, April  
Canadian Chemical Society Meeting, Montreal, May  
Lithium Battery Meeting, Bordeaux, May  
National Institute of Chemical Physics and Biophysics, Tallinn, Estonia, June  
NMR Gordon Conference, June  
International Society of Magnetic Resonance, Rhodes, Greece, August  
Duracell, Boston, August  
International Bunsen Discussion meeting; Solid State Electrolytes, Munster, Germany,  
October  
Union College, Schenectady, New York, October  
U. C. Berkeley, November  
U. C. Davis, November

**2002** University of Picardie, Amiens, France, January  
Lille University, France, January  
Hunter College, February  
University of Windsor, Canada, April  
Experimental NMR Conference, Monterey, April  
Argonne National Laboratory, May  
ACS Meeting, Boston, August  
3<sup>rd</sup> International Materials Conference, Konstanz, September  
Georgia Tech., October  
Long Island University, November  
Temple University, November

**2003** International Battery Association Meeting, Kona, Hawaii, January  
National Institute of Advanced Industrial Science and Technology,  
AIST Shikoku, Takamatsu, Japan, January  
SONY Corporation, Yokohama, Japan, January  
“World of Physics”, Stony Brook Outreach seminar series, February  
Exxon Mobil Corporation, March  
Solid State Ionics Conference, California, June  
ACS Meeting, New York, September  
Alpine NMR Conference, Chamonix, France, September

Drexel University, Pennsylvania, October  
Washington State University, St. Louis, MO.  
Indo-Pacific Catalysis Association Symposium, Taipei, Taiwan, November,  
Pre-conference school, Indo-Pacific Catalysis Association Symposium, Tsinghua University,  
Hsinchu, Taiwan, November

**2004** Southampton University, UK, January  
University of Nijmegen, the Netherlands, January  
University of Bonn, Germany, January  
Northwestern University, January  
Princeton University, March  
Physics Department, SUNY Stony Brook, April  
University of Iowa, April  
International Meeting on Lithium Ion Batteries, Nara, Japan, June  
RSC Dalton Discussion Meeting, St. Andrews, UK, July  
Solid State Gordon Research Conference, July  
ACS Meeting, Philadelphia, August  
Solid State Chemistry 2004, Prague, September  
“Recent Advances and Applications of Solid-State NMR  
from Superconducting Physics to Molecular Biology”, Warwick, September  
New Opportunities in Materials Chemistry, London, September  
84<sup>th</sup> International Bunsen Discussion Meeting, Münster, Germany, October  
SERMACS meeting, Raleigh, North Carolina, November  
MRS Meeting, Boston, November  
New York Academy of Sciences, New York, December

**2005** U. Michigan, Ann Arbor, January  
U. C. Santa Barbara, March  
Caltech, March  
ACS Meeting, San Diego, March  
Lithium Battery Discussion Meeting, Arachon, France, May  
ECS Polymer Batteries and Fuel Cells Conference, Las Vegas, June  
EUROMAR ENC Conference, Veldhoven, the Netherlands, July  
Rocky Mountain Conference, Denver Colorado, August  
EMSI (Environmental Molecular Science) Meeting, Arlington, VA , August  
ACS Meeting, Baltimore, August  
ECS Meeting, Los Angeles, October  
University of Delaware, October  
Cornell University, Ithaca, November  
MRS Meeting, Boston, November

**2006** ICMR/ICTP Workshop on Recent Developments in Inorganic Materials, International  
Center for Theoretical Physics Workshop, Trieste, Italy November  
Texas A&M University, College Station, Texas, January,

- Trinity College, Connecticut, February  
 University of Rhode Island, March  
 Frontiers in Inorganic Materials Chemistry, Santa Barbara, April  
 Experimental NMR Conference, Asilomar, April  
 Canadian Chemical Society Meeting, Halifax, Nova Scotia, May  
 British Zeolite Association, Ambleside, July  
 57<sup>th</sup> Annual Meeting of the International Society of Electrochemistry, Edinburgh, August  
 University of Utah, Salt Lake City, September  
 RSC Symposium, "From Single Molecules to extended lattices" Cambridge, UK, October  
 MRS Symposia, "Inorganic Materials", and "Magnetic Resonance Symposium in Materials Science," Boston, November
- 2007** US/Africa Workshop, "Frontiers in Materials Research and Education", Abuja, Nigeria, January  
 Oxford University, February  
 École Normale Supérieure Lyon, March  
 University of Picardie, Amiens, March  
 Institut de Ciència de Materials de Barcelona, March  
 University of St. Andrews, March  
 "Cryo MAS Open Day" Symposium, University of Southampton, June  
 "NMR of Metals in Biological Systems and in Materials", Delaware, June  
 ICMAT 2007, Singapore, July  
 49<sup>th</sup> Rocky Mountain Conference, Breckenridge, Colorado, July  
 IZC Pre-conference summer school, Dalian, China, August  
 International Zeolite Conference (IZC), Beijing, China, August  
 "Lauterbur's Legacy: Looking at Life". A memorial symposium for Prof. P. Lauterbur, Stony Brook, September  
 Battery Division Research Award Address, ECS Meeting, Washington D.C., October  
 ISMAR, Taiwan, October  
 NAE "Japan-America Frontiers of Engineering" Symposium, Palo Alto, November  
 ICMCB-CNRS, Bordeaux, France, November  
 Vassar College, New York, November  
 NYU, New York, December  
 ICMS-ICMR Winter School on Chemistry and Physics of Materials, JNCASR, Bangalore, December  
 GE Corporate Research, Bangalore, December  
 Indian Institute of Science, Bangalore, December
- 2008** GRC on Electrochemistry, Ventura, CA, January  
 U.C. Santa Barbara, January  
 Focused Battery Technical Workshop III, Material Challenges for High Energy Density and Long-life Lithium-Ion cells, Caltech, February  
 Joint U.C.S.B.- Max Planck Meeting on Energy, Lake Arrowhead, February  
 Zing Conference on Solid-State Chemistry, Cancun, Mexico, March



MRS Meeting, San Francisco, March  
Fairfield University, Connecticut, April  
Georgetown University, Washington DC, April  
UOP, Frontiers of Chemistry Lecture, May  
International Meeting on Lithium Ion Batteries, Tianjin, China, June  
Euromar, St. Petersburg, Russia, July  
Synchrotron Radiation in Materials Science, Campenas, Brazil, July  
Vaughan Lecture, Rocky Mountain Conference on Analytical Chemistry, Breckenridge, Colorado, July 2008  
American Chemical Society Meeting, Philadelphia, August  
University of New Orleans, New Orleans, September  
University of Buffalo, Buffalo, October  
Frontiers in Chemistry Lectureship, Case Western University, Ohio, October,  
49th Battery Symposium, Osaka, Japan, November  
Fundamentals on LIBs, Tegernsee, Germany, November  
MRS Meeting, Boston, December

**2009** GM, Michigan, January  
Department of Chemistry, Columbia University, New York, February  
1st International Workshop on Advanced Materials, Dubai, Arab Emirates, February  
ACS Meeting, Salt Lake City, March  
Experimental NMR Conference, Pacific Grove, CA, March  
Armourers and Brasiers Cambridge Forum, Cambridge, UK, June  
Chinese Academy of Sciences - Cambridge University Workshop, Cambridge, UK, July  
Nano Materials for Energy Storage and Conversion BioNanotechnology (SLONANO), Slovenia, October  
New York State Advanced Energy Conference, Hauppauge, New York, October

**2010** British Embassy, "Battery technology workshop", London, January  
Solid State Day, Gottfried Wilhelm Leibniz University Hannover, Institute for Physical Chemistry and Electrochemistry, Hannover, Germany, January  
EURACT- NMR Workshop, The Institute for Nuclear Waste Management, Germany, January  
Department of the Navy, Naval Research Laboratory, Chemistry Colloquium, Washington, D.C., April  
E-MRS, (Solid State Ionics Symposium) Strasbourg, June  
Gordon Research Conference on Inorganic Chemistry, Maine, June  
Smith School of Enterprise and the Environment, World Forum 2010, Oxford, June  
Gordon Research Conference on Catalysis, New Hampshire, June  
EUROMAR Meeting, Florence, July  
Gordon Research Conference on Solid State Chemistry, New Hampshire, August  
Solid State Protonic Conduction 15 (SSPC-15), Santa Barbara, August 29, 2010  
ACS Meeting, Boston, August

EU/Department of Energy Transatlantic Workshop on Storage, Washington, October: "Next Generation Batteries for Grid Storage"  
Warwick, 850 MHz Solid State NMR Opening Ceremony, October  
Chemistry Department, Durham University, November  
RSC John Jeyes Award Lecture, Bath, November  
MRS, Boston, December  
RSC NMR Discussion Day, London, December  
RSC Solid State Chemistry Meeting, UCL, London, December

**2011** LMU Chemistry Department, Munich, January  
The Kelvin Club, Peterhouse Scientific Society, February: "Recharging the Planet: New Approaches to Optimising the Performance of Lithium Ion Batteries"  
MIT Chemistry Department, February  
RSC John Jeyes Award Lecture Award Lectures, Glasgow and Surrey, February  
52th Experimental NMR Conference, Asilomar, April  
MRS, "Frontiers of Solid State Ionics", San Francisco, April  
Energy Frontier Research Centers Summit and Forum, Washington DC, May  
2011 Lithium Ion Battery Discussion Meeting, Arcachon, June  
Solid State Ionics, Plenary Lecture, Warsaw, July  
Presentation to the Department of Energy and Climate Change (DECC), London, July.  
RSC Public Lecture, Burlington House, London, September  
Strongly Correlated Electron Systems (SCES) 2011, Cambridge, September  
International Symposium on Advanced Complex Inorganic Nanomaterials (ACIN 2011), Namur, September  
Kavli Public Lecture, The Royal Society, London, October  
The Cavendish Laboratory, Cambridge, October  
Chemistry Department, University College London, November  
CAPE, Cambridge, November  
ANZMAG, Torquay, Australia, November  
Deakin University, Melbourne, December  
CSIRO, Melbourne, December

**2012** Electrochemistry Gordon Conference, Ventura, January  
Battery EV Tech, London, February  
Batteries Gordon Conference, Ventura, February  
Johnson Matthey Academic Conference (JMAC12), March  
Wuhan University of Technology, China, April  
Nanjing University, China, April  
Cardiff Spring Conference 2012, May  
IMLB 2012 Conference, JeJu Island, Korea, June  
Euromar, Dublin, July  
ISACS 8, Toronto, Canada, July  
nCAM2012, Cambridge, September  
German Chemical Society Conference, Darmstadt, September

- 2013** iNano Opening, Plenary Talk, Billund, January  
 Chemistry Department, ENS Lyon, January  
 RS, Theo Murphy International Scientific Meeting, 28 & 29 January  
 STFC, Hydrogen & Fuels Workshop, Oxford, February  
 Chemistry Department, University of Wisconsin, February  
 IBA2013, Research Award Address, Barcelona, March  
 ACS, New Orleans, March  
 54th ENC, Laukien Award Address, Asilomar, CA, April  
 ISMAR 2013, Rio de Janeiro, Brazil, May  
 University of Basel, Basel, May  
 SSI-19 Conference, Kyoto, June  
 RSC MC11, Warwick University, July  
 ICMRM, Cambridge, August  
 Electrochem2013, Southampton University, Southampton, September  
 RSC ISACS12, Cambridge, September  
 pNMR workshop, Chamonix, September  
 8<sup>th</sup> Alpine Meeting on Solid State NMR, Chamonix, September  
 LG Chemicals, Daejeon, Korea, October  
 Korea Basic Science Institute, Daegu, Korea, October  
 Department of Energy Science, Sungkyunkwan University, Korea, October  
 Samsung Advanced Institute of Technology (SAIT), Seoul, Korea, October  
 RSC-Korean Li Air Forum, Seoul Korea, October  
 Institute of Energy & Climate Research, Forschungszentrum Juelich, Germany, November  
 MRS, December  
 Alistore Meeting, Bordeaux, December
- 2014** Physics Department, Nottingham University, January  
 ISMAR Lecture, 20th Meeting of the National Magnetic Resonance Society (India),  
 "NMRS-2014", Assam, India, February  
 Chemistry Department, Birmingham University, March  
 School of Chemistry, Trinity College Dublin, March  
 BMW, Munich Battery Discussions, Munich, March  
 WE Heraeus-Seminar "Analytical Tools for Fuel Cells and Batteries", Bad Honnef,  
 Germany, March  
 Power our Future-14, CIC energigune, Vitoria, Spain, April  
 IMLB 2014, Como, June  
 Euromar 2014, Zurich, June  
 56<sup>th</sup> Rocky Mountain Conference on Magnetic Resonance, Breckenridge, July  
 AGICHEM Meeting, Edinburgh, July  
 "Not a fish out of water: Operando studies of energy materials". EMC<sup>2</sup> EFRC Center,  
 Cornell, August  
 ISE Lausanne, September  
 Thomas Young Centre, Energy Materials Workshop, UCL, London, September

Nanqiang Lecture, Xiamen, October,  
Queen Mary College, Departmental Seminar, London, November  
Japanese Battery Meeting, Kyoto, Japan, November  
UK Energy Storage Conference 2014, Warwick, November

- 2015** Chemistry Department, Liverpool University, February  
International Workshop on Advanced Materials, Ras al Khaimah, UAE, March  
Wincools – ETH/EMFL Winter School, Champéry, March  
Adlinger Center, Princeton University, March  
Dupont CR&D, Wilmington DE, March  
Beyond Lithium VIII, Oakridge, June  
Solid State Ionics, Colorado, June  
USIC Conference, Universities of Scotland, July  
ISMAR, Shanghai, August  
German Chemical Society Meeting (AS Award Address), Dresden, August  
Joint Anglo-German Discussion Meeting, Darmstadt, September  
Energy Materials Symposium, Bath, September  
Size & Strain Conference, Oxford, September  
ECS, Phoenix, October  
Dutch NMR Discussion Group, November  
African MRS, Ghana, December
- 2016** LMU Munich, talk to the Chemistry Department, January  
17th International Materials Engineering Conference (IMEC 17), Israel, February  
Weitzman Institute Departmental Seminar, Israel, February  
Paul Scherrer Institute, Switzerland, March  
Chemistry Department, ETH, Switzerland, March  
International Battery Association meeting, Nantes, March  
Graphene Flagship Meeting, Chalmers University, Gothenburg, Sweden, April  
Hume Rothery Lecture, Department of Materials, Oxford, April  
Chemistry Department, University of Reading, May  
Electrochemical Society Meeting, San Diego, May  
NSF Ceramics Workshop, San Diego, May  
International Meeting on Lithium Ion Batteries (IMLB), Chicago, June  
Euromar, Aarhus, Denmark, July  
SMARTER 5 Conference, Germany, September  
Challenges & Prospects for Solid-State Chemistry 2016 (CPSSC 16), Seville, September  
Solid-State Protonic Conductors (SSPC-18), Oslo, Norway, September  
pNMR Final Workshop, Italy, September  
University of Lancaster, Chemistry Department Opening and Lecture, October  
EPFL Chemistry Dept. and Marvel Centre Distinguished Lecture, Switzerland, October  
Materials for Tomorrow Conference, Chalmers University, Sweden, November  
CHAINS: Chemistry as Innovating Science 2016, Netherlands, December

**2017** Joint seminar to the Chemistry and Physics Departments at St Andrews, February  
International Workshop on Advanced Materials: IWAM-2017, Ras al Khaimah, February  
58th Experimental NMR Conference, Monterey, March 2017  
ACS, San Francisco, Talks in the Presidential and Synthesis & Characterization of Materials  
for Energy Applications Symposia, and the 2016 E.V. Murphree Award in Industrial &  
Engineering Chemistry Symposium in honor of Michael M. Thackeray, April 2017  
Applied Materials, Palo Alto, April 2017

## PUBLICATIONS:

1. "Paramagnetic shift probes in high-resolution solid-state NMR", A.K. Cheetham, C.M. Dobson, C.P. Grey and R.J.B. Jakeman, *Nature* (London), **328**, 706-707, (1987).
2. "Studies of rare-earth stannates by  $^{119}\text{Sn}$  MAS NMR - The use of paramagnetic shifts probes in the solid state", C.P. Grey, C.M. Dobson, A.K. Cheetham and R.J.B. Jakeman, *J. Am. Chem. Soc.*, **111**, 505-511, (1989).
3. "Oxidative coupling of methane over tin-containing rare-earth pyrochlores", A. Ashcroft, A.K. Cheetham, M.L.H. Green, C.P. Grey and P.D. Vernon, *J. Chem. Soc. Chem. Comm.*, 1667-1669, (1989).
4. "High resolution  $^{13}\text{C}$  MAS NMR-spectra of paramagnetic lanthanide complexes", A.N. Clayton, C.M. Dobson and C.P. Grey, *J. Chem. Soc. Chem. Comm.*, 72-74, (1990).
5. "Y-89 MAS NMR study of rare-earth pyrochlores - Paramagnetic shifts in the solid-state", C.P. Grey, M.E. Smith, A.K. Cheetham, C.M. Dobson and N. Dupré, *J. Am. Chem. Soc.*, **112**, 4670-4675, (1990).
6. "Selective oxidation of methane to synthesis gas-using transition-metal catalysts", A.T. Ashcroft, A.K. Cheetham, J.S. Foord, M.L.H. Green, C.P. Grey, A.J. Murrell and P.D.F. Vernon, *Nature* (London), **344**, 319-321, (1990).
7. "An investigation into the conversion of methanol to hydrocarbons over a SAPO-34 catalyst using Magic-Angle-Spinning NMR and gas-chromatography", Y. Xu, C.P. Grey, J.M. Thomas and A.K. Cheetham, *Catal. Lett.*, **4**, 251-260, (1990).
8. "ESR and solid state MAS NMR study of the silica-supported  $\text{H}_{3+n}\text{PV}_n\text{Mo}_{12-n}\text{O}_{40}$  ( $n=0,1,2,3$ ) Heteropolyacids", E.M. Serwicka and C.P. Grey, *Colloid Surface*, **45**, 69-82, (1990).
9. "A study on the reaction-mechanism of methanol conversion to hydrocarbons by solid-state NMR and gas-chromatography on a SAPO-34 catalyst", Y. Xu, C.P. Grey, J.M. Thomas and A.K. Cheetham, *Catal. Sci. Technol.*, Proc. Tokyo Conf., Eds. S. Yoshida, N. Takezawa, T. Ono, 1: 79-84 (1991).
10. "Isomorphous substitution in nonlinear optical  $\text{KTiOPO}_4$  - powder diffraction and magic angle spinning Nuclear-Magnetic-Resonance study of  $(\text{K}_{1/2}\text{Na}_{1/2})\text{TiOPO}_4$  and  $(\text{Rb}_{1/2}\text{Na}_{1/2})\text{TiOPO}_4$ ", S.J. Crennell, J.J. Owen, C.P. Grey, A.K. Cheetham, J.A. Kaduk and R.H. Jarman, *J. Mat. Chem.*, **1**, 113-119, (1991).
11. "Structure of cobaltacene in  $\text{SnS}_2$ : a single crystal solid state  $^2\text{H}$  NMR study", C.P. Grey, J.S.O. Evans, S.J. Heyes and D. O'Hare, *J.C.S. Chem Comm.*, 1380-1382, (1991).
12. "Multiple-frequency decoupling in the Magic-Angle-Spinning NMR of paramagnetic solids", D.P. Raleigh, C.P. Grey, N. Soffe and C.M. Dobson, *J. Magn. Reson.*, **97**, 162-170, (1992).
13. "Structural information from NMR studies of paramagnetic solids - Na-23 MAS spectra of sodium lanthanide salts of ethylenediaminetetraacetic acid", A.R. Brough, C.P. Grey and C.M. Dobson, *J. Chem. Soc. Chem. Comm.*, 742-743, (1992).
14. "The detection of weak heteronuclear coupling between Spin-1 and spin-1/2 nuclei in MAS NMR;  $^{14}\text{N}/^{13}\text{C}/^1\text{H}$  triple resonance experiments", C.P. Grey and W.S. Veeman, *Chem. Phys. Lett.*, **192**, 379-385, (1992).

15. "Susceptibility matching in MAS NMR - the determination of hyperfine tensors from paramagnetic stannates", C.P. Grey, C.M. Dobson and A.K. Cheetham, *J. Magn. Reson.*, **98**, 414-420, (1992).
16. "Uranium bioaccumulation by a citrobacter sp as a result of enzymatically mediated growth of polycrystalline  $\text{HUO}_2\text{PO}_4$ ", L.E. Macaskie, R.M. Empson, A.K. Cheetham, C.P. Grey and A.J. Skarnulis, *Science*, **257**, 782-784, (1992).
17. "Multinuclear solid-state Nuclear-Magnetic-Resonance study of 2-aminoethylferrocene and its intercalation compounds with the layered host lattices  $\text{MoO}_3$ ,  $\alpha\text{-Zr}(\text{HPO}_4)_2\cdot\text{H}_2\text{O}$  and  $2\text{H-TaS}_2$ ", S. Mason, L.M. Bull, C.P. Grey, S.J. Heyes and D. O'Hare, *J. Mat. Chem.*, **2**, 1189-1194, (1992).
18. "Temperature-dependent solid state  $^{119}\text{Sn}$  MAS NMR of  $\text{Nd}_2\text{Sn}_2\text{O}_7$ ,  $\text{Sm}_2\text{Sn}_2\text{O}_7$  and  $\text{Y}_{1.8}\text{Sm}_{0.2}\text{Sn}_2\text{O}_7$ : 3 sensitive chemical-shift thermometers", C.P. Grey, A.K. Cheetham and C.M. Dobson, *J. Magn. Reson. Ser. A*, **101**, 299-306, (1993).
19. "Rotational echo  $^{14}\text{N}/^{13}\text{C}/^1\text{H}$  triple-resonance solid-state Nuclear-Magnetic-Resonance - A probe of  $^{13}\text{C}$ - $^{14}\text{N}$  internuclear distances", C.P. Grey, W.S. Veeman and A.J. Vega, *J. Chem. Phys.*, **98**, 7711-7724, (1993).
20. "Paramagnetic-ions as structural probes in solid-state NMR - Distance measurements in crystalline lanthanide acetates", A.R. Brough, C.P. Grey and C.M. Dobson, *J. Am. Chem. Soc.*, **115**, 7318-7327, (1993).
21. "Population Transfers for NMR of Quadrupolar Spins in Solids", J. Haase, M.S. Conradi, C.P. Grey and A.J. Vega, *J. Magn. Reson. Ser. A*, **109**, 90-97, (1994).
22. " $^{14}\text{N}$  population transfers in 2-dimensional  $^{13}\text{C}/^{14}\text{N}/^1\text{H}$  MAS triple-resonance Magic-Angle-Spinning Nuclear-Magnetic-Resonance spectroscopy", C.P. Grey, A.P.A.M. Eyckelboom and W.S. Veeman, *Solid State Nucl. Mag.* **4**, 113-120, (1995).
23. " $\text{Pr}_2\text{Sn}_2\text{O}_7$  and  $\text{Sm}_2\text{Sn}_2\text{O}_7$  as high-temperature shift thermometers in variable-temperature  $^{119}\text{Sn}$  Mas NMR", G.-J.M.P. van Moorsel, E.R.H. van Eck and C.P. Grey, *J. Magn. Reson. A*, **113**, 159-163, (1995).
24. "High resolution solid state  $^{19}\text{F}$  MAS NMR-study of ionic motion in  $\alpha\text{ PbF}_2$ ", F. Wang and C.P. Grey, *J. Am. Chem. Soc.*, **117**, 6637-6638, (1995).
25. "Determination of the quadrupole coupling-constant of the invisible aluminum spins in zeolite HY with  $^1\text{H}/^{27}\text{Al}$  TRAPDOR NMR", C.P. Grey and A.J. Vega, *J. Am. Chem. Soc.*, **117**, 8232-8242, (1995).
26. " $^{15}\text{N}/^{27}\text{Al}$  double resonance study of monomethylamine adsorbed on Zeolite HY", C.P. Grey and B.S.A. Kumar, *J. Am. Chem. Soc.*, **117**, 9071-9072, (1995).
27. "A  $^{19}\text{F}$  and  $^{27}\text{Al}$  MAS NMR study of the dehydrofluorination reaction of hydrofluorocarbon-134 over basic faujasite zeolites", C.P. Grey and D.R. Corbin, *J. Phys. Chem. -US*, **99**, 16821-16823, (1995).
28. "NMR studies of hydrofluorocarbon-zeolite interactions", C.P. Grey and D.R. Corbin, *Studies in Surface Science and Catalysis* (J. Weitkamp, H.G. Karge, H. Pfeifer and W. Hölderich Eds.), **98**, 89-90, (1995).

29. "Neutron and Raman spectroscopies of 134 and 134a hydrofluorocarbons encaged in Na-X zeolite", T.J. Udovic, J.M. Nicol, R.R. Cavanagh, J.J. Rush, M.K. Crawford, C.P. Grey and D.R. Corbin, *Mater. Res. Soc. Symp. Proc.* **376** (Neutron Scattering in Materials Science II), 751-756, (1995).
30. "Nucleation in lithium disilicate glass: The role of Q species distribution", Q. Zeng, H. Nekvasil and C.P. Grey, (*Trans. Am. Geophys. Union* 76), **46**, F661, (1995).
31. "Probing the bronsted and Lewis acidity of zeolite HY: A  $^1\text{H}/^{27}\text{Al}$  and  $^{15}\text{N}/^{27}\text{Al}$  TRAPDOR NMR study of monomethylamine adsorbed on HY", H.-M. Kao and C.P. Grey, *J. Phys. Chem.*, 100, 5105-5117, (1996).
32. "Synthesis and structure of  $\text{KIn}(\text{PO}_4)(\text{OH})$ : chains of hydroxide-bridged  $\text{InO}_4(\text{OH})_2$  octahedra", J.A. Hriljac, C.P. Grey, A.K. Cheetham, P.D. VerNooy and C.C. Torardi, *J. Solid State Chem.*, **123**, 243-248, (1996).
33. "NMR studies of the hydrofluorocarbon-cation interactions and cation migrations on adsorption of hydrofluorocarbon-134 on zeolites NaY and CsY", C.P. Grey, F.I. Poshni, Y. Ba and D.R. Corbin, *Mater. Res. Soc. Symp. Proc.*, (*Micropor. Mesopor. Mat.*), **431**, 177-184, (1996).
34. "Characterization of the Lewis acid sites in zeolite HY, with probe molecule trimethylphosphine and  $^{31}\text{P}/^{27}\text{Al}$  double resonance NMR", H.M. Kao and C.P. Grey, *Chem. Phys. Lett.*, **259**, 459-464, (1996).
35. "A study of the mobility of poly(methyl methacrylate) silicate interpenetrating networks with  $^2\text{H}$  NMR", C.P. Grey and K.G. Sharp, *Mater. Res. Soc. Symp. Proc.* (Better Ceramics Through Chemistry VII), **435**, 179-185, (1996).
36. "Determination of the  $^{31}\text{P}-^{27}\text{Al}$  J-coupling constant of trimethylphosphine bound to the Lewis Acid site in Zeolite HY", H.M. Kao and C.P. Grey, *J. Am. Chem. Soc.*, **119**, 627-628, (1997).
37. "Combined MAS NMR and X-ray powder diffraction structural characterization of hydrofluorocarbon-134 adsorbed on zeolite NaY: Observation of cation migration and strong sorbate-cation interactions", C.P. Grey, F.I. Poshni, A. Gualtieri, P. Norby, J.C. Hanson and D.R. Corbin, *J. Am. Chem. Soc.*, **119**, 1981-1989, (1997).
38. "Probing the mechanism of fluoride-ion conduction in  $\text{LaF}_3$  and strontium-doped  $\text{LaF}_3$  with high resolution  $^{19}\text{F}$  MAS NMR", F. Wang and C.P. Grey, *Chem. Mater.*, **9**, 1069-1071, (1997).
39. "Solid state NMR spectroscopy of non-integer spin nuclei" in "New Trends in Materials Chemistry", C.P. Grey, *NATO ASI Series*, C498, (1997).
40. "Cation migration in zeolites. An in-situ X-ray powder diffraction and MAS NMR study of the structure of zeolite CsY during dehydration", P. Norby, F.I. Poshni, A.F. Gualtieri, J.C. Hanson and C.P. Grey, *J. Phys. Chem. B*, **102**, 839-856, (1998).
41. "A 1- and 2-D  $^{19}\text{F}$  MAS NMR Study of Fluoride-Ion Mobility in  $\alpha$   $\text{PbF}_2$ ", F.Wang and C.P. Grey, *J. Am. Chem. Soc.*, 120, 970-980, (1998).
42. "Detection and estimation of the number of Brønsted acid sites within NaY and NaX", V.J. Rao, D.L. Perlstein, R.J. Robbins, P.H. Lakshminarasimhan, H.-M. Kao, C.P. Grey and V. Ramamurthy", *J.C.S., Chem. Commun.*, 269, (1998).



43. "Optimizing the  $^{13}\text{C}/^{14}\text{N}$  REAPDOR NMR experiment: a theoretical and experimental study", Y. Ba, H.M.Kao, C.P. Grey, L. Chopin and T. Gullion, *J. Magn. Reson.* **133**, 104-114, (1998).
44. "Activation conditions play a key role in the activity of zeolite CaY: NMR and product studies of Brønsted acidity," H.-M.Kao, C.P. Grey, K. Pitchumani, P.H. Lakshminarasimhan and V. Ramamurthy, *J. Phys. Chem. A*, **102**, 5627-5638, (1998).
45. "INEPT experiments involving quadrupolar nuclei in solids", H.-M. Kao and C.P. Grey, *J. Magn. Reson.*, **133**, 313-323, (1998).
46. " $^{19}\text{F}/^{23}\text{Na}$  cross-polarization NMR study of hydrofluorocarbon-zeolite binding on zeolite NaY, K.H. Lim and C.P. Grey, *J.C.S. Chem. Commun*, 2257-2258, (1998).
47. "Probing the defect structure of anion-excess  $\text{Ca}_{1-x}\text{Y}_x\text{F}_{2+x}$  ( $x=0.03-0.32$ ) with high-resolution  $^{19}\text{F}$  MAS NMR spectroscopy," F. Wang and C.P. Grey, *Chem. Mater.*, **10**, 3081-3091, (1998).
48. "High-resolution  $^{19}\text{F}$  MAS and  $^{19}\text{F}$ - $^{113}\text{Cd}$  REDOR NMR study of oxygen/fluorine ordering in oxyfluorides", L.S. Du, F. Wang and C.P. Grey, *J. Solid State Chem.*, **140**, 285-294, (1998).
49. "Energy transfer, proton transfer and electron transfer reactions within zeolites, V. Ramamurthy, P. H. Lakshminarasimhan, C.P. Grey and L.J. Johnston, *Chem. Commun*, 2411-2424, (1998).
50. "Analysis of the anisotropic dimension in the RIACT (II) multiple quantum MAS NMR experiment for  $I = 3/2$  Nuclei", K.H. Lim and C.P. Grey, *Solid State Nucl. Mag.*, **13**, 101-112 (1998).
51. " $^6\text{Li}$  MAS NMR studies of lithium manganate cathode materials", Y.J. Lee, F. Wang and C.P. Grey, *J. Am. Chem. Soc.*, **120**, 12601-12613 (1998).
52. "Hydrochlorofluorocarbon reactivity and structural characterization of cation-exchanged ZnX", M.F. Ciruolo, P. Norby, C.P. Grey, J.C. Hanson and D.R. Corbin, *Proc. 12th IZC*, 2295-2300, (1999).
53. "Hydrofluorocarbon zeolite interactions: double resonance NMR and X-ray diffraction studies", C.P. Grey, K.-H. Lim, P. Norby and M.F. Ciruolo, *Proc. 12th IZC*, 2301-2308, (1999).
54. "NMR studies of oxygen-zeolite interactions at low temperatures", H.M. Liu, H.-M. Kao and C.P. Grey, *Proc. 12th IZC*, 2317-2324, (1999).
55. "Structural characterization and hydrochlorofluorocarbon reactivity zinc-exchanged NaX," M.F. Ciruolo, P. Norby, J.C. Hanson, D.R. Corbin and C.P. Grey, *J. Phys. Chem. B*, **103**, 346-356, (1999).
56. "A Raman spectroscopy study of the separation of hydrofluorocarbons using zeolites", M.K. Crawford, K.D. Dobbs, R.J. Smalley, D.R. Corbin, N. Maliszewskyj, T.J. Udovic, R.R. Cavanagh, J.J. Rush and C.P. Grey, *J. Phys. Chem. B*, **103**, 431-434, (1999).
57. "Adsorption of hydrofluorocarbons HFC-134 and HFC-134a on X and Y zeolites: Effect of ion-exchange on selectivity and heat of adsorption", S. Savitz, F.R. Siperstein, R. Huber, S.M. Tieri, R.J. Gorte, A.L. Myers, C.P. Grey and D.R. Corbin, *J. Phys. Chem. B*, **103**, 8283-8289, (1999).

58. <sup>1</sup>H MAS and <sup>1</sup>H/<sup>27</sup>Al TRAPDOR NMR studies of oxygen-zeolite interactions at low temperatures: Probing bronsted acid site accessibility”, H.M. Liu, H.-M. Kao and C.P. Grey, *J. Phys. Chem. B*, **103**, 4786-4796, (1999).
59. “High-order spin-diffusion mechanisms in <sup>19</sup>F 2-D NMR of oxyfluorides”, L.-S. Du, C.P. Grey and M.H. Levitt, *J. Magn. Reson.*, **140**, 242-249, (1999).
60. “Proton environments in hydrous aluminosilicate glasses: A <sup>1</sup>H MAS, <sup>1</sup>H/<sup>27</sup>Al and <sup>1</sup>H/<sup>23</sup>Na TRAPDOR NMR study,” Q. Zeng, H. Nekvasil and C.P. Grey, *J. Phys. Chem. B*, **103**, 7406-7415, (1999).
61. “Triple quantum cross-polarization NMR of <sup>1</sup>H/<sup>27</sup>Al and <sup>19</sup>F/<sup>23</sup>Na spin systems in solids”, K.H. Lim and C.P. Grey, *Chem. Phys. Lett.*, **312**, 45-56, (1999).
62. “<sup>6</sup>Li and <sup>7</sup>Li MAS NMR and *in situ* X-ray diffraction studies of lithium manganate cathode materials,” Y.J. Lee, F. Wang, C.P. Grey, S. Mukerjee and J. McBreen, *Mater. Res. Soc. Symp. Proc.*, **548**, 197-202, (1999).
63. “Structural studies and order-disorder phenomenon in a series of new quaternary tellurates of the type A<sup>2+</sup><sub>2</sub>M<sup>4+</sup>Te<sup>6+</sup>O<sub>6</sub> and A<sub>2</sub><sup>1+</sup>M<sup>4+</sup>Te<sup>6+</sup>O<sub>6</sub>,” P.M. Woodward, A.W. Sleight, L.-S. Du and C.P. Grey, *J. Solid State Chem.*, **147**, 99-116, (1999).
64. “In support of a depolymerization model for water in sodium aluminosilicate glasses: Information from NMR spectroscopy,” Q. Zeng, H. Nekvasil and C.P. Grey, *Geochim Cosmochim. Ac.*, **64**, 883-896, (2000).
65. “<sup>6</sup>Li and <sup>7</sup>Li Magic-Angle Spinning Nuclear Magnetic Resonance and *in situ* x-ray diffraction studies of the charging and discharging of Li<sub>x</sub>Mn<sub>2</sub>O<sub>4</sub> at 4V” Y.J. Lee, F. Wang, S. Mukerjee, J. McBreen and C.P. Grey, *J. Electrochem. Soc.*, **147**, 803-812, (2000).
66. “<sup>19</sup>F/<sup>23</sup>Na multiple quantum cross polarization NMR in solids”, K.H. Lim and C.P. Grey, *J. Chem. Phys.*, **112**, 7490-7504, (2000).
67. “Determining the structure of trimethylphosphine bound to the Brønsted acid site in zeolite HY: Double-resonance NMR and *ab-initio* studies”, H.-M. Kao, H.M. Liu, J.C. Jiang, S.H. Lin and C.P. Grey, *J. Phys. Chem. B.*, **104**, 4923-4933, (2000).
68. “Characterization of extra-framework cation positions in zeolites NaX and NaY with very fast <sup>23</sup>Na MAS and multiple quantum MAS NMR spectroscopy”, K. H. Lim and C.P. Grey, *J. Am. Chem. Soc.*, **122**, 9768-9780, (2000).
69. “<sup>19</sup>F/<sup>23</sup>Na double resonance MAS NMR study of oxygen/fluorine ordering in the oxyfluoride Na<sub>5</sub>W<sub>3</sub>O<sub>9</sub>F<sub>5</sub>”, L.-S. Du, A. Samoson, T. Tuhern and C.P. Grey, *Chem. Mater.*, **12**, 3611-3616, (2000).
70. “<sup>6</sup>Li MAS NMR study of electron correlations, magnetic ordering, and stability of lithium manganese (III) oxides”, Y.J. Lee and C.P. Grey, *Chem. Mater.*, **12**, 3871-3878, (2000).
71. “A new porous lithosilicate with a high ionic conductivity and ion-exchange capacity”, S.-H. Park, J.B. Parise, H. Gies, H.M. Liu, C.P. Grey and B.H. Toby, *J. Am. Chem. Soc.*, **122**, (44); 11023-11024, (2000).
72. “Ion mobility in α-PbF<sub>2</sub>: a computer simulation study,” M.J. Castiglione, M. Wilson, P.A. Madden and C.P. Grey, *J. Phys.: Cond. Mat*, **13**, 51-66, (2001).

73. "Characterization of  $^{93}\text{Nb}$ ,  $^{19}\text{F}$  spin pairs in solid potassium heptafluoroniobate (V) by solid-state  $^{93}\text{Nb}$  and  $^{19}\text{F}$  NMR", L.-S. Du, R.W. Schurko, K.H. Lim and C.P. Grey, *J. Phys. Chem. A*, **105**, 760-768, (2001).
74. "In-Situ X-ray diffraction and Solid State NMR study of the fluorination of  $\gamma\text{-Al}_2\text{O}_3$  with  $\text{HCF}_2\text{Cl}$ ", P.J. Chupas, M.F. Ciruolo, J.C. Hanson and C.P. Grey, *J. Am. Chem. Soc.*, **123**, 1694-1702, (2001).
75. " $^6\text{Li}$  magic angle spinning NMR study of the cathode material  $\text{LiNi}_x\text{Mn}_{2-x}\text{O}_4$  - The effect of the Ni doping on the local structure during charging", Y.J. Lee, C. Eng and C.P. Grey, *J. Electrochem. Soc.*, **148**, A249-A257, (2001).
76. "Plasma-fluorination synthesis of high surface area aluminum trifluoride from a zeolite precursor", J.L. Delattre, P.J. Chupas, C.P. Grey and A.M. Stacy, *J. Am. Chem. Soc.*, **123**, 5364-5365, (2001).
77. "An *in-situ* X-ray powder diffraction study of the adsorption of hydrofluorocarbons in zeolites", M.F. Ciruolo, J.C. Hanson, P. Norby and C.P. Grey, *J. Phys. Chem. B.*, **105**, 2604-2611, (2001).
78. "Kinetics and mechanism of the  $\beta$ - to  $\alpha$ -  $\text{CuAlCl}_4$  phase transition: A time-resolved  $^{63}\text{Cu}$  MAS NMR and powder X-ray diffraction study", H.M. Liu, R.M. Sullivan, J.C. Hanson, C.P. Grey and J.D. Martin, *J. Am. Chem. Soc.*, **123**, 7564-7573, (2001).
79. " $^2\text{H}$  MAS NMR studies of the manganese dioxide tunnel structures and hydroxides used as cathode materials in primary batteries", Y. Paik, J.P. Osegovic, F. Wang, W. Bowden and C.P. Grey, *J. Am. Chem. Soc.*, **123**, 9367-9377, (2001).
80. "Double resonance NMR and molecular simulations of hydrofluorocarbon binding on faujasite zeolites NaX and NaY: the importance of hydrogen bonding in controlling adsorption geometries", K.H. Lim, F. Jousse, S.M. Auerbach and C.P. Grey, *J. Phys. Chem. B.*, **105**, 9918-9929 (2001).
81. "Yttrium aluminum garnet (YAG) films through a precursor plasma spraying technique" S.D. Parukuttyamma, J. Margolis, H.M. Liu, C.P. Grey, S. Sampath, H. Herman and J.B. Parise, *J. Am. Ceram. Soc.*, **84**, 1906-1908, (2001).
82. "Solid-state rubidium exchange of zeolite  $\text{NH}_4\text{Y}$ " M.F. Ciruolo, J.C. Hanson and C.P. Grey, *Micropor. Mesopor. Mat.*, **49**, 111-124, (2001).
83. "Molecular dynamics studies of hydrofluorocarbons in faujasite-type zeolites: Modeling guest-induced cation migration in dry zeolites", E. Jaramillo, C.P. Grey and S.M. Auerbach, *J. Phys. Chem. B.*, **105**, 12319-12329, (2001).
84. "Combined X-ray and neutron powder refinement and NMR study of hydrochlorofluorocarbon HCFC-124a ( $\text{CF}_2\text{HCF}_2\text{Cl}$ ) binding on NaX", M.F. Ciruolo, J.C. Hanson, B.H. Toby and C.P. Grey, *J. Phys. Chem. B*, **105**, 12330-12337, (2001).
85. "Study of fluoride-ion motions in  $\text{PbSnF}_4$  and  $\text{BaSnF}_4$  compounds with molecular dynamics simulations and solid state NMR techniques, S. Chaudhuri, M. Castiglione, F. Wang, M. Wilson, P.A. Madden and C.P. Grey, *MRS Proceedings*, GG10.9, (2001).

86. "Cation ordering and electrochemical properties of the cathode materials  $\text{LiZn}_x\text{Mn}_{2-x}\text{O}_4$ ; a  $^6\text{Li}$  magic-angle spinning NMR spectroscopy and diffraction study", Y.J. Lee, S.-H. Park, C. Eng, J.B. Parise and C.P. Grey, *Chem. Mater.*, **14**, 194-205, (2002).
87. "Magnetism and structural chemistry of the  $n=1$  Ruddlesden-Popper phases  $\text{La}_4\text{LiMnO}_8$  and  $\text{La}_3\text{SrLiMnO}_8$ ", J.C. Burley, P.D. Battle, D.J. Gallon. J. Sloan. C.P. Grey and M.J. Rosseinsky, *J. Am. Chem. Soc.*, **124**, 620-628, (2002).
88. " $^6\text{Li}$  magic angle spinning NMR study of the cathode materials  $\text{Li}_{1+\alpha}\text{Mn}_{2-\alpha}\text{O}_{4-\delta}$ : - The effect on the local structure on the electrochemical properties," Y.J. Lee and C.P. Grey, *J. Electrochem. Soc.*, **149**, A103-A114, (2002).
89. "Probing  $\text{Cs}^+$  cation accessibility with  $\text{O}_2$  and  $^{133}\text{Cs}$  MAS NMR spectroscopy", H.M. Liu and C.P. Grey, *Micropor. Mesopor. Mat.*, **53**, 109 - 120, (2002).
90. "Determining the lithium local environments in the lithium manganates  $\text{LiZn}_{0.5}\text{Mn}_{1.5}\text{O}_4$  and  $\text{Li}_2\text{MnO}_3$  by analysis of the  $^6\text{Li}$  MAS NMR spinning sideband manifolds", Y.J. Lee and C.P. Grey, *J. Phys. Chem. B*, **106**, 3576-3582, (2002).
91. " $^6\text{Li}$  MAS NMR studies of the local structure and electrochemical properties of Cr-doped lithium manganese and lithium cobalt oxide cathode materials for lithium-ion batteries", C.J. Pan, Y.J. Lee, B. Ammundsen and C.P. Grey, *Chem. Mater.*, **14**, 2289-2299, (2002).
92. "Probing oxygen motion in disordered anionic conductors with  $^{17}\text{O}$  and  $^{51}\text{V}$  MAS NMR spectroscopy", N. Kim and C.P. Grey, *Science*, **297**, 1317-1320, (2002).
93. "Solid-state  $^{93}\text{Nb}$ ,  $^{19}\text{F}$  and  $^{113}\text{Cd}$  NMR study of niobium oxyfluorides: Characterization of local distortions and oxygen/fluorine ordering", L.-S. Du, R.W. Schurko, N. Kim and C.P. Grey, *J. Phys. Chem. A*, **106**, 7876-7886, (2002).
94. "Resolving the different dynamics of the fluorine sublattices in the anionic conductor  $\text{BaSnF}_4$  by using high-resolution MAS NMR techniques", S. Chaudhuri, F. Wang and C.P. Grey, *J. Am. Chem. Soc.*, **124**, 11746-11757, (2002).
95. "Nuclear magnetic resonance studies of lithium-ion battery materials", C.P. Grey and S.G. Greenbaum, *MRS Bull.*, **27**, 613-618, (2002).
96. "Investigation of the local structure of the  $\text{LiNi}_{0.5}\text{Mn}_{0.5}\text{O}_2$  cathode material during electrochemical cycling by X-ray absorption and NMR spectroscopy", W.S. Yoon, Y. Paik, X.-Q. Yang, M. Balasubramanian, J. McBreen and C.P. Grey, *Electrochem. Solid St.*, **5**, A263-A266, (2002).
97. "Lithium and deuterium NMR studies of acid-leached layered lithium manganese oxides", Y. Paik, C.P. Grey, C.S. Johnson, J.-S. Kim and M.M. Thackeray, *Chem. Mater.*, **14**, 5109-5115, (2002).
98. "Study of ion-exchanged microporous lithosilicate Na-RUB-29 using synchrotron X-ray single-crystal diffraction and  $^6\text{Li}$  MAS NMR spectroscopy" S.-H. Park, M. Kleinsorge, C.P. Grey and J.B. Parise, *J. Solid State Chem.*, **167**, 310-323, (2002).

99. “ $^{17}\text{O}$  MQMAS NMR studies of Na-A and Ca-A”, J.E. Readman, N. Kim, M. Ziliox and C.P. Grey, *Chem. Commun.*, 2808-2809, (2002).
100. “Single-step deposition of Eu-doped  $\text{Y}_2\text{O}_3$  phosphor coatings through a precursor plasma spraying technique”, P.S. Devi, J. Margolis, J.B. Parise, C.P. Grey, S. Sampath, H. Herman and H.D. Gafney, *J. Mater. Res.* **17**, 2771-2774, (2002).
101. “Understanding the NMR shifts in layered paramagnetic transition metal oxides by using density functional theory calculations”, D. Carlier, M. Menetrier, C.P. Grey, C. Delmas and G. Ceder, *Phys. Rev. B*, **67**, 174103, (2003).
102. “A combined solid-state NMR and diffraction study of the structures and acidity of fluorinated aluminas: Implications for catalysis,” P.J. Chupas, D. R. Corbin, V.N.M. Rao, J.C. Hanson and C.P. Grey, *J. Phys. Chem. B*, **107**, 8327-8336, (2003).
103. “Reduction of  $\gamma$ - $\text{MnO}_2$  in deuterium media; MAS NMR and electrochemical studies” W. Bowden, C.P. Grey, R. Sirotina, T. Richards, F. Wang and Y. Paik, *ITE Lett. Batteries, New Technol. Med.*, **4**, 148-157, (2003).
104. “Structural chemistry and magnetic properties of  $\text{La}_2\text{LiRuO}_6$ ”, P.D. Battle, C.P. Grey, M. Hervieu, C. Martin, C.A. Moore and Y. Paik, *J. Solid State Chem.*, **175**, 20-26, (2003).
105. “Lithium MAS NMR studies of cathode materials for lithium-ion batteries”, C.P. Grey and Y.J. Lee, *Solid State Sciences*, **5**, 883-894, (2003).
106. “In situ X-ray absorption spectroscopic study on  $\text{LiNi}_{0.5}\text{Mn}_{0.5}\text{O}_2$  cathode material during electrochemical cycling”, W.S. Yoon, C.P. Grey, M. Balasubramanian, X.-Q. Yang and J. McBreen, *Chem. Mater.*, **15**, 3161-3169, (2003).
107. “ $^{17}\text{O}$  MAS NMR study of the oxygen local environments in the anionic conductors  $\text{Y}_2(\text{B}_{1-x}\text{B}'_x)_2\text{O}_7$  ( $\text{B}, \text{B}'=\text{Sn}, \text{Ti}, \text{Zr}$ )”, N. Kim and C.P. Grey, *J. Solid State Chem.*, **175**, 110-115, (2003).
108. “ $^6\text{Li}$  MAS NMR and in situ X-ray studies of lithium nickel manganese oxides”, W.S. Yoon, N. Kim, X.-Q. Yang, J. McBreen and C.P. Grey, *J. Power Sources*, **119**, 649-653, (2003).
109. “Sorptive reconstruction of the  $\text{CuAlCl}_4$  framework upon reversible ethylene binding”, R.M. Sullivan, H.M. Liu, D.S. Smith, J.C. Hanson, D. Osterhout, M.F. Ciruolo, C.P. Grey and J.D. Martin, *J. Am. Chem. Soc.*, **125**, 11065-11079, (2003).
110. “Phase, structural and microstructural investigations of plasma sprayed hydroxyapatite coatings”, L.M. Sun, C.C. Berndt and C.P. Grey, *Mat. Sci. Eng. A-Struct.*, **360**, 70-84, (2003).
111. “Hydrothermal synthesis and structural characterization of four scandium phosphate frameworks”, I. Bull, V. Young, S.J. Teat, L.M. Peng, C.P. Grey and J.B. Parise, *Chem. Mater.*, **15**, 3818-3825, (2003).
112. “Structural and magnetic properties of  $\text{Li}_3\text{RuO}_4$ ”, A. Alexander, P.D. Battle, J.C. Burley, D.J. Gallon and C.P. Grey, *J. Mater. Chem.*, **13**, 2612-2616, (2003).

113. "Nuclear magnetic resonance studies of zeolites", C.P. Grey, Chapter 6 in Handbook of Zeolite Science and Technology, S.M Auerbach, K.A. Carrado and P.K. Dutta, ed., *Marcel Dekker, Inc., New York*, (2003).
114. "Rapid-acquisition pair distribution function (RA-PDF) analysis," P.J. Chupas, X.Y. Qiu, J.C. Hanson, P.L. Lee, C.P. Grey and S.J.L. Billinge, *J. Appl. Crystallogr.*, **36**, 1342-1347, (2003).
115. "Study of the nature and mechanism of the rhombohedral-to-cubic phase transition in  $\alpha$ -AlF<sub>3</sub> with molecular dynamics simulations", S. Chaudhuri, P.J. Chupas, M. Wilson, P.A. Madden and C.P. Grey, *J. Phys. Chem. B*, **108**, 3437-3445, (2004).
116. "Magnetism and structural chemistry of the n=2 Ruddlesden-Popper phase La<sub>3</sub>LiMnO<sub>7</sub>" P.D. Battle, J.C. Burley, D.J. Gallon, C.P. Grey and J. Sloan, *J. Solid State Chem.*, **177**, 119-125, (2004).
117. "Combined NMR and XAS study on local environments and electronic structures of electrochemically Li-Ion deintercalated Li<sub>1-x</sub>Co<sub>1/3</sub>Ni<sub>1/3</sub>Mn<sub>1/3</sub>O<sub>2</sub> electrode system" W.-S. Yoon, C.P. Grey, M. Balasubramanian, X.-Q. Yang, D.A. Fischer and J. McBreen, *Electrochem. Solid St.*, **7**, A53-A55, (2004).
118. "Understanding the crystal structure of layered LiNi<sub>0.5</sub>Mn<sub>0.5</sub>O<sub>2</sub> by electron diffraction and powder diffraction simulation", Y.S. Meng, G. Ceder, C.P. Grey, W.-S. Yoon and Y. Shao-Horn *Electrochem. Solid St.*, **7**, A155-A158, (2004).
119. "Local structure and cation ordering in O3 lithium nickel manganese oxides with stoichiometry Li[Ni<sub>x</sub>Mn<sub>(2-x)/3</sub>Li<sub>(1-2x)/3</sub>]O<sub>2</sub> - NMR studies and first principles calculations", W.-S. Yoon, S. Iannopollo, C.P. Grey, D. Carlier, J. Gorman, J. Reed and G. Ceder, *Electrochem. Solid St.*, **7**, A167-A171, (2004).
120. "Electrochemical and Structural Properties of xLi<sub>2</sub>M'O<sub>3</sub>·(1-x)LiMn<sub>0.5</sub>Ni<sub>0.5</sub>O<sub>2</sub> Electrodes for Lithium Batteries (M' = Ti, Mn, Zr; 0<x<0.3)" J.-S. Kim, C.S. Johnson, J.T. Vaughey, M.M. Thackeray, S.A. Hackney, W. Yoon and C.P. Grey, *Chem. Mater.*, **116**, 1996-2006, (2004).
121. "Electrochemical activity of Li in the transition-metal sites of O3 Li[Li<sub>(1-2x)/3</sub>Mn<sub>(2-x)/3</sub>Ni<sub>x</sub>]O<sub>2</sub>", C.P. Grey, W.-S. Yoon, J. Reed and G. Ceder, *Electrochem. Solid St.*, **7**, A290-A293, (2004).
122. "<sup>2</sup>H MAS NMR studies of deuterated goethite ( $\alpha$ -FeOOD)" K.E. Cole, Y. Paik, R.J. Reeder, M. Schoonen and C.P. Grey, *J. Phys. Chem. B*, **108**, 6938-6940, (2004).
123. "Probing local and long-range structure simultaneously: An in-situ study of the high-temperature phase transition of  $\alpha$ -AlF<sub>3</sub>," P.J. Chupas, S. Chaudhuri, J.C. Hanson, X.Y. Qiu, P.L. Lee, S.D. Shastri, S.J.L. Billinge and C.P. Grey, *J. Am. Chem. Soc.*, **126**, 4756-4757, (2004). Highlighted in the Annual Report of the Advanced Photon Source, May p.25-26, (2004).
124. "<sup>2</sup>H MAS NMR and stepped potential electrochemical spectroscopy studies of  $\gamma$ -MnO<sub>2</sub> in zinc alkaline primary batteries", Y. Paik, W. Bowden, T. Richards, R. Sirotina and C.P. Grey, *J. Electrochem. Soc.*, **151**, A998-A1011, (2004).

125. "Surface modification of fluorinated aluminas: Application of solid state NMR spectroscopy to the study of acidity and surface structure", P.J. Chupas and C.P. Grey, *J. Catal.*, **224**, 69-79, (2004).
126. "[Li-Si-O]-MFI: A new microporous lithosilicate with the MFI topology", S.-H. Park, H.M. Liu, M. Kleinsorge, C.P. Grey, B.H. Toby and J.B. Parise, *Chem. Mater.*, **16**, 2605-2614, (2004).
127. "<sup>7</sup>Li and <sup>51</sup>V MAS NMR study of the electrochemical behavior of Li<sub>1+x</sub>V<sub>3</sub>O<sub>8</sub>", N. Dupré, J. Gaubicher, D. Guyomard and C.P. Grey, *Chem. Mater.*, **16**, 2725-2733, (2004).
128. "Combined neutron diffraction, NMR and electrochemical investigation of the layered-to-spinel transformation in LiMnO<sub>2</sub>", A.R. Armstrong, N. Dupré, A.J. Paterson, C.P. Grey and P.G. Bruce, *Chem. Mater.*, **16**, 3106-3118, (2004).
129. "Cation and Spin Ordering in the n=1 Ruddlesden-Popper phase La<sub>2</sub>Sr<sub>2</sub>LiRuO<sub>8</sub>", J.A. Rodgers, P.D. Battle, N. Dupré, C.P. Grey and J. Sloan, *Chem. Mater.* **16**, 4257-4266, (2004).
130. "Comparison of the <sup>17</sup>O NMR spectra of zeolites LTA and LSX", J.E. Readman, C.P. Grey, M. Ziliox and L.M. Bull, *Solid State Nucl. Mag.*, **26**, 153-159, (2004).
131. "NMR studies of cathode materials for lithium-ion rechargeable batteries", C.P. Grey and N. Dupré, *Chem. Rev.*, **104**, 4493-4512, (2004).
132. "Solid-state NMR study of the anionic conductor Ca-doped Y<sub>2</sub>Ti<sub>2</sub>O<sub>7</sub>", N. Kim and C.P. Grey, *Dalton Trans.*, (19), 3048 -3052, (2004).
133. "Measuring Brønsted acid densities in zeolite HY with diphosphine molecules and solid state NMR spectroscopy", L.M. Peng, P.J. Chupas and C.P. Grey, *J. Am. Chem. Soc.*, **126**, 12254-12255, (2004). Featured in C&E News "Concentrates", Sept. 27, p.22, (2004).
134. "Syntheses and structure determination of new organically templated scandium fluorophosphate framework and its indium analogue", H.S. Park, I. Bull, L.M. Peng, G.Y.J. Victor Jr., C.P. Grey and J.B. Parise, *Chem. Mater.*, **16**, 5350-5356, (2004).
135. "High field multinuclear NMR investigation of the SEI layer in lithium rechargeable batteries", B.M. Meyer, N. Leifer, S. Sakamoto, S.G. Greenbaum and C.P. Grey, *Electrochem. Solid St.*, **8**, A145-A148, (2005).
136. "Detection of Brønsted acid sites in zeolite HY with high-field <sup>17</sup>O-MAS-NMR techniques", L.M. Peng, Y. Liu, N.J. Kim, J.E. Readman and C.P. Grey, *Nat. Mater.*, **4**, 216-219, (2005).
137. "The effect of heat-treatment on electrolytic manganese dioxide, a <sup>2</sup>H and <sup>6</sup>Li MAS NMR study", Y. Paik, W. Bowden, T. Richards and C.P. Grey, *J. Electrochem. Soc.*, **152**, A1539-A1547, (2005).
138. "Detecting different oxygen-ion jump pathways in Bi<sub>2</sub>WO<sub>6</sub> with 1-and 2-Dimensional <sup>17</sup>O MAS NMR spectroscopy", N. Kim, R.-N. Vannier and C.P. Grey, *Chem. Mater.*, **17**, 1952-1958, (2005).

139. "Cation ordering in layered O3 Li[Ni<sub>x</sub>Li<sub>1/3-2x/3</sub>Mn<sub>2/3-x/3</sub>]O<sub>2</sub> (0 ≤ x ≤ 1/2) compounds", Y.S. Meng, G. Ceder, C.P. Grey, W.S. Yoon, M. Jiang, J. Bréger and Y. Shao-Horn, *Chem. Mater.*, **17**, 2386-2394, (2005).
140. "Sol gel synthesis of Li<sup>+</sup>V<sub>3</sub>O<sub>8</sub>. 1. From precursors to xerogel", M. Dubarry, J. Gaubicher, D. Guyomard, O. Durupthy, N. Steunou, J. Livage, N. Dupré and C.P. Grey, *Chem. Mater.*, **17**, 2276-2283, (2005).
141. "Effect of A-site cation radius on ordering of BX<sub>6</sub> octahedra in (K,Na)MgF<sub>3</sub> perovskite", C.D. Martin, S. Chaudhuri, C.P. Grey and J.B. Parise, *Am. Mineral.*, **90**, 1522-1533, (2005).
142. "Ex situ NMR and neutron diffraction study of lithium motion in Li<sub>7</sub>MnN<sub>4</sub>", J. Cabana, N. Dupré, G. Rousse, C.P. Grey and M.R. Palacín, *Solid State Ionics*, **176**, 2205-2218, (2005).
143. "Short- and long-range order in the positive electrode material Li(NiMn)<sub>0.5</sub>O<sub>2</sub>: A joint X-ray and neutron diffraction, pair distribution function analysis and NMR study", J. Bréger, N. Dupré, P.J. Chupas, P.L. Lee, T. Proffen, J.B. Parise and C.P. Grey, *J. Am. Chem. Soc.*, **127**, 7529-7537, (2005).
144. "High-resolution X-ray diffraction, DIFFaX, NMR and first principles study of disorder in the Li<sub>2</sub>MnO<sub>3</sub>-Li(NiMn)<sub>1/2</sub>O<sub>2</sub> solid solution", J. Bréger, M. Jiang, N. Dupré, Y.S. Meng, Y. Shao-Horn, G. Ceder and C.P. Grey, *J. Solid State Chem.*, **178**, 2575-2585, (2005).
145. "Lithium manganese oxynitride: Alternative electrode material for lithium ion batteries", J. Cabana, N. Dupré, C.P. Grey, M.T. Caldes, G. Subias-Peruga and M.R. Palacín, *J. Electrochem Soc. A*, **52**, A2266-A2255, (2005).
146. "Phase evolution in the YO<sub>1.5</sub>-TiO<sub>2</sub>-ZrO<sub>2</sub> system around the pyrochlore region" T.A. Schaedler, W. Francillon, A.S. Gandhi, C.P. Grey, S. Sampath and C.G. Levi, *Acta Mater.*, **53**, 2957-2968, (2005).
147. "Structural chemistry and magnetic properties of Nd<sub>2</sub>BaLiRuO<sub>7</sub>", J.A. Rodgers, P.D. Battle and C.P. Grey, J. Sloan, *Chem. Mater.*, **17**, 4362-4373, (2005).
148. "Investigating sorption on iron-oxhydroxide soil minerals by solid-state NMR spectroscopy: A <sup>6</sup>Li MAS NMR study of adsorption and absorption on goethite", U.G. Nielsen, Y. Paik, K. Julmis, M.A.A. Schoonen, R.J. Reeder and C.P. Grey, *J. Phys. Chem. B*, **109**, 18310-18315, (2005).
149. "Dynamic effects in MAS and MQMAS NMR spectra of half-integer quadrupolar nuclei: Calculations and an application to the double perovskite cryolite", M. Kotecha, S. Chaudhuri, C.P. Grey and L. Frydman, *J. Am. Chem. Soc.*, **127**, 16701-16712, (2005).
150. "Investigation of the charge compensation mechanism on the electrochemically Li-ion deintercalated Li<sub>1-x</sub>Co<sub>1/3</sub>Ni<sub>1/3</sub>Mn<sub>1/3</sub>O<sub>2</sub> electrode system by a combination of soft and hard X-ray absorption spectroscopy", W.-S. Yoon, M. Balasubramanian, K.Y. Chung, X.-Q. Yang, J. McBreen, C.P. Grey and D.A. Fischer, *J. Am. Chem. Soc.*, **127**, 17479-17487, (2005).



151. “Li<sub>1+α</sub>V<sub>3</sub>O<sub>8</sub> gels: a new insight: Part II: from xerogel to the anhydrous material”, M. Dubarry, J. Gaubicher, D. Guyomard, N. Steunou, J. Livage, N. Dupré and C.P. Grey, *Chem. Mater.*, **18**, 629-636, (2006).
152. “Structural chemistry of Ln<sub>2</sub>BaLiRuO<sub>7</sub> (Ln = La, Pr)”, P.D. Battle, C.P. Grey, J.A. Rodgers and J. Sloan, *Solid State Sci.*, **8**, 280-288, (2006).
153. “Electrodes with high power and high capacity for rechargeable lithium batteries,” K.S. Kang, Y.S. Meng, J. Bréger, C.P. Grey and G. Ceder, *Science*, **311**, 977-980, (2006).
154. “Lithiation of ramsdellite-pyrolusite MnO<sub>2</sub>; NMR, XRD, TEM and electrochemical investigation of the discharge mechanism”, W. Bowden, C.P. Grey, S. Hackney, F. Wang, Y. Paik, N. Iltchev and R. Sirotnina, *J. Power Sources*, **153**, 265-273, (2006).
155. “LiNi<sub>0.5+δ</sub>Mn<sub>0.5+δ</sub>O<sub>2</sub> - A high-rate, high-capacity cathode for lithium rechargeable batteries”, S.B. Shougaard, J. Bréger, M. Jiang, C.P. Grey and J.B. Goodenough, *Adv. Mater.*, **18**, 905-909, (2006).
156. “Octahedral tilt instability of ReO<sub>3</sub>-type crystals”, P.B. Allen, Y.R. Chen, S. Chaudhuri and C.P. Grey, *Phys. Rev. B*, **73**, 172102, (2006).
157. “An atomistic MD simulation and pair-distribution-function study of disorder and reactivity of α-AlF<sub>3</sub> nanoparticles”, S. Chaudhuri, P.J. Chupas, B.J. Morgan, P.A. Madden and C.P. Grey, *Phys. Chem. Chem. Phys.*, **8**, 5045-5055, (2006).
158. “The effect of high voltage on the structure and electrochemistry of LiNi<sub>0.5</sub>Mn<sub>0.5</sub>O<sub>2</sub>; A joint experimental and theoretical study”, J. Bréger, Y.S. Meng, Y. Hinuma, S. Kumar, Y. Shao-Horn, G. Ceder and C.P. Grey, *Chem. Mater.*, **18**, 4768 -4781, (2006).
159. “Layered Oxysulfides Sr<sub>2</sub>MnO<sub>2</sub>Cu<sub>2m-0.5</sub>S<sub>m+1</sub> (m = 1, 2 and 3) as Insertion Hosts for Li-Ion batteries”, S. Indris, J. Cabana, O.J. Rutt, S.J. Clarke and C.P. Grey, *J. Am. Chem. Soc.*, **128**, 13354-13355, (2006).
160. “New manganese dioxides for lithium batteries”, W. Bowden, T Bofinger, F. Zhang, N. R. Sirotnina, Y. Paik, H. Chen, C.P. Grey and S. Hackney, *J. Power Sources*, **165**, 609-615, (2007).
161. “Similarities in 2- and 6-line ferrihydrite based on pair distribution function analysis of X-ray total scattering”, F.M. Michel, L. Ehm, G. Liu, W.Q. Han, S.M. Antao, P.J. Chupas, P.L. Lee, K. Knorr, H. Eulert, J. Kim, C.P. Grey, A.J. Celestian, J. Gillow, M.A.A. Schoonen, D.R. Strongin and J.B. Parise, *Chem. Mater.*, **19**, 1489-1496, (2007).
162. “Layered Li<sub>x</sub>Ni<sub>y</sub>Mn<sub>y</sub>Co<sub>1-2y</sub>O<sub>2</sub> cathodes for lithium ion batteries: Understanding local structure via magnetic properties”, N.A. Chernova, M. Ma, J. Xiao, M.S. Whittingham, J. Bréger and C.P. Grey, *Chem. Mater.*, **19**, 4682-4693, (2007).
163. “Characterization of defects and the local environment in natural and synthetic alunite (K, Na, H<sub>3</sub>O)Al<sub>3</sub>(SO<sub>4</sub>)<sub>2</sub>(OH)<sub>6</sub> by multi-nuclear solid-state NMR spectroscopy”, U.G. Nielsen, J. Majzlan, B. Phillips, M. Ziliox and C.P. Grey, *Am. Mineral.*, **92**, 587-597, (2007).

164.  $^{17}\text{O}$  magic angle spinning NMR studies of Brønsted acid sites in zeolites HY and HZSM-5, L.M. Peng, H. Huo, Y. Liu and C.P. Grey, *J. Am. Chem. Soc.*, **129**, 335-346, (2007).
165. "The structural evolution of layered  $\text{Li}_x\text{Mn}_y\text{O}_2$ : a combined neutron, NMR and electrochemical study", A.R. Armstrong, A.J. Patterson, N. Dupré, C.P. Grey and P.G. Bruce, *Chem. Mater.*, **19**, 1016-1023, (2007).
166. " $^{17}\text{O}$  NMR studies of local structure and phase evolution for materials in the  $\text{Y}_2\text{Ti}_2\text{O}_7$ - $\text{ZrTiO}_4$  binary system" J.L. Palumbo, T.A. Schaedler, L.M. Peng, C.G. Levi and C.P. Grey, *J. Solid State Chem.*, **180**, 2175-2185, (2007).
167. "Chemistry for a sustainable future", V.H. Grassian, G. Meyer, H. Abruña, G.W. Coates, L.E. Achenie, T. Allison, B. Brunschwig, J. Ferry, M. Garcia-Garibay, J. Gardea-Torresdey, C.P. Grey, J. Hutchison, C.-J. Li, C. Liotta, A. Ragauskas, S. Minteer, K. Mueller, J. Roberts, O. Sadik, R. Schmehl, W. Schneider, A. Selloni, P. Stair, J. Stewart, D. Thorn, J. Tyson, B. Voelker, J.M. White and F. Wood-Black, *Environ. Sci. Technol.*, **41**, 4840-4846, (2007).
168. "NMR, PDF and RMC study of the positive electrode material  $\text{Li}(\text{NiMn})_{0.5}\text{O}_2$  synthesized by ion-exchange methods", J. Bréger, K. Kang, J. Cabana, G. Ceder and C.P. Grey, *J. Mater. Chem.*, **17**, 3167-3174, (2007).
169. "Changes in the cation ordering of layered  $\text{O}_3 \text{Li}_x\text{Ni}_{0.5}\text{Mn}_{0.5}\text{O}_2$  during electrochemical cycling to high voltages: An electron diffraction study" H.H. Li, N. Yabuuchi, Y.S. Meng, S. Kumar, J. Bréger, C.P. Grey and Y. Shao-Horn, *Chem. Mater.*, **19**, 2551-2565, (2007).
170. "Cation ordering in  $\text{Li}[\text{Ni}_x\text{Mn}_x\text{Co}_{(1-2x)}]\text{O}_2$ -layered cathode materials: A nuclear magnetic resonance (NMR), pair distribution function, X-ray absorption spectroscopy and electrochemical study", D.L. Zeng, J. Cabana, J.L. Bréger, W.-S. Yoon and C.P. Grey, *Chem. Mater.*, **19**, 6277-6289, (2007).
171. "Watching nanoparticles grow: The mechanism and kinetics for the formation of  $\text{TiO}_2$ -supported platinum nanoparticles", P.J. Chupas, K.W. Chapman, G. Jennings, P.L. Lee and C.P. Grey, *J. Am. Chem. Soc.*, (Communication), **129**, 13822-13824, (2007). Highlighted as an "Editors' Choice" in *Science*, Nov. 9, p.889, (2007).
172. "Report from the third workshop on future directions of solid-state chemistry: The status of solid-state chemistry and its impact in the physical sciences," M.G. Kanatzidis, K.R. Poeppelmeier, S. Bobev, A.M. Guloy, S.-J. Hwu, A. Lachgar, S.E. Latturmer, S.E. Raymond, D.-K. Seo, S.C. Sevov, A. Stein, B. Dabrowski, J.E. Greedan, M. Greenblatt, C.P. Grey, A.J. Jacobson, D.A. Keszler, J. Li, M.A. Subramanian, Y. Xia, T. Cagin, U. Haeussermann, T. Hughbanks, S.D. Mahanti, D. Morgan, D.-K. Seo, N.A. Spaldin, W.E. Buhro, D.E. Giammar, J.A. Hollingsworth, D.C. Johnson, A.J. Nozik, X. Peng, R.L. Bedard, N.E. Brese, G. Cao, S.S. Dhingra, C.R. Kagan, D.B. Mitzi, M.J. Geselbracht, G.C. Lisensky, M.W. Lufaso, P.A. Maggard, M. O'Keefe, A.P. Wilkinson, H.C. zur Loye, T. Egami, J.E. Greedan, J.P. Hodges, J.D. Martin, J.B. Parise, B.H. Toby, T.A. Vanderah, P.C. Burns, J.Y. Chan, A.E. Meyer, C.B. Murray, A.P. Ramirez, M.D. Ward, L. Yu, M. Alario-Franco, P.D. Battle, T. Bein, C.L. Cahill, P.S. Halasyamani, A. Maignan and R. Seshadri, *Prog. Solid State Chem.*, **36**, 1-133, (2007).
173. "Probing bronsted acid sites in zeolite HY with low temperature O-17 MAS NMR spectroscopy", H. Huo, L.M. Peng, C.P. Grey, 15th Inter. Zeolite Conf., Beijing, Peoples R.

- China, (12-17 Aug 2007). Editors: R. Xu, Z. Gao, J. Chen, W. Yan,. From zeolites to porous MOF materials: The 40<sup>th</sup> Anniversary of Inter. Zeolite Conf. Proc. of the 15<sup>th</sup> Inter. Zeolite Conf., *Elsevier Science BV.*, **170**: 783-789, (2007).
174. "Determination and quantification of the local environments in stoichiometric and defect jarosite by solid-state <sup>2</sup>H NMR spectroscopy," U.G. Nielsen, J. Majzlan and C.P. Grey, *Chem. Mater.*, **20**, 2234-2241, (2008).
175. "Local environments and lithium adsorption on the iron oxyhydroxides lepidocrocite ( $\gamma$ -FeOOH) and goethite ( $\alpha$ -FeOOH): A <sup>2</sup>H and <sup>7</sup>Li solid-state MAS NMR study", J. Kim, U.G. Nielsen and C.P. Grey, *J. Am. Chem. Soc.*, **130**, 1285-1295, (2008).
176. "Tuning the structural and physical properties of Cr<sub>2</sub>Ti<sub>3</sub>Se<sub>8</sub> by lithium intercalation: A study of the magnetic properties, investigation of ion mobility with NMR Spectroscopy and electronic band structure calculations", J. Wontcheu, W. Bensch, M. Wilkening, P. Heitjans, S. Indris, P. Sideris, C.P. Grey, S. Mankovsky and H. Ebert, *J. Am. Chem. Soc.*, **130**, 288-299, (2008).
177. "<sup>17</sup>O MQMAS NMR studies of zeolite HY", L.M. Peng, H. Huo, Z. Gan and C.P. Grey, *Micropor. Mesopor. Mat.*, 109, 156-162, (2008).
178. "Molten salt synthesis and high rate performance of the "Desert-Rose" form of LiCoO<sub>2</sub>", H.L. Chen and C.P. Grey, *Adv. Mater.*, **20**, 2206-2210, (2008).
179. "Pressure-induced polymerization of diiodobutadiyne in assembled cocrystals", C. Wilhelm, S.A. Boyd, S. Chawda, F.W. Fowler, N.S. Goroff, G.P. Halada, C.P. Grey, J.W. Lauher, L. Luo, C.D. Martin, J.B. Parise, C. Tarabrella and J.A. Webb, *J. Am. Chem. Soc.*, **130**, 4415-4420, (2008).
180. "Diphosphine probe molecules and solid-state NMR investigations of proximity between acidic sites in zeolite HY", L.M. Peng and C.P. Grey, *Micropor. Mesopor. Mat.*, **116**, 277-283, (2008).
181. "Variable temperature <sup>17</sup>O NMR study of oxygen motion in the anionic conductor Bi<sub>26</sub>Mo<sub>10</sub>O<sub>69</sub>", L. Holmes, L.M. Peng, I. Heinmaa, L.A. O'Dell, M.E. Smith, R.-N. Vannier and C.P. Grey, *Chem. Mater.*, **20**, 3638-3648, (2008).
182. "A versatile sample-environment cell for non-ambient X-ray scattering experiments", P.J. Chupas, K.W. Chapman, C. Kurtz, J.C. Hanson, P.L. Lee and C.P. Grey, *J. Applied. Crystallogr.*, **41**, 822-824, (2008).
183. "Mg/Al ordering in layered double hydroxides revealed by multinuclear NMR spectroscopy", P.J. Sideris, U.-G. Nielsen, Z. Gan and C.P. Grey, *Science*, **321**, 113-117, (2008).
184. "Poly(diiododiacetylene): Preparation, isolation, and full characterization of a very simple poly(diacetylene)", L. Luo, C. Wilhelm, A.W. Sun, C.P. Grey, J.W. Lauher and N.S. Goroff, *J. Am. Chem. Soc.*, **130**, 7702-7709, (2008).
185. "Spectroscopic signatures of nitrogen-substituted zeolites", K.D. Hammond, F. Dogan, G.A. Tompsett, V. Agarwal, W.C. Conner, C.P. Grey and S.M. Auerbach, *J. Am. Chem. Soc.*, **130**, 14912-14913, (2008).

186. "The formation of a complete solid solution between the triphylite and fayalite olivine structures", N. Recham, M. Casas-Cabanas, J. Cabana, C.P. Grey, J.C. Jumas, M. Armand and J.-M. Tarascon, *Chem. Mat.*, **20**, 6798-6809, (2008).
187. "Influence of benzoquinone sorption on the structure and electrochemical performance of the MIL-53(Fe) hybrid porous material in a lithium-ion battery", G. de Combarieu, M. Morcrette, F. Millange, N. Guillou, J. Cabana, C.P. Grey, I. Margiolaki, G. Ferey and J.-M. Tarascon, *Chem. Mater.*, **21**, 1602-1611, (2009).
188. "Real-time NMR investigations of structural changes in silicon electrodes for lithium-ion batteries", B. Key, R. Bhattacharyya, M. Morcrette, V. Seznéc, J.-M. Tarascon and C.P. Grey, *J. Am. Chem. Soc.*, **131**, 9239-9249, (2009).
189. "Electrochemical and structural study of the layered, "Li-excess" lithium-ion battery electrode material  $\text{Li}[\text{Li}_{1/9}\text{Ni}_{1/3}\text{Mn}_{5/9}]\text{O}_2$ ", M. Jiang, B. Key, Y.S. Meng and C.P. Grey, *Chem. Mater.*, **21**, 2733-2745, (2009).
190. "Investigation of the conversion reaction mechanisms for binary copper (II) compounds by solid-state NMR spectroscopy and X-ray diffraction", N. Yamakawa, M. Jiang and C.P. Grey, *Chem. Mater.*, **21**, 3162-3176, (2009).
191. "The effects of moderate thermal treatments under air on  $\text{LiFePO}_4$ -based nano powders", S. Hamelet, P. Gibot, M. Casas-Cabanas, D. Bonnin, C.P. Grey, J. Cabana, J.-B. Leriche, J. Rodriguez-Carvajal, M. Courty, S. Levasseur, P. Carlach, M. van Thournout, J.-M. Tarascon and C. Masquelier, *J. Mater. Chem.*, **19**, 3979-3991, (2009).
192. "Identifying the local structures formed during lithiation of the conversion material, iron fluoride, in a Li ion battery: A solid-state NMR, X-ray diffraction, and pair distribution function analysis study", N. Yamakawa, M. Jiang, B. Key and C.P. Grey, *J. Am. Chem. Soc.*, **131**, 10525-10536, (2009).
193. "Structural and electrochemical characterization of composite layered-spinel electrodes containing Ni and Mn for Li-ion batteries", J. Cabana, S.-H. Kang, C.S. Johnson, M.M. Thackeray and C.P. Grey, *J. Electrochem. Soc.*, **156**, A730-A736, (2009).
194. "Synthesis, short range structure, and electrochemical properties of new phases in the Li-Mn-N-O system", J. Cabana, N. Dupré, F. Gillot, A.V. Chadwick, C.P. Grey and M.R. Palacín, *Inorg. Chem.*, **48**, 5141-5153, (2009).
195. "A one-step mechanochemical route to core-shell  $\text{Ca}_2\text{SnO}_4$  nanoparticles followed by  $^{119}\text{Sn}$  MAS NMR and  $^{119}\text{Sn}$  Mössbauer spectroscopy", V. Sepelak and K.D. Becker, I. Bergmann, S. Suzuki, S. Indris, A. Feldhoff, P. Heitjans and C.P. Grey, *Chem. Mater.*, **21**, 2518-2524, (2009).
196. "Lithium salt of tetrahydroxybenzoquinone: Toward the development of a sustainable Li-ion battery", H.Y. Chen, M. Armand, M. Courty, M. Jiang, C.P. Grey, F. Dolhem, J.-M. Tarascon and P. Poizot, *J. Am. Chem. Soc.*, **131**, 8984-8988, (2009).
197. "Low temperature  $^1\text{H}$  MAS NMR spectroscopy studies of proton motion in zeolite HZSM-5", H. Huo, L.M. Peng and C.P. Grey, *J. Phys. Chem. C*, **113**, 8211-8219, (2009).

198. "Application of high-energy X-rays and pair-distribution-function analysis to nano-scale structural studies in catalysis", P.J. Chupas, K.W. Chapman, H.L. Chen and C.P. Grey, *Catalysis Today*, **145**, 213-219, (2009).
199. "Searching for microporous, strongly basic catalysts: Experimental and calculated  $^{29}\text{Si}$  NMR spectra of heavily nitrogen-doped Y zeolites", F. Dogan, K.D. Hammond, G.A. Tompsett, H. Huo, W.C. Conner, Jr., S.M. Auerbach and C.P. Grey, *J. Am. Chem. Soc.*, **131**, 11062-11079, (2009).
200. "Enhancing MQMAS of low  $\gamma$  nuclei by using a high  $B_1$  field balanced probe circuit", Z.H. Gan, P.L. Gor'kov, W.W. Brey, P.J. Sideris and C.P. Grey, *J. Magn. Reson.*, **200**, 2-5, (2009).
201. "Solid-state NMR in biological and materials physics", C.P. Grey and R. Tycko, *Phys. Today*, **62**, 44-49, (2009).
202. "Ultrafast synthesis of  $\text{Li}_{1+\alpha}\text{V}_3\text{O}_3$  gel precursors for lithium battery applications", M. Dubarry, J. Gaubicher, D. Guyomard, N. Dupré and C. Grey, *Solid State Ionics*, **180**, 1511-1516, (2009).
202. "Density functional theory study of ferrihydrite and related Fe-oxyhydroxides", N. Pinney, J.D. Kubicki, D.S. Middlemiss, C.P. Grey and D. Morgan, *Chem. Mater.*, **21**, 5727-5742, (2009).
203. "Investigation of the structural changes in  $\text{Li}[\text{Ni}_y\text{Mn}_y\text{Co}_{(1-2y)}]\text{O}_2$  ( $y = 0.05$ ) upon electrochemical lithium deintercalation", D.L. Zeng, J. Cabana, W.S. Yoon and C. P. Grey, *Chem. Mater.*, **22**, 1209-1219, (2010).
204. "High rate performance of lithium manganese nitride and oxynitride as negative electrodes in lithium batteries", J. Cabana, C.M. Ionica-Bousquet, C.P. Grey and M. R. Palacín, *Electrochem. Commun.*, **12**, 315-318, (2010).
205. "MAS NMR study of the metastable solid solutions found in the  $\text{LiFePO}_4/\text{FePO}_4$  system", J. Cabana, J. Shirakawa, G.Y. Chen, T.J. Richardson and C.P. Grey, *Chem. Mater.*, **22**, 1249-1262, (2010).
206. "Optimizing the synthesis of nitrogen-substituted zeolites", K.D. Hammond, M. Gharibeh, G.A. Tompsett, F. Dogan, A.V. Brown, C.P. Grey, S.M. Auerbach and W.C. Conner, Jr., *Chem. Mater.*, **22**, 130-142, (2010).
207. "Investigation of surface structures by powder diffraction: A differential pair distribution function study on arsenate sorption on ferrihydrite", R. Harrington, D.B. Hausner, N. Bhandari, D.R. Strongin, K.W. Chapman, P.J. Chupas, D.S. Middlemiss, C.P. Grey and J.B. Parise, *Inorg. Chem.*, **49**, 325-330, (2010).
208. "Solid-state NMR calculations for metal oxides and gallates: Shielding and quadrupolar parameters for perovskites and related phases", D.S. F. Blanc, C.J. Pickard and C.P. Grey, *J. Magn. Reson.*, **204**, 1-10, (2010).
209. "Linking local environments and hyperfine shifts: A combined experimental and theoretical  $^{31}\text{P}$  and  $^7\text{Li}$  solid-state NMR study of paramagnetic Fe(III) phosphates", J. Kim, D.S.

- Middlemiss, N.A. Chernova, B.Y.X. Zhu, C. Masquelier and C.P. Grey, *J. Am. Chem. Soc.*, **132**, 16825-16840, (2010).
210. “*In situ* NMR observation of the formation of metallic lithium microstructures in lithium batteries”, R. Bhattacharyya, B. Key, H. L. Chen, A.S. Best, A.F. Hollenkamp and C.P. Grey, *Nat. Mater.*, **9**, 504-520 (2010).
211. “Surface science studies of environmentally relevant iron (oxy)hydroxides ranging from the nano to the macro-regime”, D.R. Strongin, C.P. Grey, J.B. Parise and J.D. Kubicki, *Surf. Sci.*, **604**, 1065-1069, (2010).
212. “ $^2\text{H}$  and  $^7\text{Li}$  solid-state MAS NMR study of local environments and lithium adsorption on the iron (III) oxyhydroxide, akaganeite ( $\beta\text{-FeOOH}$ )”, J. Kim and C.P. Grey, *Chem. Mater.*, **22**, 5453-5462, (2010).
213. “Chemically modified  $\text{Ba}_6\text{Mn}_{24}\text{O}_{48}$  tunnel manganite as a lithium insertion host,” E.A. Pomerantseva, T.L. Kulova, D.L. Zeng, A.M. Skundin, C.P. Grey, E.A. Goodilin and Y.D. Tretyakov, *Solid State Ionics*, **181**, 1002-1008, (2010).
214. “Structural complexity of layered-spinel composite electrodes for Li-ion batteries”, J. Cabana, C.S. Johnson, X.Q. Yang, K.Y. Chung, W.S. Yoon, S.H. Kang, M.M. Thackeray and C.P. Grey, *J. Mater. Res.*, **25**, 1601-1616, (2010).
215. “Probing the local structures and protonic conduction pathways in scandium substituted  $\text{BaZrO}_3$  by multinuclear solid-state NMR spectroscopy” L. Buannic, F. Blanc, I. Hung, Z.H. Gan and C.P. Grey, *J. Mater. Chem.*, **20**, 6322-6332, (2010).
216. “Spin crossover in the  $\text{CsFeII}[\text{Cr-III}(\text{CN})_6]$  Prussian blue analog: Phonons and thermodynamics from hybrid functionals”, D.S. Middlemiss, D. Portinari, C.P. Grey, C.A. Morrison and C.C. Wilson, *Phys. Rev. B*, **81**, 184410, (2010).
217. “Pair distribution function analysis and solid state NMR studies of silicon electrodes for lithium ion batteries: Understanding the (De)lithiation mechanisms”, B. Key, M. Morcrette, J.-M. Tarascon and C.P. Grey, *J. Am. Chem. Soc.*, **133**, 503-512, (2011).
218. “ $\text{LiCoO}_2$  Concaved cuboctahedrons from symmetry-controlled topological reactions” H.L. Chen, L.J. Wu, L.H. Zhang, Y.M. Zhu and C.P. Grey, *J. Am. Chem. Soc.*, **133**, 262–270, (2011).
219. “Measuring Brønsted acid site O–H distances in zeolites HY and HZSM-5 with low-temperature  $^{17}\text{O}$ - $^1\text{H}$  double resonance MAS NMR spectroscopy”, H. Huo, L.M. Peng and C.P. Grey, *J. Phys. Chem. C*, **115**, 2030–2037, (2011).
220. “High-resolution  $^{27}\text{Al}$  MAS NMR spectroscopic studies of the response of spinel aluminates to mechanical action”, V. Sepelak, I. Bergmann, S. Indris, A. Feldhoff, H. Hahn, K. Dieter Becker, C.P. Grey and P. Heitjans, *J. Mater. Chem.*, **21**, 8332-8337, (2011).
221. “Effect of ball-milling and lithium insertion on the lithium mobility and structure of  $\text{Li}_3\text{Fe}_2(\text{PO}_4)_3$ ”, J. Cabana, J. Shirakawa, M. Nakayama, M. Wakihara and C.P. Grey, *J. Mater. Chem.*, **21**, 10012-10020, (2011).

222. "Characterization and carbonization of highly oriented poly(diiododiacetylene) nanofibers", L. Luo, C. Wilhelm, C.N. Young, C.P. Grey, G.P. Halada, K. Xiao, I.N. Ivanov, J.Y. Howe, D.B. Geohegan and N.S. Goroff, *Macromolecules*, **44**, 2626-2631, (2011).
223. "Liquid phase aldol condensation reactions with MgO-ZrO<sub>2</sub> and shape-selective nitrogen-substituted NaY", W.Q. Shen, G.A. Tompsett, K.D. Hammond, R. Xing, F. Dogan, C.P. Grey, W.C. Conner, S.M. Auerbach and G.W. Huber, *Appl. Catal. A-Gen.*, **392**, 57-68, (2011).
224. "C-13 solid state NMR suggests unusual breakdown products in SEI formation on lithium ion electrodes", N. Leifer, M.C. Smart, G.K.S. Prakash, L. Gonzalez, L. Sanchez, K.A. Smith, P. Bhalla, C.P. Grey and S.G. Greenbaum, *J. Electrochem. Soc.*, **158**, A471-A480, (2011).
225. "Phosphate adsorption on the iron oxyhydroxides goethite ( $\alpha$ -FeOOH), akaganeite ( $\beta$ -FeOOH), lepidocrocite ( $\gamma$ -FeOOH): a <sup>31</sup>P NMR study", J. Kim, L. Wei, B. L. Philips, and C. P. Grey, *EES*, **4**, 4298-4305 (2011).
225. "Insight into the local magnetic environments and deuteron mobility in jarosite (AFe<sub>3</sub>(SO<sub>4</sub>)<sub>2</sub>(OD,OD<sub>2</sub>)<sub>6</sub>, A = K, Na, D<sub>3</sub>O) and hydronium alunite ((D<sub>3</sub>O)Al<sub>3</sub>(SO<sub>4</sub>)<sub>2</sub>(OD)<sub>6</sub>), from variable-temperature <sup>2</sup>H MAS NMR spectroscopy", U.G. Nielsen, I. Heinmaa, A. Samoson, J. Majzlan and C.P. Grey, *Chem. Mat.*, **23**, 3176-3187, (2011).
226. "Citric acid- and ammonium-mediated morphological transformations of olivine LiFePO<sub>4</sub> particles", Z. Lu, H. Chen, R. Robert, B.Y.X. Zhu, J. Deng, L. Wu, C.Y. Chung and C.P. Grey, *Chem. Mat.*, **23**, 2848-2859, (2011).
227. "Conversion reaction mechanisms in lithium ion batteries: Study of the binary metal fluoride electrodes", F. Wang, R. Robert, N.A. Chernova, N. Pereira, F. Omenya, F. Badway, X. Hua, M. Ruotolo, R. Zhang, L. Wu, V. Volkov, D. Su, B. Key, M.S. Whittingham, C.P. Grey, G.G. Amatucci, Y. Zhu, J. Graetz, *J. Am. Chem. Soc.*, **133**, 18828-18836 (2011).
228. "Defects in doped LaGaO<sub>3</sub> anionic conductors: Linking NMR spectral features, local environments and defect thermodynamics", F. Blanc, D.S. Middlemiss, Z. Gan, C.P. Grey, *J. Am. Chem. Soc.*, **133**, 17662-17672 (2011).
229. "Real-time NMR studies of electrochemical double-layer capacitors", H. Wang, T.K.J. Köster, N.M. Trease, J. Segalini, P.-L. Taberna, P. Simon, Y. Gogotsi and C.P. Grey, *J. Am. Chem. Soc.*, **133**, 19270-19273 (2011).
230. "Room-temperature carbonization of poly(diiododiacetylene) by reaction with Lewis bases" L. Luo, D. Resch, C. Wilhelm, C.N. Young, G.P. Halada, R.J. Gambino, C.P. Grey, N.S. Goroff, *J. Am. Chem. Soc.*, **133**, 19274-19277 (2011).
231. "Resolving the different silicon clusters in Li<sub>12</sub>Si<sub>7</sub> by <sup>29</sup>Si and <sup>6,7</sup>Li solid-state NMR spectroscopy", T.K.-J. Köster, E. Salager, A.J. Morris, B. Key, V. Seznec, M. Morcrette, C.J. Pickard and C.P. Grey, *Angew. Chem. Int. Ed.*, **50**, (2011).
232. "Energetics of hydrogen/lithium complexes in silicon analyzed using the Maxwell construction", A.J. Morris, C.P. Grey, R.J. Needs and C.J. Pickard, *Phys. Rev. B.*, **84**, 224106-1 -5, (2011).

233. "Structure of aluminum fluoride coated  $\text{Li}[\text{Li}_{1/9}\text{Ni}_{1/3}\text{Mn}_{5/9}]\text{O}_2$  cathodes for secondary lithium-ion batteries", K.J. Rosina, M. Jiang, D. Zeng, E. Salager, A.S. Best, C.P. Grey, *J. Mat. Chem.*, **22**, 20602-20610, (2012).
234. "Structure, defects and thermal stability of delithiated olivine phosphates", G.M. Nolis, F. Omenya, R. Zhang, B. Fang, S. Upreti, N.A. Chernova, F. Wang, J. Graetz, Y-Y Hu, C.P. Grey, and M. Stanley Whittingham, *J. Mat. Chem.*, **22**, 20482-20489, (2012).
235. "Role of structure and interfaces in the performance of  $\text{TiSnSb}$  as an electrode for Li-ion batteries", C. Marino, M.T. Sougrati, B. Gerke, R. Pöttgen, H. Huo, M. Ménétrier, C.P. Grey, L. Monconduit, *Chem. Mat.*, **24**, 4735-4743, (2012).
236. "Nonequilibrium structure of  $\text{Zn}_2\text{SnO}_4$  spinel nanoparticles", V. Sepelak, S.M. Becker, I. Bergmann, S. Indris, M. Scheuermann, A. Feldhoff, C. Kubel, M. Bruns, N. Sturzl, A.S. Ulrich, M. Ghafari, H. Hahn, C.P. Grey, K.D. Becker and P. Heitjans, *J. Mater. Chem.*, **22**, 3117-3126, (2012).
237. "Isotropic high field NMR spectra of Li-Ion battery materials with anisotropy  $>1$  MHz", I. Hung, L. Zhou, F. Pourpoint, C.P. Grey and Z. Gan, *J. Am. Chem. Soc.*, **134**, 1898-1901 (2012).
238. "Crystal structure, physical properties, and electrochemistry of copper substituted  $\text{LiFePO}_4$  single crystals", S. Upreti, N.A. Chernova, J. Xiao, J.K. Miller, O.V. Yakubovich, J. Cabana, C.P. Grey, V.L. Chevrier, G. Ceder, J.L. Musfeldt, M.S. Whittingham, *Chem. Mat.*, **24**, 166-173, (2012).
239. "Nanoparticulate  $\text{TiO}_2$  B: An anode for lithium-ion batteries", Y. Ren, Z. Liu, F. Pourpoint, A.R. Armstrong, C.P. Grey, P.G. Bruce, *Angew. Chem. Int. Ed.*, **51**, 2164-2167, (2012).
240. "Thermal phase transformations in  $\text{LaGaO}_3$  and  $\text{LaAlO}_3$  perovskites: An experimental and computational solid-state NMR study", F. Blanc, D.S. Middlemiss, L. Buannic, J.L. Palumbo, I. Farnan and C.P. Grey, *Solid State Nucl. Magn. Reson.*, **42**, 87-97, (2012).
241. " $^7\text{Li}$  MRI of Li batteries reveals location of microstructural lithium", S. Chandrashekar, S.M. Trease, H.J. Chang, L.S. Du, C.P. Grey and A. Jerschow, *Nat. Mater.*, **11**, 311-315, (2012).
242. "In situ NMR of lithium ion batteries: Bulk susceptibility effects and practical considerations", N.M. Trease, L. Zhou, H.J. Chang, B.Y. Zhu, C.P. Grey, *Solid State Nucl. Magn. Reson.*, **42**, 62-70 (2012).
243. "Electronic spin transition in nanosize stoichiometric lithium cobalt oxide", D. Qian, Y. Hinuma, H. Chen, L.S. Du, K.J. Carroll, G. Ceder, C.P. Grey, Y.S. Meng, *J. Am. Chem. Soc.*, **134**, 6096-6099, (2012).
244. "Solid-state MAS NMR studies of Brønsted acid sites in zeolite H-mordenite", H. Huo, L. Peng, Z. Gan, C.P. Grey, *J. Am. Chem. Soc.*, **134**, 9708-9720, (2012).
245. "Probing cation and vacancy ordering in the dry and hydrated yttrium substituted  $\text{BaSnO}_3$  perovskite by NMR spectroscopy and first principles calculations: Implications for proton mobility", L. Buannic, F. Blanc, D.S. Middlemiss, C.P. Grey, *J. Am. Chem. Soc.*, **134**, 14483-14498, (2012).



246. “Degradation and (de)lithiation processes in the high capacity battery material  $\text{LiFeBO}_3$ ”, S.H. Bo, F. Wang, Y. Janssen, D.L. Zeng, K.W. Nam, W.Q. Xu, L.S. Du, J. Graetz, X.Q. Yang, Y.M. Zhu, J.B. Parise, C.P. Grey, P.G. Khalifah, *J. Mater. Chem.*, **22**, 8799-8809, (2012).
247. “Investigation of cation ordering in triclinic sodium birnessite via Na-23 MAS NMR spectroscopy”, K.A. Aldi, J. Cabana, P.J. Sideris, C.P. Grey, *American Mineralogist*, **97**, 883-889, (2012).
248. “Structural modulation in the high capacity battery cathode material  $\text{LiFeBO}_3$ ”, Y. Janssen, D.S. Middlemiss, S.H. Bo, C.P. Grey, P.G. Khalifah, *J. Am. Chem. Soc.*, **134**, 12516-12527, (2012).
249. “Direct detection of discharge products in lithium-oxygen batteries by solid-state NMR spectroscopy”, M. Leskes, N.E. Drewett, L.J. Hardwick, P.G. Bruce, G.R. Goward, C.P. Grey, *Angew Chem. Int. Ed. Engl.*, 1521-3773, (2012).
250. “Scanning x-ray fluorescence imaging study of lithium insertion into copper based oxysulfides for Li-ion batteries”, R. Robert, D. Zeng, A. Lanzirrotti, P. Adamson, S.J. Clarke, and C.P. Grey, *Chem. Mat.*, **24**, 2684-2691, (2012).
251. “Identification of cation clustering in Mg-Al layered double hydroxides using multinuclear solid state nuclear magnetic resonance spectroscopy”, P.J. Sideris, F. Blanc, Z. Gan, C.P. Grey, *Chem. Mat.*, **24**, 2449-2461, (2012).
252. “New insights into the crystal and electronic structures of  $\text{Li}_{1+x}\text{V}_{1-x}\text{O}_2$  from solid state NMR, pair distribution function analyses, and first principles calculations”, F. Pourpoint, X. Hua, D.S. Middlemiss, P. Adamson, D. Wang, P.G. Bruce, C.P. Grey, *Chem. Mat.*, **24**, 2880-2893, (2012).
254. “Spin-transfer pathways in paramagnetic lithium transition-metal phosphates from combined broadband isotropic solid-state MAS NMR spectroscopy and DFT calculations”, R. J. Clément, A.J. Pell, D.S. Middlemiss, F.C. Strobridge, J.K. Miller, M.S. Whittingham, L. Emsley, C.P. Grey, and G. Pintacuda, *J. Am. Chem. Soc.*, **134**, 17178-17185, (2012).
255. “Multinuclear NMR spectroscopic studies of structure and dynamics in hydrous  $\text{NaAlSi}_3\text{O}_8$  and  $\text{Ca}_{0.5}\text{AlSi}_3\text{O}_8$  glasses”, S. Indris, P. Heitjans, C.P. Grey, *J. Non-Crystal. Sol.*, **358**, 2862-2867, (2012).
255. “Composition-structure relationships in the Li-ion battery electrode material  $\text{LiNi}_{0.5}\text{Mn}_{1.5}\text{O}_4$ ”, J. Cabana, M. Casas-Cabanas, F.O. Omenya, N.A. Chernova, D. Zeng, M.S. Whittingham, C.P. Grey, *Chem. Mat.*, **24**, 2952-2964, (2012).
256. “Comprehensive insights into the structural and chemical changes in mixed-anion FeOF electrodes by using operando PDF and NMR spectroscopy”, K.M. Wiaderek, O.J. Borkiewicz, E. Castillo-Martínez, R. Robert, N. Pereira, G.G. Amatucci, C.P. Grey, P.J. Chupas, K.W. Chapman, *J. Am. Chem. Soc.*, **135**, 4070-4078 (2013).
257. “Dynamic nuclear polarization enhanced natural abundance  $^{17}\text{O}$  spectroscopy”, F. Blanc, L. Sperrin, D.A. Jefferson, S. Pawsey, M. Rosay, and C.P. Grey, *J. Am. Chem. Soc.*, **135**, 2975-2978, (2013).

258. “Frequency-stepped acquisition in nuclear magnetic resonance spectroscopy under magic angle spinning”, A.J. Pell, R.J. Clement, C.P. Grey, L. Emsley, G. Pintacuda, *J. Chem. Phys.*, **138**, (2013).
259. “Nuclear magnetic resonance study of ion adsorption on microporous carbide-derived carbon”, A.C. Forse, J.M. Griffin, H. Wang, N.M. Trease, V. Presser, Y. Gogotsi, P. Simon and C.P. Grey, *Phys. Chem. Chem. Phys.*, **15**, 7722-7730, (2013).
260. “Ligand-directed control over crystal structures of inorganic-organic frameworks and formation of solid solutions”, H.H.-M. Yeung, W. Li, P.J. Saines, T.K. Köster, C.P. Grey, A.K. Cheetham, *Angew Chem. Int. Ed. Engl.*, **52**, 5544-5547, (2013).
261. “Lithiation of silicon via lithium Zintl-defect complexes from first principles”, A.J. Morris, R.J. Needs, E. Salager, C.P. Grey, C.J. Pickard, *Phys. Rev. B*, **87**, 174108-1 – 174108-4, (2013).
262. “Proton trapping in yttrium-doped barium zirconate”, Y. Yamazaki, F. Blanc, Y. Okuyama, L. Buannic, J.C. Lucio-Vega, C.P. Grey, and S.M. Haile, *Nat. Mat.*, **12**, 647 – 651 (2013).
263. “Understanding the conduction mechanism of the protonic conductor CsH<sub>2</sub>PO<sub>4</sub> by solid-state NMR spectroscopy”, G. Kim, F. Blanc, Y.-Y. Hu, and C.P. Grey, *J. Phys. Chem. C.*, **117**, 6504-6515, (2013).
264. “Paramagnetic electrodes and bulk magnetic susceptibility effects in the in situ NMR studies of batteries: Application to Li<sub>1.08</sub>Mn<sub>1.92</sub>O<sub>4</sub> spinels”, L. Zhou, M. Leskes, A.J. Ilott, N.M. Trease, and C.P. Grey, *J. Mag. Res.*, **234**, 44-57 (2013).
265. “Density functional theory-based bond pathway decompositions of hyperfine shifts: Equipping solid-state NMR to characterize atomic environments in paramagnetic materials”, D.S. Middlemiss, A.J. Ilott, R.J. Clément, F.C. Strobridge, and C.P. Grey, *Chem. Mat.*, **25**, 1723-1734 (2013).
266. “Study of the transition metal ordering in layered Na<sub>x</sub>Ni<sub>x/2</sub>Mn<sub>1-x/2</sub>O<sub>2</sub> ( $2/3 \leq x \leq 1$ ) and consequences of Na/Li Exchange”, J. Cabana, N.A. Chernova, J. Xiao, M. Roppolo, K.A. Aldi, M. S. Whittingham, and C. P. Grey, *Inorg. Chem.*, **52**, 8540-8550 (2013).
267. “Long-range-ordered coexistence of 4-, 5-, and 6-coordinate niobium in the mixed ionic-electronic conductor gamma-Ba<sub>4</sub>Nb<sub>2</sub>O<sub>9</sub>”, M.T. Dunstan, F. Blanc, M Avdeev, G.J. McIntyre, C.P. Grey, C.D. Ling, *Chem. Mat.*, **25**, 3154-3161 (2013).
268. “Sidorenkite (Na<sub>3</sub>MnPO<sub>4</sub>CO<sub>3</sub>): A new intercalation cathode material for Na-ion batteries”, H. Chen, Q. Hao, O. Zivkovic, G. Hautier, L.-S. Du, Y. T, Y.-Y. Hu, X. Ma, C.P. Grey, and G. Ceder, *Chem. Mat.*, **25**, 2777-2786 (2013).
269. “In situ solid-state NMR spectroscopy of electrochemical cells: Batteries, supercapacitors, and fuel cells”, F. Blanc, M. Leskes, and C.P. Grey, *Acc. Chem. Res.*, **46**, 1952-1963, (2013).
270. “On the cause of the excess capacities in metal oxide/fluoride battery electrodes”, Y.-Y. Hu, Z. Liu, K. -W. Nam, O. J. Borkiewicz, X. Hua, J. Cheng, M. Dunstan, X. Yu, L.-S. Du, K. W. Chapman, P. J. Chupas, X. Yang, Clare P. Grey, *Nat. Mater.* **12**, 1130 – 1136 (2013).

271. "Electrochemical reaction of lithium with nanostructured silicon anodes: a study by in-situ synchrotron x-ray diffraction and electron energy-loss spectroscopy", F. Wang, L. Wu, B. Key, X-Q Yang, C.P. Grey, Y. Zhu, J. Graetz, *Adv. Energy Mater.*, **3**, 1324-1331, (2013).
272. "In situ NMR spectroscopy of supercapacitors: insight into the charge storage mechanism", H. Wang, A.C. Forse, J.M. Griffin, N.M. Trease, L. Trognko, P.L. Taberna, P. Simon, C.P. Grey, *J. Am. Chem. Soc.*, **135**, 18968-18980 (2013).
273. "Reversible CO<sub>2</sub> absorption by the 6H Perovskite Ba<sub>4</sub>Sb<sub>2</sub>O<sub>9</sub>", M.T. Dunstan, W. Liu, A.F. Pavan, J.A. Kimpton, C.D. Ling, S.A. Scott, J.S. Dennis, C.P. Grey, *Chem. Mat.*, **25**, 4881-4891 (2013).
274. "Monitoring the electrochemical processes in the lithium-air battery by solid state NMR spectroscopy", M. Leskes, A.J. Moore, G.R. Goward, C.P. Grey, *J. Phys. Chem. C*, **117**, 26929-26939 (2013).
275. "Joint experimental and computational O-17 solid state NMR study of Brownmillerite Ba<sub>2</sub>In<sub>2</sub>O<sub>5</sub>", R. Dervisoglu, D.S. Middlemiss, F. Blanc, L.A. Holmes, Y.L. Lee, D. Morgan, C.P. Grey, *Phys. Chem. Chem. Phys.*, **16**, 2597-2606 (2014).
276. "Identifying the critical role of Li substitution in P2-Na-x[LiyNizMn1-y-z]O-2 (0 < x, y, z < 1) intercalation cathode materials for high-energy Na-ion batteries", J. Xu, D.H. Lee, R.J. Clement, X.Q. Yu, M. Leskes, A. J. Pell, G. Pintacuda, X. -Q. Yang, C. P. Grey, Y. S. Meng, *Chem. Mat.*, **26**, 260-1269 (2014).
277. "Revealing lithium-silicide phase transformations in nano-structured silicon-based lithium ion batteries via in situ NMR spectroscopy", K. Ogata, E. Salager, C.J. Kerr, A.E. Fraser, C. Ducati, A.J. Morris, S. Hofmann, C.P. Grey, *Nature Commun.*, **5**, (2014).
278. "Capturing metastable structures during high rate cycling of LiFePO<sub>4</sub> nanoparticle electrodes", H. Liu, F. C. Strobridge, O. J. Borkiewicz, K. M. Wiaderek, K. W. Chapman, P. J. Chupas, C. P. Grey, *Science*, **344**, no 6191 (2014).
279. "Local structure and dynamics in the Na ion battery positive electrode material Na<sub>2</sub>V<sub>2</sub>(PO<sub>4</sub>)<sub>2</sub>F<sub>3</sub>", Z. Liu, Y.Y. Hu, M.T. Dunstan, H. Huo, X. G. Gao, H. Zou, G. M. Zhong, Y. Yang, C. P. Grey, *Chem. Mater.*, **26**, 2513-2521 (2014).
280. "Structures of delithiated and degraded LiFeBO<sub>3</sub>, and their distinct changes upon electrochemical cycling", S.H. Bo, K.W. Nam, O.J. Borkiewicz, Y.Y. Hu, X.Q. Yang, P.J. Chupas, K.W. Chapman, L. Wu, L. Zhang, F. Wang, C.P. Grey, P.G. Khalifah, *Inorg. Chem.* **53**, 6585 (2014).
281. "Three-dimensional characterization of electrodeposited lithium microstructures using synchrotron X-ray phase contrast imaging", D.S. Eastwood, P.M. Bayley, H.J. Chang, O.O. Taiwo, J. Vila-Comamala, D.J. Brett, C. Rau, P.J. Withers, P.R. Shearing, C.P. Grey, P.D. Lee, *Chem. Commun.* **51**, 266 (2015).
282. "Thin-film and bulk investigations of LiCoBO<sub>3</sub> as a Li-ion battery cathode.' S.H. Bo, G.M. Veith, M.R. Saccomanno, H. Huang, P.V. Burmistrova, A.C. Malingowski, R.L. Sacci, K.R. Kittilstved, C.P. Grey, P.G. Khalifah, *Appl. Mater. Interfaces*, **6**, 10840 (2014).

283. Visualizing skin effects in conductors with MRI:  $^7\text{Li}$  MRI experiments and calculations” A.J. Illott, S. Chandrashekar, A. Klöckner, H.J. Chang, N.M. Trease, C.P. Grey, L. Greengard, A. Jerschow, *Journal of Magnetic Resonance* (2014) **245**, 143.
284. “Thermodynamically stable lithium silicides and germanides from density-functional theory calculations”, A.J. Morris, C.P. Grey, C.J. Pickard, *Phys. Rev. B*, **90** (2014).
285. “Ring current effects: factors affecting the NMR chemical shift of molecules adsorbed on porous carbons”, A.C. Forse, J.M., V. Presser; Y. Gogotsi, C.P. Grey, *J. Phys. Chem. C*, **118**, 7508-7514 (2014).
286. “Dynamic nuclear polarization NMR of low-gamma nuclei: structural insights into hydrated yttrium-doped  $\text{BaZrO}_3$ ”, F. Blanc, L. Sperrin, D. Lee, Daniel, R. Dervisoglu, Y. Yamazaki, S. Haile, G. De Paepe, C. P. Grey, *J. Phys. Chem. Lett.*, **5**, 2431-2436 (2014).
287. “Comprehensive study of the  $\text{CuF}_2$  conversion reaction mechanism in a lithium ion battery”, X. Hua, R. Robert, L-S. Du, K.M. Wiaderek, M. Leskes, K.W. Chapman, P.J. Chupas, C.P. Grey, *J. Phys. Chem.*, **118**, 15169-15184 (2014).
288. “Analysis of charged state stability for monoclinic  $\text{LiMnBO}_3$  cathode”, J.C. Kim; X. Li, C.J. Moore, S-H Bo, P.G. Khalifah, C.P. Grey, G. Ceder, *Chem. Mat.*, **26**, 4200-4206 (2014).
289. “Characterising local environments in high energy density Li-ion battery cathodes: a combined NMR and first principles study of  $\text{LiFe}_x\text{Co}_{1-x}\text{PO}_4$ ”, F.C. Strobridge, D.S. Middlemiss, A.J. Pell, M. Leskes, R.J. Clement, F. Pourpoint, Z. Lu, J.V. Hanna, G. Pintacuda, L. Emsley, A. Samoson, C.P. Grey, *J. Mater. Chem. A*, **2**, 11948-11957 (2014).
290. “Topotactic elimination of water across a C-C ligand bond in a dense 3-D metal-organic framework”, H.H. Yeung, M. Kosa, J.M. Griffin, C.P. Grey, D.T. Major, A.K. Cheetham, *Chem. Commun.*, **50**, 13292 (2014).
291. “Investigating local structure in layered double hydroxides with O-17 NMR spectroscopy”, L. Zhao, Z. Qi, F. Blanc, G.Y. Yu, M. Wang, N.H. Xue, X.K. Ke, X.F. Guo, W.P. Ding, C.P. Grey, L.M. Peng, *Adv. Funct. Mater.*, **24**, 1696-1702 (2014).
292. “Multinuclear in situ magnetic resonance imaging of electrochemical double-layer capacitors”, A.J. Illott, N.M. Trease, C.P. Grey, A. Jerschow, *Nature Commun.*, **5**, 4536 (2014).
293. “Architecture dependence on the dynamics of nano- $\text{LiFePO}_4$  electrodes”, B. Orvananos, R. Malik, H.C. Yu, A. Abdellahi, C.P. Grey, G. Ceder, K. Thornton, *Electrochimica Acta*, **137**, 245-257 (2014).
294. “Relationships between  $\text{Mn}^{3+}$  content, structural ordering, phase transformation, and kinetic properties in  $\text{LiNi}_x\text{Mn}_{2-x}\text{O}_4$  cathode materials”, H. Duncan, B. Hai, M. Leskes, C. P. Grey, G.Y. Chen, *Chem. Mat.*, **26**, 5374-5382 (2014).
295. “Identifying the structure of the intermediate,  $\text{Li}_{2/3}\text{CoPO}_4$ , formed during electrochemical cycling of  $\text{LiCoPO}_4$ ”, F.C. Strobridge, R.J. Clement, M. Leskes, D.S. Middlemiss, O.J. Borkiewicz, K.M. Wiaderek, K.W. Chapman, P.J. Chupas, C.P. Grey, *Chem. Mat.*, **26**, 6193-6205 (2014).

296. "Ab initio structure search and in situ Li-7 NMR studies of discharge products in the Li-S battery system", K.A. See, M. Leskes, J.M. Griffin, S. Britto, P.D. Matthews, A. Emly, A. Van der Ven, D.S. Wright, A.J. Morris, C.P. Grey, R. Seshadri, *J. Am. Chem. Soc.*, **136**, 16368-16377 (2014).
297. "Beta-NaMnO<sub>2</sub>: a high-performance cathode for sodium-ion batteries", J. Billaud, R.J. Clement, A.R. Armstrong, J. Canales-Vazquez, P. Rozier, C.P. Grey, P.G. Bruce, *J. Am. Chem. Soc.*, **136**, 17243-17248 (2014).
298. "Ion counting in supercapacitor electrodes using NMR spectroscopy", J.M. Griffin, A.C. Forse, H. Wang, N.M. Trease, P.L. Taberna, P. Simon, C.P. Grey, *Faraday Discussions*, **176**, 49 (2015).
299. "Three-dimensional characterization of electrodeposited lithium microstructures using synchrotron X-ray phase contrast imaging", D.S. Eastwood, P.M. Bayley, H.J. Chang, O.O. Taiwo, J. Vila-Comamala, D.J.L. Brett, C. Rau, P.J. Withers, P.R. Shearing, C.P. Grey, P.D. Lee, *Chem. Commun.*, 51, 266-268 (2015).
300. "Mapping the inhomogeneous electrochemical reaction through porous LiFePO<sub>4</sub>-electrodes in a standard coin cell battery, F. C. Strobridge, B. Orvananos, M. Croft, H. C. Yu, R. R. Robert, H. Liu, Z. Zhong, T. Connolly, M. Drakopoulos, T. Thornton, C. P. Grey, *Chem. Mater.*, **27**, 2374 – 2386 (2015).
301. "Kinetics of nanoparticle interactions in battery electrodes", B. Orvananos, H.C. Yu, A. Abdellahi, R. Malik, C.P. Grey, G. Ceder, K. Thornton, *J. Electrochem. Soc.*, **162**, A965-A973, (2015).
302. "Effect of a size-dependent equilibrium potential on nano-LiFePO<sub>4</sub> particle interactions", B. Orvananos, H.C. Yu, R. Malik, A. Abdellahi, C.P. Grey, G. Ceder, K. Thornton, *J. Electrochem. Soc.*, **162**, A1718-A1724 (2015).
303. "Finite pulse effects in CPMG pulse trains on paramagnetic materials", M. Leskes, C.P. Grey, *Phys. Chem. Chem. Phys.*, **17**, 22311-22320 (2015).
304. "Elucidating the origins of phase transformation hysteresis during electrochemical cycling of Li-Sb electrodes", D.H. Chang, H. Huo, K.E. Johnston, M. Menetrier, L. Monconduit, C.P. Grey, A. Van der Ven, *J. Mater. Chem.*, **3**, 18928-18943 (2015).
305. "Divergence from the classical hydroboration reactivity; boron containing materials through a hydroboration cascade of small cyclic dienes", A. Andreou, M. Leskes, P.G. Jambrina, G.J. Tustin, C.P. Grey, E. Rosta, O.A. Scherman, *Chem. Sci.*, **6**, 6262-6269 (2015).
306. "Review-manganese-based P2-type transition metal oxides as sodium-ion battery cathode materials", R.J. Clement, P.G. Bruce, C.P. Grey, *J. Electrochem. Soc.*, **162**, A2589-A2604 (2015).
307. "IR near-field spectroscopy and imaging of single Li<sub>x</sub>FePO<sub>4</sub> microcrystals", I.T. Lucas, A.S. McLeod, J.S. Syzdek, D.S. Middlemiss, C.P. Grey, D.N. Basov, R. Kostecki, *Nano Letters*, **15** (2015).

308. "Elucidation of the local and long-range structural changes that occur in germanium anodes in lithium-ion batteries", H. Jung, P.K. Allan, Y-Y Hu, O.J. Borkiewicz, X.L. Wang, W.Q. Han, L.S. Du, C.J. Pickard, P.J. Chupas, K.W. Chapman, A.J. Morris, C.P. Grey, *Chem. Mater.*, **27**, 1031-1041 (2015).
309. "Lattice simulation method to model diffusion and NMR spectra in porous materials", C. Merlet, A.C. Forse, J.M. Griffin, D. Frenkel, C.P. Grey, *J. Chem. Phys.*, **142**, (2015).
310. "Characterization of the dynamics in the protonic conductor  $C_5H_2PO_4$  by O-17 solid-state NMR spectroscopy and first-principles calculations: correlating phosphate and protonic motion", G. Kim, J.M. Griffin, F. Blanc, S.M. Haile, C.P. Grey, *J. Am. Chem. Soc.*, **137**, 3867-3876 (2015).
311. "Ordered and disordered polymorphs of  $Na(Ni_{2/3}Sb_{1/3})O_2$ : honeycomb-ordered cathodes for Na-ion batteries", J. Ma, S.H. Bo, L.J. Wu, Y.M. Zhu, C.P. Grey, P.G. Khalifah, *Chem. Mater.*, **27**, 2387-2399, (2015).
312. "Mapping the inhomogeneous electrochemical reaction through porous  $LiFePO_4$ -electrodes in a standard coin cell battery", F.C. Strobridge, B. Orvananos, M. Croft, H.C. Yu, R. Robert, H. Liu, Z. Zhong, T. Connolley, M. Drakopoulos, K. Thornton, C.P. Grey, *Chem. Mater.*, **27**, 2374-2386 (2015).
313. "Theory and practice: bulk synthesis of  $C_3B$  and its  $H_2$  and Li-storage capacity", T.C. King, P.D. Matthews, H. Glass, J.A. Cormack, J.P. Holgado, M. Leskes, J.M. Griffin, O.A. Scherman, P.D. Barker, C.P. Grey, S.E. Dutton, R.M. Lambert, G. Tustin, A. Alavi, D.S. Wright, *Angew. Chem. Int. Ed.*, **54**, 5919-5923 (2015).
314. "Mechanism of the delithiation/lithiation process in  $LiFe_{0.4}Mn_{0.6}PO_4$ : in situ and ex situ investigations on long-range and local structures", I. Bezza, M. Kaus, R. Heinzmann, M. Yavuz, M. Knapp, S. Mangold, S. Doyle, C.P. Grey, H. Ehrenberg, S. Indris, I. Saadoun, *J. Phys. Chem. C*, **119**, 9016-9024 (2015).
315. "H-2 and Al-27 solid-state NMR study of the local environments in Al-doped 2-line ferrihydrite, goethite, and lepidocrocite", J. Kim, A.J. Ilott, D.S. Middlemiss, N.A. Chernova, N. Pinney, D. Morgan, C.P. Grey, *Chem. Mater.*, **27**, 3966-3978 (2015).
316. "Joint experimental and computational  $^{17}O$  and  $^1H$  solid state NMR study of  $Ba_2In_2O_4(OH)_2$  structure and dynamics", R. Dervisoglu, D.S. Middlemiss, F. Blanc, Y.L. Lee, D. Morgan, C.P. Grey, *Chem. Mater.*, **27**, 3861-3873 (2015).
317. "NMR study of ion dynamics and charge storage in ionic liquid supercapacitors", A.C. Forse, J.M. Griffin, C. Merlet, P.M. Bayley, H. Wang, P. Simon, C.P. Grey, *J. Am. Chem. Soc.*, **137**, 7231-7242 (2015).
318. "Dependence on crystal size of the nanoscale chemical phase distribution and fracture in  $LixFePO_4$ ", Y.S. Yu, C. Kim, D.A. Shapiro, M. Farmand, D. Qian, T. Tyliczszak, A.L.D. Kilcoyne, R. Celestre, S. Marchesini, J. Joseph, P. Denes, T. Warwick, F.C. Strobridge, C.P. Grey, H. Padmore, Y.S. Meng, R. Kostecki, J. Cabana, *Nano Lett.*, **15**, 4282-4288, (2015).
319. "Multiple redox modes in the reversible lithiation of high-capacity, peierls-distorted vanadium sulfide", S. Britto, M. Leskes, X. Hua, C.A. Hebert, H.S. Shin, S. Clarke, O. Borkiewicz,

- K.W. Chapman, R. Seshadri, J. Cho, C.P. Grey, *J. Am. Chem. Soc.*, **137**, 8499-8508 (2015).
320. "Defect-tolerant diffusion channels for Mg<sup>2+</sup> ions in ribbon-type borates: structural insights into potential battery cathodes MgVBO<sub>4</sub> and Mg<sub>x</sub>Fe<sub>2-x</sub>B<sub>2</sub>O<sub>5</sub>", S.H. Bo, C.P. Grey, P.G. Khaifah, *Chem. Mater.*, **27**, 4630-4639 (2015).
321. "Structural and mechanistic insights into fast lithium-ion conduction in Li<sub>4</sub>SiO<sub>4</sub>-Li<sub>3</sub>PO<sub>4</sub> solid electrolytes", Y. Deng, C. Eames, J.N. Chotard, F. Lalere, V. Seznec, S. Emge, O. Pecher, C.P. Grey, C. Masquelier, M.S. Islam, *J. Am. Chem. Soc.*, **137**, 9136-9145 (2015).
323. "Investigating Li microstructure formation on Li anodes for lithium batteries by *in situ* Li-6/Li-7 NMR and SEM", H.J. Chang, N.M. Trease, A.J. Ilott, D.L. Zeng, L.S. Du, A. Jerschow, C.P. Grey, *J. Phys. Chem. C*, **119**, 16443-16451 (2015).
323. "In situ NMR and electrochemical quartz crystal microbalance techniques reveal the structure of the electrical double layer in supercapacitors", J.M. Griffin, A.C. Forse, W.Y. Tsai, P.L. Taberna, P. Simon, C.P. Grey, *Nat. Mater.*, **14**, 812 (2015)
324. "Mapping structural changes in electrode materials: application of the hybrid eigenvector-following density functional theory (DFT) method to layered Li<sub>0.5</sub>MnO<sub>2</sub>", I.D. Seymour S. Chakraborty, D.S. Middlemiss, D.J. Wales, C.P. Grey, *Chem. Mater.*, **27**, 5550-5561 (2015).
325. "New insights into the structure of nanoporous carbons from NMR, Raman, and pair distribution function analysis", A.C. Forse, C. Merlet, P.K. Allan, E.K. Humphreys, J.M. Griffin, M. Aslan, M. Zeiger, V. Presser, Y. Gogotsi, C.P. Grey, *Chem. Mater.*, **27**, 6848-6857 (2015).
326. "The morphology of TiO<sub>2</sub> (B) nanoparticles", X. Hua, Z. Liu, P.G. Bruce, C.P. Grey, *J. Am. Chem. Soc.*, **137**, 13612-13623 (2015).
327. "Ion dynamics in Li<sub>2</sub>CO<sub>3</sub> studied by solid-state NMR and first-principles calculations", M.T. Dunstan, J.M. Griffin, F. Blanc, M. Leskes, C.P. Grey, *J. Phys. Chem. C*, **119**, 24255-24264 (2015).
328. "Cycling Li-O<sub>2</sub> batteries via LiOH formation and decomposition", T. Liu, M. Leskes, WJ Yu, A.J. Moore, L.N. Zhou, P.M. Bayley, G. Kim, C.P. Grey, *Science*, **350**, 530-533 (2015).
329. "Correlating microstructural lithium metal growth with electrolyte salt depletion in lithium batteries using Li-7 MRI", H.J. Chang, A.J. Ilott, N.M. Trease, M. Mohammadi, A. Jerschow, C.P. Grey, *J. Am. Chem. Soc.*, **137**, 15209-15216 (2015).
330. "A neutron diffraction study of the electrochemical double layer capacitor electrolyte tetrapropylammonium bromide in acetonitrile", E.K. Humphreys, P.K. Allan, R.J.L. Welbourn, T.G.A. Youngs, A.K. Soper, C.P. Grey, S.M. Clarke, *J. Phys. Chem. B*, **119**, 15320-15333 (2015).
331. "Probing dynamic processes in lithium-ion batteries by *in situ* NMR spectroscopy: Application to Li<sub>1.08</sub>Mn<sub>1.92</sub>O<sub>4</sub> electrodes", L. Zhou, M. Leskes, T. Liu, C.P. Grey, *Angew. Chem. Int. Ed. Engl.*, **54**, 14782 (2015).
332. "Crystal structure and proton conductivity of BaSn<sub>0.6</sub>Sc<sub>0.4</sub>O<sub>3-δ</sub>: insights from neutron

- powder diffraction and solid-state NMR spectroscopy”, F.G. Kinyanjui, S.T. Norberg, C.S. Knee, I. Ahmed, S. Hull, L. Buannic, I. Hung, Z. Gan, F. Blanc, C.P. Grey, S.G. Eriksson, *J. Mater. Chem. A*, **4**, 5088 (2016).
333. “Synthesis and extensive characterisation of phosphorus doped graphite”, P.D. Matthews, T.C. King, H. Glass, P.C.M.M. Magusin, G.J. Tustin, P.A.C. Brown, J.A. Cormack, R. García-Rodríguez, M. Leskes, S.E. Dutton, P.D. Barker, F.M. Grosche, A. Alavi, C.P. Grey, D.S. Wright, *RSC Advances*, **6**, 62140 (2016).
334. “Challenges and new opportunities of in situ NMR characterization of electrochemical processes”, O. Pecher, A. Vyalikh, C.P. Grey, *ESTORM 2015*, 1765, UNSP 020011 (2016).
335. “Influence of particle size, cycling rate and temperature on the lithiation process of anatase TiO<sub>2</sub>”, H. Liu, C.P. Grey, *J. Mater. Chem. A*, **4**, 6433 (2016).
336. “Structural evolution in synthetic, Ca-based sorbents for carbon capture”, W. Liu, B. Gonzalez, M.T. Dunstan, D.S. Sultan, A. Pavan, C.D. Ling, C.P. Grey, J.S. Dennis, *Chem. Eng. Science*, 139, 15-26, (2016).
337. “[Ge<sub>2</sub>]<sup>4+</sup> dumbbells with very short Ge-Ge distances in the zintl phase Li<sub>3</sub>NaGe<sub>2</sub>: A solid-state equivalent to molecular O<sub>2</sub>”, L.M. Scherf, A.J. Karttunen, O. Pecher, P.C. Magusin, C.P. Grey, T.F. Fässler, *Angew Chem Int Ed Engl*, **55**, 1075 (2015).
338. “Voltage dependent solid electrolyte interphase formation in silicon electrodes: monitoring the formation of organic decomposition products”, A.L. Michan, M. Leskes, C.P. Grey, *Chem. Mat.*, **28**, 385 (2016).
339. “Role of amine-cavity interactions in determining the structure and mechanical properties of the ferroelectric hybrid perovskite [NH<sub>3</sub>NH<sub>2</sub>]Zn(HCOO)<sub>3</sub>”, G. Kieslich, A.C. Forse, S. Sun, K.T. Butler, S. Kumagai, Y. Wu, M.R. Warren, A. Walsh, C.P. Grey, A.K. Cheetham, *Chem. Mat.*, **28**, 312 (2016).
340. “Insights into electrochemical sodium metal deposition as probed with in situ <sup>23</sup>Na NMR”, P.M. Bayley, N.M. Trease, C.P. Grey, *J. Am. Chem. Soc.*, **138**, 1955 (2016).
341. “NMR reveals the surface functionalisation of Ti<sub>3</sub>C<sub>2</sub> MXene”, M.A. Hope, A.C. Forse, K.J. Griffith, M.R. Lukatskaya, M. Ghidui, Y. Gogotsi, C.P. Grey, *Phys. Chem. Chem., Phys.*, **18**, 5099 (2016).
342. “Tracking sodium-antimonide phase transformations in sodium-ion anodes: insights from operando pair distribution function analysis and solid-state NMR spectroscopy”, P.K. Allan, J.M. Griffin, A. Darwiche, O.J. Borkiewicz, K.M. Wiaderek, K.W. Chapman, A.J. Morris, P.J. Chupas, L. Monconduit, C.P. Grey, *J. Am. Chem. Soc.*, **138**, 2352 (2016).
343. “Solid-state NMR studies of supercapacitors”, J.M. Griffin, A.C. Forse, C.P. Grey, *Sol. St. Nucl. Mag. Res.*, **74-75** (2016).
344. “Designing disordered materials using DNA-coated colloids of bacteriophage fd and gold”, Z. Ruff, S.H. Nathan, R.R. Unwin, M. Zupkauskas, D. Joshi, G.P.C. Salmond, C.P. Grey, E. Eiser, *Faraday Discussions*, **186** (2016).



345. “New perspectives on the charging mechanisms of supercapacitors”, A.C. Forse, C. Merlet, J.M. Griffin, C.P. Grey, *J. Am. Chem. Soc.*, **38**, 5731-5744 (2016).
346. “Solid electrolyte interphase growth and capacity loss in silicon electrodes.” A. L. Michan, G. Divitini, A. J. Pell, M. Leskes, C. Ducati, C. P. Grey, *J. Am. Chem. Soc.*, **138**, 7918 (2016).
347. “Automatic tuning matching cyler (ATMC) in situ NMR spectroscopy as a novel approach for real-time investigations of Li- and Na-ion batteries”, O. Pecher, P.M. Bayley, H. Liu, Z. Liu, N.M. Trease, C.P. Grey, *J. Mag. Reson.* **265**, 200 (2016).
348. “High-rate intercalation without nanostructuring in metastable Nb<sub>2</sub>O<sub>5</sub> bronze phases” K. J. Griffith, A. C. Forse, J. M. Griffin, C. P. Grey, *J. Am. Chem. Soc.*, **138**, 8888-8899 (2016). (ACS Editor’s Choice)
349. “Effects of relaxation on conversion negative electrode materials for Li-ion batteries: a study of TiSnSb using <sup>119</sup>Sn Mossbauer and <sup>7</sup>Li MAS NMR spectroscopies”, K.E. Johnston, M.T. Sougrati, L. Stievano, A. Darwiche, N. Dupre, C.P. Grey, L. Monconduit, *Chem. Mater.*, **28**, 4032 (2016).
350. “Unraveling the complex delithiation mechanisms of olivine-type cathode materials, LiFe<sub>x</sub>Co<sub>1-x</sub>PO<sub>4</sub>”, F.C. Strobridge, H. Liu, M. Leskes, O.J. Borkiewicz, K.M. Wiaderek, P.J. Chupas, K.W. Chapman, C.P. Grey, *Chem. Mater.*, **28**, 3676 (2016).
351. “Mg(PF<sub>6</sub>)<sub>2</sub>-based electrolyte systems: understanding electrolyte-electrode interactions for the development of Mg-ion batteries”, E.N. Keyzer, H.F.J. Glass, Z. Liu, P.M. Bayley, S.E. Dutton, C.P. Grey, D.S. Wright, *J. Am. Chem. Soc.*, **138**, 8682 (2016).
352. “Characterizing oxygen local environments in paramagnetic battery materials via O-17 NMR and DFT calculations”, I.D. Seymour, D.S. Middlemiss, D.M. Halat, N.M. Trease, A.J. Pell, C.P. Grey, *J. Am. Chem. Soc.*, **138**, 9405 (2016).
353. “In situ studies of materials for high temperature CO<sub>2</sub> capture and storage”, M.T. Dunstan, S.A. Maugeri, W. Liu, M.G. Tucker, O.O. Taiwo, B. Gonzalez, P.K. Allan, M.W. Gaultois, P.R. Shearing, D.A. Keen, A.E. Phillips, M.T. Dove, S.A. Scott, J.S. Dennis, C.P. Grey, *Faraday Discuss.* (2016).
354. “Probing oxide-ion mobility in the mixed ionic–electronic conductor La<sub>2</sub>NiO<sub>4+δ</sub> by Solid-State <sup>17</sup>O MAS NMR Spectroscopy”, D.M. Halat, R. Dervişoğlu, G. Kim, M.T. Dunstan, F. Blanc, D.S. Middlemiss, C.P. Grey, *J. Am Chem. Soc.*, **138**, 11958 (2016).
355. “Zintl Phases K<sub>4-x</sub>Na<sub>x</sub>Si<sub>4</sub> (1 ≤ x ≤ 2.2) and K<sub>7</sub>NaSi<sub>8</sub>: synthesis, crystal structures, and solid-state NMR spectroscopic investigations”, K.J. Griffith, L.M. Scherf, O. Pecher, F. Haarmann, C.P. Grey, T.F. Fassler, *European J. Inorg. Chem.* (2016)
356. “Real-time 3D imaging of microstructure growth in battery cells using indirect MRI”, A.J. Ilott, M. Mohammadi, H.J. Chang, C.P. Grey, A. Jerschow, *Proc. Nat. Ac. Sci. USA*, **113**, 10779 (2016)
357. “What happens to LiMnPO<sub>4</sub> upon chemical delithiation?”, Y. Huang, N.A. Chernova, Q. Yin, Q. Wang, N.F. Quackenbush, M. Leskes, J. Fang, F. Omenya, R. Zhang, M.J. Wahila, L.F.J. Piper, G. Zhou, C.P. Grey, M.S. Whittingham, *Inorg. Chem.*, **55**, 4335 (2016)

358. “Large scale computational screening and experimental discovery of novel materials for high temperature CO<sub>2</sub> capture”, M.T. Dunstan, A. Jain, W. Liu, S.P. Ong, T. Liu, J. Lee, K.A. Persson, S.A. Scott, J.S. Dennis, C.P. Grey, *Energy Environ. Sci.*, **9**, 1346 (2016).
359. “Mechanistic insights into sodium storage in hard carbon anodes using local structure probes”, J.M. Stratford, P.K. Allan, O. Pecher, P.A. Chater, C.P. Grey, *Chem. Commun. (Camb)*, **52**, 12430 (2016).
360. “Preventing structural rearrangements on battery cycling: a first-principles investigation of the effect of dopants on the migration barriers in layered Li<sub>0.5</sub>MnO<sub>2</sub>”, I.D. Seymour, D.J. Wales, C.P. Grey, *Journal of Physical Chemistry C*, **120**, 19521 (2016).
361. “Sodium intercalation mechanism of 3.8 V class alluaudite sodium iron sulfate”, G. Oyama, O. Pecher, K.J. Griffith, S.I. Nishimura, R. Pigliapochi, C.P. Grey, A. Yamada, *Chem. Mater.*, **28**, 5321 (2016).
362. “Structurally stable Mg-doped P<sub>2</sub>-Na<sub>2/3</sub>Mn<sub>1-y</sub>Mg<sub>y</sub>O<sub>2</sub> sodium-ion battery cathodes with high rate performance: insights from electrochemical, NMR and diffraction studies,” R.J. Clement, J. Billaud, A. R. Armstrong, G. Singh, T. Rojo, P. G. Bruce, C.P. Grey, *Energy Environ. Sci.*, **9**, 3240-3250 (2016).
363. “Insights into the Nature and Evolution upon Electrochemical Cycling of Planar Defects in the beta-NaMnO<sub>2</sub> Na-Ion Battery Cathode: An NMR and First-Principles Density Functional Theory Approach”, R.J. Clement, D.S. Middlemiss, I.D. Seymour, A.J. Illott, C.P. Grey, *Chem. Mater.* **28**, 8228 (2016).
364. “Fluoroethylene carbonate and vinylene carbonate reduction: Understanding lithium-ion battery electrolyte additives and solid electrolyte interphase formation”, A.L. Michan, B.S. Parimalam, M. Leskes, R.N. Kerber, T. Yoon, C.P. Grey, B.L. Lucht, *Chem. Mater.* **28**, 8149 (2016).
365. “Mechanistic Insights into the Challenges of Cycling a Nonaqueous Na-O<sub>2</sub> Battery”, T. Liu, G. Kim, M.T.L. Casford, C.P. Grey, *J. Phys. Chem. Lett.*, **7**, 4841, (2016)
366. “A systematic study of <sup>25</sup>Mg NMR in paramagnetic transition metal oxides: applications to Mg-ion battery materials”, J. Lee, I.D. Seymour, A.J. Pell, S.E. Dutton, C.P. Grey, *Phys. Chem. Chem. Phys.*, **19**, 613 (2016)
367. “Sustainability and in situ monitoring in battery development”, C.P. Grey, J.M. Tarascon, *Nat. Mater.* **16**, 45 (2016).
368. “Efficient storage mechanisms for building better supercapacitors”, M. Salanne, B. Rotenberg, K. Naoi, K. Kaneko, P.L. Taberna, C.P. Grey, B. Dunn, P. Simon, *Nature Energy*, **1**, 16070 (2016).
369. “A radially accessible tubular in situ X-ray cell for spatially resolved operando scattering and spectroscopic studies of electrochemical energy storage devices”, H. Liu, P.K. Allan, O.J. Borkiewicz, C. Kurtz, C.P. Grey, K.W. Chapman, P.J. Chupas, *Journal of Applied Crystallography*, **49**, 1665-1673 Part: 5 (2016).

370. "Identifying the distribution of Al<sup>3+</sup> in LiNi<sub>0.8</sub>Co<sub>0.15</sub>Al<sub>0.05</sub>O<sub>2</sub>", N.M. Trease, I.D. Seymour, M.D. Radin, H. Liu, H. Liu, S. Hy, N. Chernova, P. Parikh, A. Devaraj, K.M. Wiaderek, P.J. Chupas, K.W. Chapman, M.S. Whittingham, Y.S. Meng, A. Van der Van, C.P. Grey, *Chem. Mater.*, **28**, 22 (2016).
371. "Insights into the electrochemical performances of Bi anodes for Mg ion batteries using <sup>25</sup>Mg solid state NMR spectroscopy", Z. Liu, J. Lee, G. Xiang, H.F.J. Glass, E.N. Keyzer, S.E. Dutton, C.P. Grey, *Chem. Commun.*, **53**, 743-746 (2017).
372. "Direct evidence for high Na<sup>+</sup> mobility and high voltage structural processes in P2-Nax[LiyNizMn1-y-z]O2 (x,y,z ≤ 1) cathodes from solid-state NMR and DFT calculations" Clément, R. J.; Xu, J.; Middlemiss, D. S.; Alvarado, J.; Ma, C.; Meng, Y. S.; Grey, C. P. *J. Mater. Chem. A*, **5**, 4129 (2017).
373. "Floating zone growth of □□Na<sub>0.9</sub>MnO<sub>2</sub> single crystals", R. Dally et al., *J. Cryst. Growth*, **459**, 203-208 (2017).
374. "Exploring oxygen activity in the high energy P2-type Na<sub>0.78</sub>Ni<sub>0.23</sub>Mn<sub>0.69</sub>O<sub>2</sub> cathode material for Na-ion batteries", C. Ma, J. Alvarado, J. Xu, R.J. Clément, M. Kodur, W. Tong, C.P. Grey, Y.S. Meng, *J. Am. Chem. Soc.*, **139**, 4835 (2017).
375. "Direct observation of ion dynamics in supercapacitor electrodes using in situ diffusion NMR spectroscopy", A.C. Forse, J.M. Griffin, C. Merlet, J. Carretero-Gonzalez, A.-R.O. Raji, N.M. Trease, C.P. Grey, *Nature Energy*, **2**, 16216 (2017). (DOI: 10.1038/nenergy.2016.216)
376. "DFT investigation of the effect of spin-orbit coupling on the NMR shifts in paramagnetic solids", R. Pigliapochi, A.J. Pell, I.D. Seymour, C.P. Grey, D. Ceresoli, M. Kaupp, *Phys. Rev. B*, **95**, 054412 (2017).
377. "Large scale in silico screening of materials for carbon capture through chemical looping", C.Y. Lau, M.T. Dunstan, W.T. Hu, C.P. Grey, S.A. Scott, *Energy & Environmental Science*, **10**, 3 (2017).
378. "Surface-selective direct O-17 DNP NMR of CeO<sub>2</sub> nanoparticles", M.A. Hope, D.M. Halat, P.C.M.M. Magusin, S. Paul, L.M. Peng, C.P. Grey, *Chemical Communications*, **53**, 13 (2017).
379. "Donor-acceptor stacking arrangements in bulk and thin-film high-mobility conjugated polymers characterized using molecular modelling and MAS and surface-enhanced solid-state NMR spectroscopy", S.R. Chaudhari, J.M. Griffin, K. Broch, A. Lesage, V. Lemaur, D. Dudenko, Y. Olivier, H. Siringhaus, L. Emsley, C.P. Grey, *Chemical Science*, **8**, 4 (2017).
380. "Reversible capacity of conductive carbon additives at low potentials: caveats for testing alternative anode materials for Li-ion batteries", K.A. See, M.A. Lumley, G.D. Stucky, C.P. Grey, R. Seshadri, *Journal of the electrochemical society*, **164**, 2 (2017).
381. "Materials' methods: NMR in battery research", O. Pecher, J. Carretero-Gonzalez, K.J. Griffith, C.P. Grey, *Chem. Mater.*, **29**, 1 (2017).
382. "Enhanced efficiency of solid-state NMR investigations of energy materials using an external automatic tuning/matching (eATM) robot", O. Pecher, D.M. Halat, J. Lee, Z.G. Liu, K.J.

- Griffith, M. Braun, C.P. Grey, *Journal of Magnetic Resonance*, **275**, 127-136 (2017).
383. “Structural evolution and atom clustering in beta-SiAlON: beta-Si<sub>6</sub>-zAl<sub>z</sub>O<sub>z</sub>N<sub>8-z</sub>”, C. Cozzan, K.J. Griffith, G. Laurita, J.G. Hu, C.P. Grey, R. Seshadri, *Inorganic Chemistry*, **56**, 4 (2017).
384. “Surface-sensitive NMR detection of the solid electrolyte interphase layer on reduced graphene oxide”, M. Leskes, G. Kim, T. Liu, A.L. Michan, AL, F. Aussenac, P. Dorffer, S. Paul, C.P. Grey, *J. Phys. Chem. Letter*, **8**, 5 (2017).
385. “Structural stability from crystallographic shear in TiO<sub>2</sub>-Nb<sub>2</sub>O<sub>5</sub> phases: cation ordering and lithiation behavior of TiNb<sub>2</sub>O<sub>6</sub>”, K.J. Griffith, A. Senyshyn, C.P. Grey, *Inorganic Chemistry*, **56**, 7 (2017).
386. “Mg<sub>x</sub>Mn<sub>2-x</sub>B<sub>2</sub>O<sub>5</sub> Pyroborates (2/3 ≤ x ≤ 4/3): high capacity and high rate cathodes for Li-ion batteries”, H.F.J. Glass, Z. Liu, P.M. Bayley, E. Suard, S.H. Bo, P.G. Khalifah, C.P. Grey, S.E. Dutton, *Chem. Mater.*, **29**, 7 (2017).
387. “Local structure evolution and modes of charge storage in secondary Li-FeS<sub>2</sub> cells”, M.M. Butala, M. Mayo, V.V.T. Doan-Nguyen, M.A. Lumley, C. Gobel, K.M. Wiaderek, O.J. Borkiewicz, K.W. Chapman, P.J. Chupas, M. Balasubramanian, G. Laurita, S. Britto, A.J. Morris, C.P. Grey, R. Seshadri, *Chem. Mater.*, **29**, 7 (2017).
388. “Metal-organic nanosheets formed via defect-mediated transformation of a hafnium metal-organic framework”, M.J. Cliffe, E. Castillo-Martinez, Y. Wu, J. Lee, A.C. Forse, F.C.N. Firth, P.Z. Moghadam, D. Fairen-Jimenez, M.W. Gaultois, J.A. Hill, O.V. Magdysyuk, B. Slater, A.L. Goodwin, C.P. Grey, *J. Am. Chem. Soc.*, **139**, 15 (2017).
389. “Investigating sodium storage mechanisms in tin anodes: a combined pair distribution function analysis, density functional theory and solid-state NMR approach”, J.M. Stratford, M. Mayo, P.K. Allan, O. Pecher, O.J. Borkiewicz, K.M. Wiaderek, K. Chapman, C.J. Pickard, A.J. Morris, C.P. Grey, *J. Am. Chem. Soc.* 2017, in press (<http://pubs.acs.org/doi/abs/10.1021/jacs.7b01398>).
390. “Unravelling the Complex Delithiation and Lkithiation mechanisms of the high capacity cathode material”, W. Meng, R. Pigliapochi, P. M. Bayley, O. Pecher, M. W. Gaultois, I. D. Seymour, H. Liang, W. Xu, K. M. Wiaderek, K. W. Chapman, C. P. Grey. V6O13 *Chem. Mater.* 2017, in press (10.1021/acs.chemmater.7b00428).

## Patents

1. “Direct synthesis and deposition of luminescent films,” World Patent, WO/2002/102903, S. P. Devi, R. Gambino, C.P. Grey, H. Herman, J. Margoles, J.B. Parise, S. Sampath.
2. “New Electrodes for Lithium Ion Batteries,” UK Patent Application No 0610888.0, S.J. Clarke, O. J. Rutt, C.P. Grey, S. Indris, J. Cabana

## Current Graduate Students

Hugh Glass, Kent Griffith, David Halat, Wei Meng, Roberta Pigliapochi, Zachary Ruff, Luke Sperrin, Yanting Jin, Evan Keyzer, Jeonjae Lee, Josh

Stratford, Simon Engelke, Michael Hope, Nis-Julian Kneusels, George Lane, Philip Reeves, Amangeldi Torayev, Steffen Emge, Anna Gunnarsdóttir, Yuning Zhou

### **Current Postdoctoral Research Associates**

Phoebe Allan, Sylvia Britto, Elizabeth Castillo-Martínez, Matthew Cliffe, Matthew Dunstan, Michael Gaultois, Matthias Groh, Erlendur Jónsson, John Kattirtzi, Rachel Kerber, Gunwoo Kim, Tao Liu, Lauren Marbella, Céline Merlet, Oliver Pecher, Abdul-Rahman Raji, Ieuan Seymour, Yuanlong Shao, Israel Temprano, Robert Wheaterup

### **Current Academic Visitors**

Javier Carretero González (CSIC, Spain) Keitaro Kitada (SONY)

### **Lab Manager**

Pieter Magusin

### **Past Graduate Students**

Francis Wang, 1998 (Duracell), Hsien-Ming Kao, 1998 (Prof., National Central University), Kwang Hun Lim, 2000 (Assist. Prof., East Carolina Univ.), Michael F. Ciruolo, 2000 (Patent attorney), Lin-Shu Du, 2000 (Stanford), Young Joo Lee, 2001 (L.G. Chemicals), Haiming Liu, 2001 (Atofina Chemicals), Peter J. Chupas, 2003 (ANL), Santanu Chaudhuri, 2003 (Research Professor, Washington State University), Younkee Paik, 2004 (Korea Basic Science Institute (Daegu), Kyungpook National University), Namjun Kim, 2004 (Stanford), Luming Peng, 2006 (Stanford), Julien Bréger, 2006 (SAFT), John Palumbo, Lesley Holmes, 2008, Meng Jiang, 2008 (SEEO), Hailong Chen, 2009 (MIT), Hua Huo, 2009 (University of Bordeaux), Jongsik Kim, 2009 (Northwestern University), Paul Sideris, 2009 (Hunter College), Fulya Dogan, 2010, Baris Key, 2010 (Argonne National Laboratory), Dongli Zeng, 2010 (Brookhaven National Laboratory), Yi Xiao, 2000 (Computer Scientist), Stephen Boyd (SUNY Hunter College), Riza Dervisoglu (U. Nijmegen), Shou-Hang Bo (MIT), Fiona Strobridge (Apple), Hao Wang (Argonne National Laboratory), Yunxu Zhu, Lina Zhou, Kenneth Rosina, Xiao Hua (Fribourg University), Hee Jung Chang (PNNL), Hyeyoung Jung, Amy Moore (Cambridge Consultants), Alexander Forse (U. C. Berkeley), Raphaële Clément, (U. C. Berkeley), Alison Michan, Beth Howe

### **Past Postdoctoral Research Associates**

Alessandro Gualtieri (Professor, U. Modena), Yong Ba (Prof., Cal. State Univ. Los Angeles), Paul Norby (U. Oslo), John Osegovic, Robert Schurko (Assoc. Prof., U. Windsor), Wonsub Yoon (BNL), Jennifer Readman (U. of Exeter), Benjamin Meyer (MaxPower), Nicolas Dupré (CNRS Nantes) Sylvio Indris (Institute of Nanotechnology, Germany), Ulla Gro Nielsen (Assistant Professor, U. of Southern Denmark), Junichi Shirakawa (Dupont, Japan), Jordi Cabana Jimenez (Lawrence Berkeley National Lab, UIC), Zhouguang Lu (City University of Hong Kong), Rangeet Bhattacharyya (U. of Southampton), Frédérique Pourpoint (Maitre de Conference, Université Lille), Thomas Köster (BMW, Germany), Elizabeth Castillo Martinez, Hua

Huo, Rosa Robert Sanchez (Paul Scherer Institute, Switzerland), Frédéric Blanc (Lectureship, University of Liverpool), Elodie Salager-Oehler (Charge de Recherche, CNRS at the CEMHTI lab, Orleans, France), Lin-Shu Du (MaxPower, Inc.), Andrew Ilott (NYU), Srinivasan Shekar (FSU-National High Magnetic Field Laboratory), Derek Middlemiss (Warwick University), Wanjing Yu, Yan-Yan Hu (Assistant Prof. Florida State), Michal Leskes (Weitzman Institute), John Griffin (Lecturer, U. Lancaster), Karen Johnson (Lecturer, U. Durham), Paul Bayley (Apple)

### **Past Masters Students**

Faiza I. Poshni (Boehringer Ingelheim)  
Chanjuan Pan 2004 (Renaissance Technologies)  
Sarah Sakamoto 2005 (Brookhaven Instruments)  
Darrin Clinton 2006 (U. S. Military Academy, West Point)  
Keinia Julmis 2006

### **RESEARCH INTERESTS**

- Synthesis, characterization and electrochemical testing of lithium ion batteries electrode materials
- Development of new *in situ* NMR methods for probing lithium-ion battery and supercapacitor function
- Application of novel local probes of structure (NMR, pair distribution function analysis) to monitor structural changes in electrode materials during and following cycling
- Oxygen-ion and proton conductivity in membranes for solid oxide fuel cells
- Structures of solid-water interfaces: investigation of ion uptake and sorption in synthetic and natural materials
- Catalysis and sorption: structure and function