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# PUBLICATIONS LIST 2014

Institut Laue-Langevin

# PUBLICATIONS

## Applied Physics, Instrumentation and Techniques

Bardelli F., Mondelli C., Didier M., Vitillo J.G., Cavicchia D.R., Robinet J.C., Leone L., Charlet L. Hydrogen uptake and diffusion in Callovo-Oxfordian clay rock for nuclear waste disposal technology *Applied Geochemistry* **49**, 168-177 (2014)

Barrière N.M., Tomsick J.A., Ackermann M.D., Bastie P., Boggs S.E., Hanlon L., Jentschel M., Lowell A., Roudil G., von Ballmoos P., Wade C. Laue lens development at UC Berkeley: Status and prospects *Proceedings SPIE* **8861**, 88610F-1-88610F-8 (2013)

Barrière N.M., Tomsick J.A., Boggs S.E., Lowell A., Wade C., Baugh M., von Ballmoos P., Abrosimov N.V., Hanlon L. Developing a method for soft gamma-ray Laue lens assembly and calibration *Nuclear Instruments and Methods in Physics Research A* **741**, 47-56 (2014)

Bellucci V., Camattari R., Guidi V. Proposal for a Laue lens relying on hybrid quasi-mosaic curved crystals *Astronomy & Astrophysics* **560**, A58-1-A58-8 (2013)

Bellucci V., Camattari R., Guidi V., Bastie P. Stack of quasi-mosaic thin lamellae as a diffracting element for Laue lenses *Experimental Astronomy* **38**, 25-40 (2014)

Bigault T., Delphin G., Vittoz A., Gaignon V., Courtois P. Recent polarizing supermirror projects at the ILL *Journal of Physics: Conference Series* **528**, 012017-1-012017-6 (2014)

Birch J., Buffet J.C., Clergeau J.F., Correa J., Van Esch P., Ferraton M., Guérard B., Halbwachs J., Hall-Wilton R., Hultman L., Höglund C., Khaplanov A., Koza M., Piscitelli F., Zbiri M. In-beam test of the Boron-10 Multi-Grid neutron detector at the IN6 time-of-flight spectrometer at the ILL *Journal of Physics: Conference Series* **528**, 012040-1-012040-10 (2014)

Camattari R., Paternò G., Battelli A., Bellucci V., Bastie P., Guidi V. High-efficiency focusing of hard X-rays exploiting the quasi-mosaic effect in a bent germanium crystal *Journal of Applied Crystallography* **47**, 799-802 (2014)

Capelli S.C. Structure of complex materials *In "Experimental Methods in the Physical Sciences"* Germer T.A. et al. Eds. (2014, Elsevier) pp. 321-362

Chizhova L.A., Rotter S., Jenke T., Cronenberg G., Geltenbort P., Wautischer G., Filter H., Abele H., Burgdorfer J. Vectorial velocity filter for ultracold neutrons based on a surface-disordered mirror system *Physical Review E* **89**, 032907-1-032907-12 (2014)

Clergeau J.F., Ferraton M., Guérard B., Khaplanov A., Piscitelli F., Platz M., Rigal J.M., Van Esch P., Daullé T. An information-theoretical approach to image resolution applied to neutron imaging detectors based upon individual discriminator signals *In "Advancements in Nuclear Instrumentation Measurement Methods and their Applications (ANIMMA)"* (2013, IEEE) pp. 1-8

Courtois P., Fernandez-Diaz M.T., Nenert G., Andersen K.H., Freund A.K., Gsell S., Fischer M., Schreck M., Link P., Meven M. The first prototype diamond monochromator at the Institut Laue-Langevin *Journal of Physics: Conference Series* **528**, 012001-1-012001-9 (2014)

Cuello G., Fouquet P. Neutron scattering in Brazil and Argentina *Neutron News* **25**, 2 (2014)

Cuello G.J., Cristiglio V., Hennem L., Puente-Orench I. Neutron scattering at high temperature and levitation techniques *Journal of Physics: Conference Series* **549**, 012002-1-012002-10 (2014)

Cuello G.J., Croibier M. The signal of sample environment as a way to measure sample transmission *Journal of Physics: Conference Series* **549**, 012005-1-012005-4 (2014)

Daum M., Franke B., Geltenbort P., Gutmiedl E., Ivanov S., Karch J., Kasprzak M., Kirch K., Kraft A., Lauer T., Lauss B., Müller A.R., Paul S., Schmidt-Wellenburg P., Zechlau T., Zsigmond G. Transmission of ultra-cold neutrons through guides coated with materials of high optical potential *Nuclear Instruments and Methods in Physics Research A* **741**, 71-77 (2014)

Dawidowski J., Rodríguez Palomino L.A., Blostein J.J., Cuello G.J. Experimental corrections in neutron scattering experiments: A modern theoretical and computational approach *Neutron News* **25**, 20-23 (2014)

Dewhurst C.D. Novel multiple-beam very-small-angle neutron scattering (VSANS) using a conventional SANS instrument *Journal of Applied Crystallography* **47**, 1180-1189 (2014)

Dijulio D.D., Lelièvre-Berna E., Courtois P., Andersen K.H., Bentley P.M. Optimisation of multi-channel neutron focusing guides for extreme sample environments *Journal of Physics: Conference Series* **528**, 012006-1-012006-8 (2014)

Farhi E., Debab Y., Willendrup P. iFit: A new data analysis framework. Applications for data reduction and optimisation of neutron scattering instrument simulations with McStas *Journal of Neutron Research* **17**, 5-18 (2014)

Farhi E., Monzat C., Arnerin R., Van Vuure T., Castán-Guerrero C., Hennane C., Harraud P.A., Campioni G., Fuard S., Ollivier J., Willendrup P. Advanced sources and optical components for the McStas neutron scattering instrument simulation package  
Journal of Neutron Research **17**, 63-74 (2014)

Formisano F., De Francesco A., Guarini E., Laloni A., Orecchini A., Petrillo C., Pilgrim W.C., Russo D., Sacchetti F. The neutron spectrometer BRISP: A new approach to the study of excitations in condensed matter at low momentum transfer in the Milli-eV energy region  
Journal of the Physical Society of Japan **82**, SA028-1-SA028-11 (2013)

Guérard B., Hall-Wilton R., Murtas F. Prospects in MPGDs development for neutron detection  
Report Arkiv (2014)

Hall-Wilton R., Theroine C. Status of the European Spallation Source ESS AB, the instrument selection process, and a fundamental physics beamline at the ESS  
Physics Procedia **51**, 8-12 (2014)

Hughes D.J., Koukovini-Platia E., Heeley E.L. Residual stress in a laser welded EUROFER blanket module assembly using non-destructive neutron diffraction techniques  
Fusion Engineering and Design **89**, 104-108 (2014)

Ispirian K.A. Gamma Cherenkov-transition radiation of high-energy electrons and methods for the measurement of the refractive index of MeV photons using total internal and external reflections (Invited talk)  
Journal of Physics: Conference Series **517**, 012008-1-012008-7 (2014)

Ivanov A., Jiménez-Ruiz M., Kulda J. IN1-LAGRANGE – The new ILL instrument to explore vibration dynamics of complex materials  
Journal of Physics: Conference Series **554**, 012001-1-012001-7 (2014)

Jain R., Petri M., Kirschbaum S., Feindt H., Steltenkamp S., Sonnenkalb S., Becker S., Griesinger C., Menzel A., Burg T.P., Techert S. X-ray scattering experiments with high-flux X-ray source coupled rapid mixing microchannel device and their potential for high-flux neutron-scattering investigations  
European Physical Journal E **36**, 109-1-109-9 (2013)

Kanaki K., Birch J., Hall-Wilton R.J., Höglund C., Hultman L., Jackson A., Kirstein O., Kittelmann T., Kolya S., Piscitelli F. An alternative small-angle neutron scattering detector  
IEEE Nuclear Science Symposium and Medical Imaging Conference, 1-7 (2013)

Kanaki K., Hall-Wilton R., Andersen K.H., Anevski D., Birch J., Cai X.X., Höglund C., Hultman L., Jansa Llamas I., Keiderling U., Khaplanov A., Kirstein O., Schulz C., Wilpert T. Statistical energy determination in neutron detector systems for neutron scattering science  
IEEE Nuclear Science Symposium and Medical Imaging Conference, 1-6 (2013)

Köster U., Cantone M.C. Radioisotope production  
In "Nuclear Physics for Medicine" Azaiez F. et al. Eds. (2014, European Science Foundation) pp. 95-144

Lemmel H. Dispersion cancellation in a triple Laue interferometer  
Journal of Optics **16**, 105704-1-105704-10 (2014)

Mutti P., Blanc A., de France G., Jentschel M., Köster U., Ruiz Martinez E., Simpson G., Soldner T., Ur C.A., Urban W. A trigger-less acquisition system for the EXILL large germanium detectors array  
In "Advancements in Nuclear Instrumentation Measurement Methods and their Applications (ANIMMA)" (2013, IEEE) pp. 1-6

Piovano A., Roux S., Kulda J. exTAS: A new concept in three-axis spectroscopy for small samples  
Journal of Physics: Conference Series **528**, 012027-1-012027-7 (2014)

Piscitelli F., Buffet J.C., Clergeau J.F., Cuccaro S., Guérard B., Khaplanov A., La Manna Q., Rigal J.M., Esch P. Study of a high spatial resolution <sup>10</sup>B-based thermal neutron detector for application in neutron reflectometry: The Multi-Blade prototype  
Journal of Instrumentation **9**, P03007-1-P03007-30 (2014)

Puente-Orench I., Clergeau J.F., Martínez S., Olmos M., Fabelo O., Campo J. The new powder diffractometer D1B of the Institut Laue Langevin  
Journal of Physics: Conference Series **549**, 012003-1-012003-5 (2014)

Rehm C., Brülé A., Freund A.K., Kennedy S.J. Kookaburra: The ultra-small-angle neutron scattering instrument at OPAL  
Journal of Applied Crystallography **46**, 1699-1704 (2013)

Rossillon F., Depradeux L., Miloudi S., Deforge D., Lemaire E., Massoud J.P. Learnings from investigations on SG divider plates: Coupling field characterisations with numerical mechanical simulation  
Nuclear Engineering and Design **269**, 45-51 (2014)

Sordo F., Fernandez-Alonso F., González M.A., Ghiglini A., Magán M., Terrón S., Martínez F., de Vicente J.P., Vivanco R., Bermejo F.J., Perlado J.M. Baseline design of a low-energy neutron source at ESS-Bilbao  
Journal of Physics: Conference Series **549**, 012001-1-012001-12 (2014)



# PUBLICATIONS

Willendrup P., Farhi E., Knudsen E., Filges U., Lefmann K.  
McStas: Past, present and future  
Journal of Neutron Research **17**, 35-43 (2014)

Willendrup P.K., Knudsen E.B., Klinkby E., Nielsen T., Farhi E.,  
Filges U., Lefmann K. New developments in the McStas neutron  
instrument simulation package  
Journal of Physics: Conference Series **528**, 012035-1-012035-11  
(2014)

Wolff M., Herbel J., Adlmann F., Dennison A.J.C., Liesche G.,  
Gutfreund P., Rogers S. Depth-resolved grazing-incidence time-of-flight  
neutron scattering from a solid-liquid interface  
Journal of Applied Crystallography **47**, 130-135 (2014)

---

## Biology

---

Appolaire A., Girard E., Colombo M., Durá M.A., Moulin M.,  
Härtlein M., Franzetti B., Gabel F. Small-angle neutron scattering  
reveals the assembly mode and oligomeric architecture of TET,  
a large, dodecameric aminopeptidase  
Acta Crystallographica D **70**, 2983-2993 (2014)

Benedetto A., Heinrich F., González M.A., Fragneto G., Watkins E.,  
Ballone P. Structure and stability of phospholipid bilayers hydrated  
by a room-temperature ionic liquid/water solution: A neutron  
reflectometry study  
Journal of Physical Chemistry B **118**, 12192-12206 (2014)

Blanc M., Coetzer T.L., Blackledge M., Haertlein M., Mitchell E.P.,  
Forsyth V.T., Jensen M.R. Intrinsic disorder within the erythrocyte  
binding-like proteins from *Plasmodium falciparum*  
Biochimica et Biophysica Acta **1844**, 2306-2314 (2014)

Brüning B., Farago B. Perfluorooctanoic acid rigidifies a model  
lipid membrane  
Physical Review E **89**, 040702-1-040702-5 (2014)

Buch M., Wine Y., Dror Y., Rosenheck S., Lebendiker M.,  
Giordano R., Leal R.M.F., Popov A.N., Freeman A., Frolow F.  
Protein products obtained by site-preferred partial crosslinking in protein  
crystals and "liberated" by redissolution  
Biotechnology and Bioengineering **111**, 1296-1303 (2014)

Casadei C.M., Gumiero A., Metcalfe C.L., Murphy E.J.,  
Basran J., Concilio M.G., Teixeira S.C.M., Schrader T.E.,  
Fielding A.J., Ostermann A., Blakeley M.P., Raven E.L., Moody P.C.E.  
Neutron cryo-crystallography captures the protonation state of ferryl  
heme in a peroxidase  
Science **345**, 193-197 (2014)

Chiappisi L., Prévost S., Grillo I., Gradzielski M. From crab shells to  
smart systems: Chitosan-alkylethoxy carboxylate complexes  
Langmuir **30**, 10608-10616 (2014)

Compton E.L.R., Page K., Findlay H.E., Haertlein M., Moulin M.,  
Zachariae U., Norman D.G., Gabel F., Javelle A. Conserved structure  
and domain organisation among bacterial Slc26 transporters  
Biochemical Journal **463**, 297-307 (2014)

Dabkowska A.P., Collins I.E., Barlow D.J., Barker R.,  
McLain S.E., Lawrence M.J., Lorenz C.D. Modulation of  
dipalmitoylphosphatidylcholine monolayers by dimethyl sulfoxide  
Langmuir **30**, 8803-8811 (2014)

de Gouvion Saint Cyr D., Wisniewski C., Schrive L., Farhi E.,  
Rivasseau C. Feasibility study of microfiltration for algae separation  
in an innovative nuclear effluents decontamination process  
Separation and Purification Technology **125**, 126-135 (2014)

Demé B., Cataye C., Block M.A., Marechal E., Jouhet J. Contribution  
of galactoglycerolipids to the 3-dimensional architecture of thylakoids  
FASEB Journal **28**, 3373-3383 (2014)

Denninger A.R., Demé B., Cristiglio V., Leduc G., Feller W.B.,  
Kirschner D.A. Neutron scattering from myelin revisited:  
Bilayer asymmetry and water-exchange kinetics  
Acta Crystallographica D **70**, 3198-3211 (2014)

Falourd X., Natali F., Peters J., Foucat L. Molecular mobility in  
*Medicago truncatula* seed during early stage of germination:  
Neutron scattering and NMR investigations  
Chemical Physics **428**, 181-185 (2014)

Fisher S.J., Blakeley M.P., Howard E.I., Petit-Haertlein I.,  
Haertlein M., Mitschler A., Cousido-Siah A., Salvay A.G.,  
Popov A., Müller-Dieckmann C., Petrova T., Podjarny A.  
Perdeuteration: Improved visualisation of solvent structure in neutron  
macromolecular crystallography  
Acta Crystallographica D **70**, 3266-3272 (2014)

Fomina M., Schirò G., Cupane A. Hydration dependence of  
myoglobin dynamics studied with elastic neutron scattering, differential  
scanning calorimetry and broadband dielectric spectroscopy  
Biophysical Chemistry **185**, 25-31 (2014)

Fragneto G. Etudier la structure des membranes biologiques:  
l'intérêt des systèmes modèles et des neutrons  
Reflète de la Physique **41**, 36-40 (2014)

Gabel F., Lensink M.F., Clantin B., Jacob-Dubuisson F., Villeret V.,  
Ebel C. Probing the conformation of FhaC with small-angle  
neutron scattering and molecular modeling  
Biophysical Journal **107**, 185-196 (2014)

- Ganguly S., Wescott A., Nagy T., Colegrove P., Williams S. Characterisation of residual stress state and distortion in welded plates stress engineered by local mechanical tensioning *Materials Science Forum* **772**, 187-191 (2014)
- Gibrat G., Hui Bon Hoa G., Craescu C.T., Assairi L., Blouquit Y., Annighöfer B., May R.P., Bellissent-Funel M.C. High-pressure SANS and fluorescence unfolding study of calmodulin *Biochimica et Biophysica Acta* **1844**, 1560-1568 (2014)
- Golden E.A., Vrielink A. Looking for hydrogen atoms: Neutron crystallography provides novel insights into protein structure and function *Australian Journal of Chemistry* **67**, 1751-1762 (2014)
- Grimaldo M., Roosen-Runge F., Zhang F., Seydel T., Schreiber F. Diffusion and dynamics of  $\gamma$ -globulin in crowded aqueous solutions *Journal of Physical Chemistry B* **118**, 7203-7209 (2014)
- Groves J.T., Boaz N.C. Biochemistry. Fishing for peroxidase protons *Science* **345**, 142-143 (2014)
- Grünberg J., Lindenblatt D., Dorrer H., Cohrs S., Zhernosekov K., Köster U., Türler A., Fischer E., Schibli R. Anti-L1CAM radioimmunotherapy is more effective with the radiolanthanide terbium-161 compared to lutetium-177 in an ovarian cancer model *European Journal of Nuclear Medicine and Molecular Imaging* **41**, 1907-1915 (2014)
- Haupt M., Blakeley M.P., Fisher S.J., Mason S.A., Cooper J.B., Mitchell E.P., Forsyth V.T. Binding site asymmetry in human transthyretin: Insights from a joint neutron and X-ray crystallographic analysis using perdeuterated protein *IUCr* **1**, 429-438 (2014)
- Howard E., Blakeley M.P., Salvay A.G., Podjarny A. Use of neutron scattering techniques for antifreeze protein mechanistic studies *Neutron News* **25**, 24-27 (2014)
- Huang G.Y., Gerlits O.O., Blakeley M.P., Sankaran B., Kovalevsky A.Y., Kim C. Neutron diffraction reveals hydrogen bonds critical for cGMP-selective activation: Insights for cGMP-dependent protein kinase agonist design *Biochemistry* **53**, 6725-6727 (2014)
- Knoll W., Peters J., Kursula P., Gerelli Y., Ollivier J., Demé B., Telling M., Kemner E., Natali F. Structural and dynamical properties of reconstituted myelin sheaths in the presence of myelin proteins MBP and P2 studied by neutron scattering *Soft Matter* **10**, 519-529 (2014)
- Kumar S., Aswal V.K., Callow P. pH dependent interaction and resultant structures of silica nanoparticles and lysozyme protein *Langmuir* **30**, 1588-1598 (2014)
- Kumar S., Aswal V.K., Callow P. Tuning structure of oppositely charged nanoparticle and protein complexes *AIP Conference Proceedings* **1591**, 161-163 (2014)
- Kynde S.A.R., Skar-Gislinge N., Pedersen M.C., Midtgaard S.R., Simonsen J.B., Schweins R., Mortensen K., Arleth L. Small-angle scattering gives direct structural information about a membrane protein inside a lipid environment *Acta Crystallographica D* **70**, 371-383 (2014)
- Langan P., Sangha A.K., Wymore T., Parks J.M., Yang Z.K., Hanson B.L., Fisher Z., Mason S.A., Blakeley M.P., Forsyth V.T., Glusker J.P., Carrell H.L., Smith J.C., Keen D.A., Graham D.E., Kovalevsky A. L-arabinose binding, isomerisation, and epimerisation by D-xylose isomerase: X-ray/neutron crystallographic and molecular simulation study *Structure* **22**, 1287-1300 (2014)
- Leonardo T., Farhi E., Boisson A.M., Vial J., Cloetens P., Bohic S., Rivasseau C. Determination of elemental distribution in green micro-algae using synchrotron radiation nano X-ray fluorescence (SR-nXRF) and electron microscopy techniques – Subcellular localisation and quantitative imaging of silver and cobalt uptake by *Coccomyxa actinobiotis* *Metallomics* **6**, 316-329 (2014)
- Magazù S., Migliardo F., Benedetto A., Vertessy B. Protein dynamics by neutron scattering: The protein dynamical transition and the fragile-to-strong dynamical crossover in hydrated lysozyme *Chemical Physics* **424**, 26-31 (2013)
- Magazù S., Migliardo F., Vertessy B.G., Caccamo M.T. Investigations of homologous disaccharides by elastic incoherent neutron scattering and wavelet multiresolution analysis *Chemical Physics* **424**, 56-61 (2013)
- Mandal S.S., Cristiglio V., Lindner P., Bhattacharyya A.J. Small-angle neutron-scattering studies of hemoglobin confined inside silica tubes of varying sizes *ChemPhysChem* **15**, 302-309 (2014)
- Maric S., Skar-Gislinge N., Midtgaard S., Thygesen M.B., Schiller J., Frielinghaus H., Moulin M., Haertlein M., Forsyth V.T., Pomorski T.G., Arleth L. Stealth carriers for low-resolution structure determination of membrane proteins in solution *Acta Crystallographica D* **70**, 317-328 (2014)
- Meilleur F., Munshi P., Robertson L., Stoica A.D., Crow L., Kovalevsky A., Koritsanszky T., Chakoumakos B.C., Blessing R., Myles D.A.A. The IMAGINE instrument: First neutron protein structure and new capabilities for neutron macromolecular crystallography *Acta Crystallographica D* **69**, 2157-2160 (2013)

## PUBLICATIONS

- Midgaard S.R., Pedersen M.C., Kirkensgaard J.J.K., Sørensen K.K., Mortensen K., Jensen K.J., Arleth L. Self-assembling peptides form nanodiscs that stabilize membrane proteins  
*Soft Matter* **10**, 738-752 (2014)
- Migliardo F., Caccamo M.T., Magazù S. Thermal analysis on bioprotectant disaccharides by elastic incoherent neutron scattering  
*Food Biophysics* **9**, 99-104 (2014)
- Migliardo F., Tallima H., El Ridi R. Is there a sphingomyelin-based hydrogen bond barrier at the mammalian host-schistosome parasite interface?  
*Cell Biochemistry and Biophysics* **68**, 359-367 (2014)
- Migliardo F., Tallima H., El Ridi R. Rigidity and resistance of larval- and adult schistosomes-medium interface  
*Biochemical and Biophysical Research Communications* **446**, 255-260 (2014)
- Munshi P., Snell E.H., Van der Woerd M.J., Judge R.A., Myles D.A.A., Ren Z., Meilleur F. Neutron structure of the cyclic glucose-bound xylose isomerase E186Q mutant  
*Acta Crystallographica D* **70**, 414-420 (2014)
- Müller C., Fischer E., Behe M., Köster U., Dorner H., Reber J., Haller S., Cohrs S., Blanc A., Grünberg J., Bunka M., Zhernosekov K., Van der Meulen N., Johnston K., Türler A., Schibli R. Future prospects for SPECT imaging using the radiolanthanide terbium-155 – Production and preclinical evaluation in tumor-bearing mice  
*Nuclear Medicine and Biology* **41**, e58-e65 (2014)
- Müller C., Reber J., Haller S., Dorner H., Köster U., Johnston K., Zhernosekov K., Türler A., Schibli R. Folate receptor targeted alpha-therapy using terbium-149  
*Pharmaceuticals* **7**, 353-365 (2014)
- Nagy G., Garab G., Pieper J.  
Neutron scattering in photosynthesis research  
In "Photosynthesis: Open Questions and What We Know Today" Allakhverdiev S.I. et al. Eds. (2014, Institute of Computer Science) pp. 69-121
- Nagy G., Ünneper R., Zsiros O., Tokutsu R., Takizawa K., Porcar L., Moyet L., Petroustos D., Garab G., Finazzi G., Minagawa J.  
Chloroplast remodeling during state transitions in *Chlamydomonas reinhardtii* as revealed by non-invasive techniques in vivo  
*Proceedings of the National Academy of Sciences* **111**, 5042-5047 (2014)
- Oksanen E., Blakeley M.P., El-Hajji M., Ryde U., Budayova-Spano M.  
The neutron structure of urate oxidase resolves a long-standing mechanistic conundrum and reveals unexpected changes in protonation  
*PloS One* **9**, e86651-1-e86651-10 (2014)
- Pettit M.W., Dyer P.D.R., Mitchell J.C., Griffiths P.C., Alexander B., Cattoz B., Heenan R.K., King S.M., Schweins R., Pullen F., Wicks S.R., Richardson S.C.W. Construction and physicochemical characterisation of a multi-composite, potential oral vaccine delivery system (VDS)  
*International Journal of Pharmaceutics* **468**, 264-271 (2014)
- Rheinstädter M.C. Basic aspects and applications of lipids and protein dynamics  
In "Liposomes, Lipid Bilayers and Model Membranes: From Basic Research to Application" Pabst G. et al. Eds. (2014, CRC Press) pp. 111-122
- Schirò G., Vetri V., Andersen C.B., Natali F., Koza M.M., Leone M., Cupane A. The boson peak of amyloid fibrils: Probing the softness of protein aggregates by inelastic neutron scattering  
*Journal of Physical Chemistry B* **118**, 2913-2923 (2014)
- Stadler A.M., Garvey C.J., Embs J.P., Koza M.M., Unruh T., Artmann G., Zaccari G. Picosecond dynamics in haemoglobin from different species: A quasielastic neutron scattering study  
*Biochimica et Biophysica Acta (BBA) – General Subjects* **1840**, 2989-2999 (2014)
- Sugiyama M., Yagi H., Yamaguchi T., Kumoi K., Hirai M., Oba Y., Sato N., Porcar L., Martel A., Kato K. Conformational characterisation of a protein complex involving intrinsically disordered protein by small-angle neutron scattering using the inverse contrast matching method: A case study of interaction between  $\alpha$ -synuclein and PbaB tetramer as a model chaperone  
*Journal of Applied Crystallography* **47**, 430-435 (2014)
- Tamamis P., Terzaki K., Kassinosopoulos M., Mastrogianis L., Mossou E., Forsyth V.T., Mitchell E.P., Mitraki A., Archontis G. Self-assembly of an aspartate-rich sequence from the adenovirus fiber shaft: Insights from molecular dynamics simulations and experiments  
*Journal of Physical Chemistry B* **118**, 1765-1774 (2014)
- Tehei M., Perlmutter J.D., Giusti F., Sachs J.N., Zaccari G., Popot J.L. Thermal fluctuations in amphipol A8-35 particles: A neutron scattering and molecular dynamics study  
*Journal of Membrane Biology* **247**, 897-908 (2014)
- Terzaki K., Kalloudi E., Mossou E., Mitchell E.P., Forsyth V.T., Rosseeva E., Simon P., Vamvakaki M., Chatzinikolaïdou M., Mitraki A., Farsari M. Mineralised self-assembled peptides on 3D laser-made scaffolds: A new route toward "scaffold-on-scaffold" hard tissue engineering  
*Biofabrication* **5**, 045002-1-045002-14 (2013)
- Thomas L.H., Forsyth V.T., Martel A., Grillo I., Altaner C.M., Jarvis M.C. Structure and spacing of cellulose microfibrils in woody cell walls of dicots  
*Cellulose* **21**, 3887-3895 (2014)



## Crystallography

- Trapp M., Tehei M., Trovaslet M., Nachon F., Martinez N., Koza M.M., Weik M., Masson P., Peters J. Correlation of the dynamics of native *human* acetylcholinesterase and its inhibited huperzine A counterpart from sub-picoseconds to nanoseconds  
Journal of the Royal Society Interface **11**, 20140372-1-20140372-9 (2014)
- Ünnep R., Nagy G., Markó M., Garab G. Monitoring thylakoid ultrastructural changes in vivo using small-angle neutron-scattering  
Plant Physiology and Biochemistry **81**, 197-207 (2014)
- Ünnep R., Zsiros O., Solymosi K., Kovács L., Lambrev P.H., Tóth T., Schweins R., Posselt D., Székely N.K., Rosta L., Nagy G., Garab G. The ultrastructure and flexibility of thylakoid membranes in leaves and isolated chloroplasts as revealed by small-angle neutron-scattering  
Biochimica et Biophysica Acta **1837**, 1572-1580 (2014)
- Vasquez D., Milusheva R., Baumann P., Constantin D., Chami M., Palivan C.G. The amine content of PEGylated chitosan *Bombyx mori* nanoparticles acts as a trigger for protein delivery  
Langmuir **30**, 965-975 (2014)
- Wanderlingh U., D'Angelo G., Branca C., Nibali V.C., Trimarchi A., Rifici S., Finocchiaro D., Crupi C., Ollivier J., Middendorf H.D. Multi-component modeling of quasielastic neutron-scattering from phospholipid membranes  
Journal of Chemical Physics **140**, 174901-1-174901-10 (2014)
- Watkins E.B., Gao H., Dennison A.J.C., Chopin N., Struth B., Arnold T., Florent J.C., Johannes L. Carbohydrate conformation and lipid condensation in monolayers containing glycosphingolipid Gb3: Influence of acyl chain structure  
Biophysical Journal **107**, 1146-1155 (2014)
- Xu H., Penfold J., Thomas R.K., Petkov J.T., Tucker I., Webster J.P.R. The formation of surface multilayers at the air-water interface from sodium diethylene glycol monoalkyl ether sulfate/AICl<sub>3</sub> solutions: The role of the alkyl chain length  
Langmuir **29**, 12744-12753 (2013)
- Yanez Arteta M., Ainalem M.L., Porcar L., Martel A., Coker H., Lundberg D., Chang D.P., Soltwedel O., Barker R., Nylander T. Interactions of PAMAM dendrimers with negatively charged model biomembranes  
Journal of Physical Chemistry B **118**, 12892-12906 (2014)
- Yearley E.J., Godfrin P.D., Perevozchikova T., Zhang H., Falus P., Porcar L., Nagao M., Curtis J.E., Gawande P., Taing R., Zarraga I.E., Wagner N.J., Liu Y. Observation of small cluster formation in concentrated monoclonal antibody solutions and its implications to solution viscosity  
Biophysical Journal **106**, 1763-1770 (2014)
- Auer H., Kohlmann H. Reinvestigation of crystal structure and non-stoichiometry in copper hydride, CuH<sub>1-x</sub> (0 ≤ x ≤ 0.26)  
Zeitschrift für Anorganische und Allgemeine Chemie **640**, 3159-3165 (2014)
- Babizhetskyy V., Jepsen O., Kremer R.K., Simon A., Ouladdiaf B., Stolovits A. Structure and bonding of superconducting LaC<sub>2</sub>  
Journal of Physics: Condensed Matter **26**, 025701-1-025701-9 (2014)
- Baratta W., Baldino S., Calhorda M.J., Costa P.J., Esposito G., Herdtweck E., Magnolia S., Mealli C., Messaoudi A., Mason S.A., Veiros L.F. CNN pincer ruthenium catalysts for hydrogenation and transfer hydrogenation of ketones: Experimental and computational studies  
Chemistry: A European Journal **20**, 13603-13617 (2014)
- Berthold R., Mihalkovic M., Burkhardt U., Prots Y., Amarsanaa A., Kreiner G. Crystal structure, disorder and composition of the 2/1 approximant in the Al-Mg-Zn system revisited  
Intermetallics **53**, 67-84 (2014)
- Besnard L., Protat M., Malloggi F., Daillant J., Cousin F., Pantoustier N., Guenoun P., Perrin P. Breaking of the Bancroft rule for multiple emulsions stabilised by a single stimuable polymer  
Soft Matter **10**, 7073-7087 (2014)
- Bianchini M., Ateba-Mba J.M., Dagault P., Bogdan E., Carlier D., Suard E., Masquelier C., Croguennec L. Multiple phases in the ε-VPO<sub>4</sub>-LiVPO<sub>4</sub>-O-Li<sub>2</sub>VPO<sub>4</sub>-O system: A combined solid state electrochemistry and diffraction structural study  
Journal of Materials Chemistry A **2**, 10182-10192 (2014)
- Bianchini M., Brisset N., Fauth F., Weill F., Elkaim E., Suard E., Masquelier C., Croguennec L. Na<sub>3</sub>V<sub>2</sub>(PO<sub>4</sub>)<sub>2</sub>F<sub>3</sub> revisited: A high-resolution diffraction study  
Chemistry of Materials **26**, 4238-4247 (2014)
- Bianchini M., Suard E., Croguennec L., Masquelier C. Li-Rich Li<sub>1-x</sub>Mn<sub>2x</sub>O<sub>4</sub> spinel electrode materials: An *operando* neutron diffraction study during Li<sup>+</sup> extraction/insertion  
Journal of Physical Chemistry C **118**, 25947-25955 (2014)
- Birkenstock J., Nénert G., Gesing T.M., Burianek M., Mühlberg M., Fischer R.X. "Forbidden" reflections in neutron diffraction on bismuth metal oxides: Symmetry reduction, λ/2 effect or Umweganregung?  
Zeitschrift für Kristallographie **228**, 611-619 (2013)
- Blanco M.C., De Paoli J.M., Ceppi S., Tirao G., Nassif V.M., Guimpel J., Carbonio R.E. Synthesis, structural characterisation and magnetic properties of the monoclinic ordered double perovskites BaLaMSbO<sub>6</sub>, with M = Mn, Co and Ni  
Journal of Alloys and Compounds **606**, 139-148 (2014)

## PUBLICATIONS

- Brown C.M., Ramirez-Cuesta A.T.J., Johnson M.R., Garcia-Sakai V. Chemical spectroscopy using neutrons *Chemical Physics* **427**, 1-2 (2013)
- Cañadillas-Delgado L., Fabelo O., Pasán J., Déniz M., Martínez-Benito C., Díaz-Gallifa P., Martín T., Ruiz-Pérez C. Three new europium(III) methanetriacetate metal-organic frameworks: The influence of synthesis on the product topology *Acta Crystallographica B* **70**, 19-27 (2014)
- Capelli S.C., Bürgi H.B., Mason S.A., Jayatilaka D. Glycyl-L-alanine: A multi-temperature neutron study *Acta Crystallographica C* **70**, 949-952 (2014)
- Capelli S.C., Falvello L.R., Forcén-Vazquez E., McIntyre G.J., Palacio F., Sanz S., Tomás M. Proton cascade in a molecular solid: H/D exchange on mobile and immobile water *Angewandte Chemie* **125**, 13705-13709 (2013)
- Cascos V., Martínez-Coronado R., Alonso J.A., Fernández-Díaz M.T. Visualisation by neutron diffraction of 2D oxygen diffusion in the  $\text{Sr}_{0.7}\text{Ho}_{0.3}\text{CoO}_{3.8}$  cathode for solid-oxide fuel cells *ACS Applied Materials & Interfaces* **6**, 9194-9200 (2014)
- Catti M., Ghaani M.R. On the lithiation reaction of niobium oxide: Structural and electronic properties of  $\text{Li}_{1.714}\text{Nb}_2\text{O}_5$  *Physical Chemistry Chemical Physics* **16**, 1385-1392 (2014)
- Chambrier M.H., Le Bail A., Giovannelli F., Redjaimia A., Florian P., Massiot D., Suard E., Goutenoire F.  $\text{La}_{10}\text{W}_2\text{O}_{21}$ : An anion-deficient fluorite-related superstructure with oxide ion conduction *Inorganic Chemistry* **53**, 147-159 (2014)
- Clausen H.F., Jørgensen M.R.V., Cenedese S., Schmøkel M.S., Christensen M., Chen Y.S., Koutsantonis G., Overgaard J., Spackman M.A., Iversen B.B. Host perturbation in a  $\beta$ -hydroquinone clathrate studied by combined X-ray/neutron charge-density analysis: Implications for molecular inclusion in supramolecular entities *Chemistry: A European Journal* **20**, 8089-8098 (2014)
- Cole J.M., Waddell P.G., Wheatley A.E.H., McIntyre G.J., Peel A.J., Tate C.W., Linton D.J. Neutron diffraction characterisation of C-H...Li interactions in a lithium aluminate polymer *Organometallics* **33**, 3919-3923 (2014)
- Corkett A.J., Free D.G., Cassidy S.J., Ramos S., Clarke S.J. Control of the superconducting properties of  $\text{Sr}_{2x}\text{Ca}_x\text{VO}_3\text{FeAs}$  through isovalent substitution *Journal of Solid State Chemistry* **216**, 91-98 (2014)
- De Aza A.H., Turrillas X., Rodríguez M.A., Duran T., Pena P. Time-resolved powder neutron diffraction study of the phase transformation sequence of kaolinite to mullite *Journal of the European Ceramic Society* **34**, 1409-1421 (2014)
- Déniz M., Hernández-Rodríguez I., Pasán J., Fabelo O., Cañadillas-Delgado L., Vallejo J., Julve M., Lloret F., Ruiz-Pérez C. Syntheses, crystal structures and magnetic properties of five new manganese(II) complexes: Influence of the conformation of different alkyl/aryl substituted malonate ligands on the crystal packing *CrystEngComm* **16**, 2766-2778 (2014)
- Díaz-Gallifa P., Fabelo O., Cañadillas-Delgado L., Pasán J., Labrador A., Lloret F., Julve M., Ruiz-Pérez C. Synthesis, crystal structure and magnetic characterisation of a series of  $\text{Cu}^{\text{II}}\text{-Ln}^{\text{III}}$  heterometallic [ $\text{Ln} = \text{La, Ce, Pr, Nd and Sm}$ ] metal-organic compounds with an unusual single-crystal to single-crystal phase transition *Crystal Growth & Design* **13**, 4735-4745 (2013)
- Díaz-Gallifa P., Fabelo O., Pasán J., Cañadillas-Delgado L., Lloret F., Julve M., Ruiz-Pérez C. Two-dimensional 3d-4f heterometallic coordination polymers: Syntheses, crystal structures, and magnetic properties of six new  $\text{Co(II)-Ln(III)}$  compounds *Inorganic Chemistry* **53**, 6299-6308 (2014)
- Fang Y.N., Ritter C., White T.J. Crystal chemical characteristics of ellestadite-type apatite: Implications for toxic metal immobilisation *Dalton Transactions*. **43**, 16031-16043 (2014)
- Fernández-Carrión A.J., Allix M., Ocaña M., García-Sevillano J., Cusso F., Fitch A.N., Suard E., Becerro A.I. Crystal structures and photoluminescence across the  $\text{La}_2\text{Si}_2\text{O}_7\text{-Ho}_2\text{Si}_2\text{O}_7$  system *Inorganic Chemistry* **52**, 13469-13479 (2013)
- Galven C., Mounier D., Pagnier T., Suard E., Le Berre F., Crosnier-Lopez M.P. Thermal structural characterisation of the acentric layered perovskite  $\text{LiHSrTa}_2\text{O}_7$ : X-ray and neutron diffraction, SHG and Raman experiments *Dalton Transactions* **43**, 14841-14850 (2014)
- García-Saiz A., de Pedro I., Migowski P., Vallcorba O., Junquera J., Blanco J.A., Fabelo O., Sheptyakov D., Waerenborgh J.C., Fernández-Díaz M.T., Rius J., Dupont J., González J.A., Rodríguez Fernández J. Anion- $\pi$  and halide-halide nonbonding interactions in a new ionic liquid based on imidazolium cation with three-dimensional magnetic ordering in the solid state *Inorganic Chemistry* **53**, 8384-8396 (2014)
- García-Saiz A., Migowski P., Vallcorba O., Junquera J., Blanco J.A., González J.A., Fernández-Díaz M.T., Rius J., Dupont J., Rodríguez Fernández J., de Pedro I. A magnetic ionic liquid based on tetrachloroferrate exhibits three-dimensional magnetic ordering: A combined experimental and theoretical study of the magnetic interaction mechanism *Chemistry: A European Journal* **20**, 72-76 (2014)
- Gatta G.D., Bosi F., McIntyre G.J., Hålenius U. Static positional disorder in ulvöspinel: A single-crystal neutron diffraction study *American Mineralogist* **99**, 255-260 (2014)

- Gatta G.D., Bosi F., McIntyre G.J., Skogby H.  
First accurate location of two proton sites in tourmaline:  
A single-crystal neutron diffraction study of oxy-dravite  
*Mineralogical Magazine* **78**, 681-692 (2014)
- Gatta G.D., Jacobsen S.D., Vignola P., McIntyre G.J., Guastella G.,  
Abate L.F. Single-crystal neutron diffraction and Raman spectroscopic  
study of hydroxylherderite,  $\text{CaBePO}_4(\text{OH}, \text{F})$   
*Mineralogical Magazine* **78**, 723-737 (2014)
- Gatta G.D., Lotti P., Nénert G., Kahlenberg V.  
On the crystal structure and low-temperature behaviour of davynite:  
A single-crystal X-ray and neutron diffraction study  
*Microporous and Mesoporous Materials* **185**, 137-148 (2014)
- Gatta G.D., Nénert G., Guastella G., Lotti P., Guastoni A., Rizzato S.  
A single-crystal neutron and X-ray diffraction study of a Li,Be-bearing  
brittle mica  
*Mineralogical Magazine* **78**, 55-72 (2014)
- Gómez-Pérez A., Pérez-Flores J.C., Ritter C., Boulahya K., Castro G.R.,  
García-Alvarado F., Amador U. Structure evolution with Sr content of  
the perovskite-like materials  $\text{La}_{2x}\text{Sr}_x\text{CoTiO}_6$  ( $0 \leq x \leq 0.5$ )  
*Journal of Applied Crystallography* **47**, 745-754 (2014)
- Gruene T., Hahn H.W., Luebben A.V., Meilleur F., Sheldrick G.M.  
Refinement of macromolecular structures against neutron data with  
*SHELXL2013*  
*Journal of Applied Crystallography* **47**, 462-466 (2014)
- Hansen T.C., Kohlmann H. Chemical reactions followed by *in situ*  
neutron powder diffraction  
*Zeitschrift für Anorganische und Allgemeine Chemie* **640**,  
3044-3063 (2014)
- Hervoches C.H., Greaves C. Variable temperature neutron  
diffraction study of crystal structure and transport pathways in oxide  
ion conductors  $\text{Bi}_{12.5}\text{Ln}_{1.5}\text{ReO}_{24.5}$  (Ln = Lu, Er)  
*Solid State Ionics* **254**, 1-5 (2014)
- Huang Z., Auckett J.E., Blanchard P.E.R., Kennedy B.J., Miiller W.,  
Zhou Q., Avdeev M., Johnson M.R., Zbiri M., Garbarino G.,  
Marshall W.G., Gu Q., Ling C.D. Pressure-induced intersite  
Bi-M (M = Ru, Ir) valence transitions in hexagonal perovskites  
*Angewandte Chemie International Edition* **53**, 3414-3417 (2014)
- Hunter S.C., Smith B.A., Hoffmann C.M., Wang X., Chen Y.S.,  
McIntyre G.J., Xue Z.L. Intermolecular interactions in solid-state  
metalloporphyrins and their impacts on crystal and molecular structures  
*Inorganic Chemistry* **53**, 11552-11562 (2014)
- Iles G.N., Devred F., Henry P.F., Reinhart G., Hansen T.C.  
Neutron diffraction studies for realtime leaching of catalytic Ni  
*Journal of Chemical Physics* **141**, 034201-1-034201-7 (2014)
- Jones A.O.F., Leech C.K., McIntyre G.J., Wilson C.C., Thomas L.H.  
Engineering short, strong hydrogen bonds in urea di-carboxylic acid  
complexes  
*CrystEngComm* **16**, 8177-8184 (2014)
- Jordá J.L., Rey F., Sastre G., Valencia S., Palomino M., Corma A.,  
Segura A., Errandonea D., Lacombe R., Manjón F.J., Gomis O.,  
Kleppe A.K., Jephcoat A.P., Amboage M., Rodríguez-Velamazán J.A.  
Synthesis of a novel zeolite through a pressure-induced reconstructive  
phase transition process  
*Angewandte Chemie International Edition* **52**, 10458-10462 (2013)
- Kayser P., Martínez-Lope M.J., Alonso J.A., Retuerto M., Croft M.,  
Ignatov A., Fernández-Díaz M.T. Crystal and magnetic structure of  
 $\text{Sr}_2\text{MlrO}_6$  (M = Ca, Mg) double perovskites – A neutron diffraction  
study  
*European Journal of Inorganic Chemistry* **2014**, 178-185 (2014)
- Kimber S.A.J., Salamat A., Evans S.R., Jeschke H.O., Muthukumar K.,  
Tomić M., Salvat-Pujol F., Valentí R., Kaisheva M.V., Zizak I., Chatterji T.  
Giant pressure-induced volume collapse in the pyrite mineral  $\text{MnS}_2$   
*Proceedings of the National Academy of Sciences* **111**, 5106-5110  
(2014)
- Klicpera M., Javorský P., Čermák P., Rudajevová A., Daniš S.,  
Brunátová T., Císařová I. Crystal structure and its stability in  
 $\text{CeCuAl}_3$  single crystal  
*Intermetallics* **46**, 126-130 (2014)
- Kojda D., Wallacher D., Bedoin S., Hansen T.C., Huber P.,  
Hofmann T. Solid phases of spatially nanoconfined oxygen:  
A neutron scattering study  
*Journal of Chemical Physics* **140**, 024705-1-024705-9 (2014)
- Köpf M., Eckstein N., Pfister D., Grotz C., Krüger I., Greiwe M.,  
Hansen T., Kohlmann H., Nilges T. Access and *in situ* growth  
of phosphorene-precursor black phosphorus  
*Journal of Crystal Growth* **405**, 6-10 (2014)
- Kuo C.Y., Drees Y., Fernández-Díaz M.T., Zhao L., Vasylechko L.,  
Sheptyakov D., Bell A.M.T., Pi T.W., Lin H.J., Wu M.K., Pellegrin E.,  
Valvidares S.M., Li Z.W., Adler P., Todorova A., Küchler R.,  
Steppeke A., Tjeng L.H., Hu Z., Komarek A.C.  
 $k = 0$  Magnetic structure and absence of ferroelectricity in  $\text{SmFeO}_3$   
*Physical Review Letters* **113**, 217203-1-217203-5 (2014)
- Lanfredi S., Darie C., Bellucci F.S., Nobre M.A.L., Colin C.V.  
Phase transitions and interface phenomena in the cryogenic  
temperature domain of a niobate nanostructured ceramic  
*Dalton Transactions* **43**, 10983-10998 (2014)

## PUBLICATIONS

- Larrégola S.A., Alonso J.A., de la Peña-O'Shea V.A., Sheptyakov D., Pomjakushin V., Fernández-Díaz M.T., Pedregosa J.C. Localisation and impact of Pb-non-bonded electronic pair on the crystal and electronic structure of  $\text{Pb}_2\text{YSbO}_6$   
Inorganic Chemistry **53**, 5609-5618 (2014)
- López C.A., Saleta M.E., Pedregosa J.C., Sánchez R.D., Alonso J.A., Fernández-Díaz M.T. Coexistence of localised and itinerant electrons in the double-perovskite  $\text{Ba}_2\text{Fe}_{2/3}\text{Mo}_{4/3}\text{O}_6$   
European Journal of Inorganic Chemistry **2014**, 3555-3563 (2014)
- Martínez-Coronado R., Alonso J.A., Aguadero A., Fernández-Díaz M.T. New  $\text{SrMo}_{1-x}\text{Cr}_x\text{O}_{3-\delta}$  perovskites as anodes in solid-oxide fuel cells  
International Journal of Hydrogen Energy **39**, 4067-4073 (2014)
- Martínez-Coronado R., Alonso J.A., Fernández-Díaz M.T. Low-temperature transitions in the  $\text{SrMo}_{1-x}\text{Cr}_x\text{O}_{3-\delta}$  ( $x = 0.1$  and  $0.2$ ) perovskite system  
Journal of Alloys and Compounds **607**, 280-284 (2014)
- Martínez-Coronado R., Alonso J.A., Fernández-Díaz M.T.  $\text{SrMo}_{0.9}\text{Co}_{0.1}\text{O}_{3-\delta}$ : A potential anode for intermediate-temperature solid-oxide fuel cells (IT-SOFC)  
Journal of Power Sources **258**, 76-82 (2014)
- Martínez-Coronado R., Singh P., Alonso-Alonso J., Goodenough J.B. Structural investigation of the oxide-ion electrolyte with  $\text{SrMO}_3$  ( $M = \text{Si/Ge}$ ) structure  
Journal of Materials Chemistry A **2**, 4355-4360 (2014)
- Maupoey Z., Azcondo M.T., Pérez-Flores J.C., Ritter C., Boulahya K., Amador U., García-Alvarado F. A-site sub-stoichiometry and oxygen vacancies as the origin of the electrical properties of  $\text{Sr}_{2-y}\text{LuNb}_{1-x}\text{Ti}_x\text{O}_{6-\delta}$  perovskite-like materials  
Dalton Transactions **43**, 14099-14108 (2014)
- Mossou E., Teixeira S.C.M., Mitchell E.P., Mason S.A., Adler-Abramovich L., Gazit E., Forsyth V.T. The self-assembling zwitterionic form of L-phenylalanine at neutral pH  
Acta Crystallographica C **70**, 326-331 (2014)
- Murshed M.M., Mendive C.B., Curti M., Nénert G., Kalita P.E., Lipinska K., Cornelius A.L., Huq A., Gesing T.M. Anisotropic lattice thermal expansion of  $\text{PbFeBO}_4$ : A study by X-ray and neutron diffraction, Raman spectroscopy and DFT calculations  
Materials Research Bulletin **59**, 170-178 (2014)
- Müller A., Pütz Y., Oberhoffer R., Becker N., Strey R., Wiedenmann A., Sottmann T. Kinetics of pressure induced structural changes in super- or near-critical  $\text{CO}_2$ -microemulsions  
Physical Chemistry Chemical Physics **16**, 18092-18097 (2014)
- Neuhaus J., Leitner M., Nicolaus K., Petry W., Hennion B., Hiess A. Role of vibrational entropy in the stabilisation of the high-temperature phases of iron  
Physical Review B **89**, 184302-1-184302-6 (2014)
- Oró-Solé J., Clark L., Kumar N., Bonin W., Sundaresan A., Atfield J.P., Rao C.N.R., Fuertes A. Synthesis, anion order and magnetic properties of  $\text{RVO}_{3-x}\text{N}_x$  perovskites ( $R = \text{La, Pr, Nd}$ ;  $0 \leq x \leq 1$ )  
Journal of Materials Chemistry C **2**, 2212-2220 (2014)
- Padilla-Pantoja J., Herrero-Martín J., Gargiani P., Valvidares S.M., Cuartero V., Kummer K., Watson O., Brookes N.B., García-Muñoz J.L. Stability of the cationic oxidation states in  $\text{Pr}_{0.50}\text{Sr}_{0.50}\text{CoO}_3$  across the magnetostructural transition by X-ray absorption spectroscopy  
Inorganic Chemistry **53**, 8854-8858 (2014)
- Pasán J., Sanchiz J., Fabelo O., Cañadillas-Delgado L., Déniz M., Díaz-Gallifa P., Martínez-Benito C., Lloret F., Julve M., Ruiz-Pérez C. Influence of the coligand in the magnetic properties of a series of copper(III)-phenylmalonate complexes  
CrystEngComm **16**, 8106-8118 (2014)
- Patino M.A., Smith T., Zhang W., Halasyamani P.S., Hayward M.A. Cation exchange in a 3D perovskite-synthesis of  $\text{Ni}_{0.5}\text{TaO}_3$   
Inorganic Chemistry **53**, 8020-8024 (2014)
- Pedersen M.C., Arleth L., Mortensen K. *WillItFit*: A framework for fitting of constrained models to small-angle scattering data  
Journal of Applied Crystallography **46**, 1894-1898 (2013)
- Pérez-Flores J.C., Gómez-Pérez A., Yuste M., Canales-Vázquez J., Climent-Pascual E., Ritter C., Azcondo M.T., Amador U., García-Alvarado F. Characterisation of  $\text{La}_{2-x}\text{Sr}_x\text{CoTiO}_6$  ( $0.6 \leq x \leq 1.0$ ) series as new cathodes of solid oxide fuel cells  
International Journal of Hydrogen Energy **39**, 5440-5450 (2014)
- Popuri S.R., Scott A.J.M., Downie R.A., Hall M.A., Suard E., Decourt R., Pollet M., Bos J.W.G. Glass-like thermal conductivity in  $\text{SrTiO}_3$  thermoelectrics induced by A-site vacancies  
RSC Advances **4**, 33720-33723 (2014)
- Rodríguez-Velamazán J.A., Cañadillas-Delgado L., Castro M., McIntyre G.J., Real J.A. Temperature- and pressure-dependent structural study of  $\{\text{Fe}(\text{pmd})_2[\text{Ag}(\text{CN})_2]_n\}$  spin-crossover compound by neutron Laue diffraction  
Acta Crystallographica B **70**, 436-443 (2014)
- Romoli F., Mossou E., Cuypers M., Van der Linden P., Carpentier P., Mason S.A., Forsyth V.T., McSweeney S. SPINE-compatible 'carboloops': A new microshaped vitreous carbon sample mount for X-ray and neutron crystallography  
Acta Crystallographica F **70**, 681-684 (2014)



Sánchez-Alarcos V., Recarte V., Pérez-Landazábal J.I., Cesari E., Rodríguez-Velamazán J.A. Long-range atomic order and entropy change at the martensitic transformation in a Ni-Mn-In-Co metamagnetic shape memory alloy  
Entropy **16**, 2756-2767 (2014)

Schmidtman M., Coster P., Henry P.F., Ting V.P., Weller M.T., Wilson C.C. Determining hydrogen positions in crystal engineered organic molecular complexes by joint neutron powder and single-crystal X-ray diffraction  
CrystEngComm **16**, 1232-1236 (2014)

Singh S., Petricek V., Rajput P., Hill A.H., Suard E., Barman S.R., Pandey D. High-resolution synchrotron X-ray powder diffraction study of the incommensurate modulation in the martensite phase of Ni<sub>2</sub>MnGa: Evidence for nearly 7M modulation and phason broadening  
Physical Review B **90**, 014109-1-014109-9 (2014)

Smart K.A., Grellier M., Coppel Y., Vendier L., Mason S.A., Capelli S.C., Albinati A., Montiel-Palma V., Muñoz-Hernandez M.A., Sabo-Etienne S. Nature of Si-H interactions in a series of ruthenium silazane complexes using multinuclear solid-state NMR and neutron diffraction  
Inorganic Chemistry **53**, 1156-1165 (2014)

Solano E., Frontera C., Puig T., Obradors X., Ricart S., Ros J. Neutron and X-ray diffraction study of ferrite nanocrystals obtained by microwave-assisted growth. A structural comparison with the thermal synthetic route  
Journal of Applied Crystallography **47**, 414-420 (2014)

Tamimi M.A., McIntosh S. High temperature *in situ* neutron powder diffraction of oxides  
Journal of Materials Chemistry A **2**, 6015-6026 (2014)

Tang W.S., Chotard J.N., Raybaud P., Janot R. Enthalpy-entropy compensation effect in hydrogen storage materials: Striking example of alkali silanides MSiH<sub>3</sub> (M = K, Rb, Cs)  
Journal of Physical Chemistry C **118**, 3409-3419 (2014)

Tao L., Rouse G., Chotard J.N., Dupont L., Bruyère S., Hanžel D., Mali G., Dominko R., Levasseur S., Masquelier C. Preparation, structure and electrochemistry of LiFeBO<sub>3</sub>: A cathode material for Li-ion batteries  
Journal of Materials Chemistry A **2**, 2060-2070 (2014)

Thomson R.I., Chatterji T., Carpenter M.A. CoF<sub>2</sub>: A model system for magnetoelastic coupling and elastic softening mechanisms associated with paramagnetic ↔ antiferromagnetic phase transitions  
Journal of Physics: Condensed Matter **26**, 146001-1-146001-13 (2014)

Tidey J.P., Wong H.L.S., Schröder M., Blake A.J. Structural chemistry of metal coordination complexes at high pressure  
Coordination Chemistry Reviews **277-278**, 187-207 (2014)

Vecchini C., Bombardi A., Chapon L.C., Beutier G., Radaelli P.G., Park S., Cheong S.W. Magnetically induced femtoscale strain modulations in HoMn<sub>2</sub>O<sub>5</sub>  
Physical Review B **89**, 125114-1-125114-7 (2014)

Wdowik U.D., Parlinski K., Rols S., Chatterji T. Soft-phonon mediated structural phase transition in GeTe  
Physical Review B **89**, 224306-1-224306-7 (2014)

Widenmeyer M., Hansen T.C., Meissner E., Niewa R. Formation and decomposition of iron nitrides observed by *in situ* powder neutron diffraction and thermal analysis  
Zeitschrift für Anorganische und Allgemeine Chemie **640**, 1265-1274 (2014)

Widenmeyer M., Hansen T.C., Niewa R. Formation and decomposition of metastable α'-Fe<sub>16</sub>N<sub>2</sub> from *in situ* powder neutron diffraction and thermal analysis  
Zeitschrift für Anorganische und Allgemeine Chemie **639**, 2851-2859 (2013)

Williams E.R., Weller M.T. Direct observation of structural changes near and at the charge-ordering temperature of ilvaite using high-flux neutron powder diffraction  
Journal of Materials Chemistry C **2**, 3890-3894 (2014)

Wilson C.C., Henry P.F., Schmidtman M., Ting V.P., Williams E., Weller M.T. Neutron powder diffraction – New opportunities in hydrogen location in molecular and materials structure  
Crystallography Reviews **20**, 162-206 (2014)

Zhao P., Lampronti G.I., Lloyd G.O., Suard E., Redfern S.A.T. Direct visualisation of carbon dioxide adsorption in gate-opening zeolitic imidazolate framework ZIF-7  
Journal of Materials Chemistry A **2**, 620-623 (2014)

---

## Liquids and Glasses

---

Burankova T., Reichert E., Fossog V., Hempelmann R., Embs J.P. The dynamics of cations in pyridinium-based ionic liquids by means of quasielastic and inelastic neutron scattering  
Journal of Molecular Liquids **192**, 199-207 (2014)

Cuello G.J., Cristiglio V., González M.A., Cabrillo C. Structure factor of liquid n-butanol at room temperature  
Journal of Physics: Conference Series **549**, 012015-1-012015-4 (2014)

Efimov V.B., Likhov A.V., Mezhev-Deglin L.P., Dewhurst C., Nesvizhevsky V.V., Kolmakov G.V. Nanocluster magnetic gel in superfluid He-II  
JETP Letters **99**, 32-36 (2014)

## PUBLICATIONS

- Falenty A., Hansen T.C., Kuhs W.F. Formation and properties of ice XVI obtained by emptying a type sII clathrate hydrate  
*Nature* **516**, 231-233 (2014)
- Fathi S., Bouazizi S., Trabelsi S., González M., Bahri M., Nasr S., Bellissent-Funel M.C. Structural investigation of liquid acetic acid by neutron scattering, DFT calculations and molecular dynamics simulations. Complementarity to X-ray scattering results  
*Journal of Molecular Liquids* **196**, 69-76 (2014)
- Holland-Moritz D., Yang F., Gegner J., Hansen T., Ruiz-Martín M.D., Meyer A. Structural aspects of glass-formation in Ni-Nb melts  
*Journal of Applied Physics* **115**, 203509-1-203509-5 (2014)
- Hosokawa S. Anomalous X-ray scattering investigations on metallic glasses  
*Materials Science Forum* **783-786**, 1907-1912 (2014)
- Kanduč M., Schlaich A., Schneck E., Netz R.R. Hydration repulsion between membranes and polar surfaces: Simulation approaches versus continuum theories  
*Advances in Colloid and Interface Science* **208**, 142-152 (2014)
- Kidkhunthod P., Skinner L.B., Barnes A.C., Klysubun W., Fischer H.E. Structure of Ba-Ti-Al-O glasses produced by aerodynamic levitation and laser heating  
*Physical Review B* **90**, 094206-1-094206-15 (2014)
- Narimani R., Yang A.C.C., Tsang E.M.W., Rubatat L., Holdcroft S., Frisken B.J. Controlling water content and proton conductivity through copolymer morphology  
*Macromolecules* **46**, 9676-9687 (2013)
- Ngai K.L., Capaccioli S., Paciaroni A. Nature of the water specific relaxation in hydrated proteins and aqueous mixtures  
*Chemical Physics* **424**, 37-44 (2013)
- Pajzderska A., González M.A., Mielcarek J., Wąsicki J. Water behavior in MCM-41 as a function of pore filling and temperature studied by NMR and molecular dynamics simulations  
*Journal of Physical Chemistry C* **118**, 23701-23710 (2014)
- Plazanet M., Sacchetti F., Petrillo C., Demé B., Bartolini P., Torre R. Water in a polymeric electrolyte membrane: Sorption/desorption and freezing phenomena  
*Journal of Membrane Science* **453**, 419-424 (2014)
- Pluhařová E., Fischer H.E., Mason P.E., Jungwirth P. Hydration of the chloride ion in concentrated aqueous solutions using neutron scattering and molecular dynamics  
*Molecular Physics* **112**, 1230-1240 (2014)
- Sanz A., Nogales A., Puente-Orench I., Jiménez-Ruiz M., Ezquerro T.A. Changes in mobility of plastic crystal ethanol during its transformation into the monoclinic crystal state  
*Journal of Chemical Physics* **140**, 054510-1-054510-6 (2014)
- Sillrén P., Matic A., Karlsson M., Koza M., Maccarini M., Fouquet P., Götz M., Bauer T., Gulich R., Lunkenheimer P., Loidl A., Mattsson J., Gainaru C., Vynokur E., Schildmann S., Bauer S., Bohmer R. Liquid 1-propanol studied by neutron scattering, near-infrared, and dielectric spectroscopy  
*Journal of Chemical Physics* **140**, 124501-1-124501-10 (2014)
- Silva-Santisteban A., Henao A., Pothoczki S., Bermejo F.J., Tamarit J.L., Guardia E., Cuello G.J., Pardo L.C. Short range order of  $\text{CCl}_4$ : RMC and MD Methods  
*Journal of Physics: Conference Series* **549**, 012014-1-012014-4 (2014)
- Wezka K., Bouzid A., Pizzey K.J., Salmon P.S., Zeidler A., Klotz S., Fischer H.E., Bull C.L., Tucker M.G., Boero M., Le Roux S., Tugène C., Massobrio C. Density-driven defect-mediated network collapse of  $\text{GeSe}_2$  glass  
*Physical Review B* **90**, 054206-1-054206-9 (2014)
- Wright A.C. Crystalline-like ordering in melt-quenched network glasses?  
*Journal of Non-Crystalline Solids* **401**, 4-26 (2014)
- Wright A.C., Clarke S.J., Howard C.K., Bingham P.A., Forder S.D., Holland D., Martlew D., Fischer H.E. The environment of  $\text{Fe}^{2+}/\text{Fe}^{3+}$  cations in a soda-lime-silica glass  
*Physics and Chemistry of Glasses* **55**, 243-252 (2014)
- Wright A.C., Sinclair R.N., Stone C.E., Shaw J.L., Feller S.A., Williams R.B., Fischer H.E., Vedishcheva N.M. A neutron diffraction study of sodium, rubidium and caesium borate glasses  
*Physics and Chemistry of Glasses* **55**, 74-84 (2014)
- Zeidler A., Wezka K., Rowlands R.F., Whittaker D.A.J., Salmon P.S., Polidori A., Drewitt J.W.E., Klotz S., Fischer H.E., Wilding M.C., Bull C.L., Tucker M.G., Wilson M. High-pressure transformation of  $\text{SiO}_2$  glass from a tetrahedral to an octahedral network: A joint approach using neutron diffraction and molecular dynamics  
*Physical Review Letters* **113**, 135501-1-135501-5 (2014)
- Zeidler A., Wezka K., Whittaker D.A.J., Salmon P.S., Baroni A., Klotz S., Fischer H.E., Wilding M.C., Bull C.L., Tucker M.G., Salanne M., Ferlat G., Micoulaut M. Density-driven structural transformations in  $\text{B}_2\text{O}_3$  glass  
*Physical Review B* **90**, 024206-1-024206-12 (2014)

## Magnetic Excitations

Ahuja B.L., Dashora A., Mund H.S., Priolkar K.R., Yusuf S.M., Itou M., Sakurai Y. Temperature-dependent spin magnetisation density in Mn-rich Ni-Mn-Sn shape memory alloy by magnetic Compton scattering  
EPL (Europhysics Letters) **107**, 27005-1-27005-6 (2014)

Bonilla C.M., Herrero-Albillos J., Figueroa A.I., Castán-Guerrero C., Bartolomé J., Calvo-Almazán I., Schmitz D., Weschke E., García L.M., Bartolomé F. Paramagnetism in HoCo<sub>2</sub> and TmCo<sub>2</sub>  
Journal of Physics: Condensed Matter **26**, 156001-1-156001-14 (2014)

Brok E., Sales M., Lefmann K., Kuhn L.T., Schmidt W.F., Roessli B., Robinson P., McEnroe S.A., Harrison R.J. Experimental evidence for lamellar magnetism in hemo-ilmenite by polarized neutron-scattering  
Physical Review B **89**, 054430-1-054430-7 (2014)

Chaix L., de Brion S., Petit S., Ballou R., Regnault L.P., Ollivier J., Brubach J.B., Roy P., Debray J., Lejay P., Cano A., Ressouche E., Simonet V. Magneto- to electroactive transmutation of spin waves in ErMnO<sub>3</sub>  
Physical Review Letters **112**, 137201-1-137201-5 (2014)

Chatterji T., Holderer O., Schneider H. Direct evidence for nuclear spin waves in Nd<sub>2</sub>CuO<sub>4</sub> by high-resolution neutron-spin-echo spectroscopy  
Journal of Physics: Condensed Matter **25**, 476002-1-476002-5 (2013)

Del Bianco L., Spizzo F., Deriu A., Orecchini A. Inelastic neutron scattering investigation of ball-milled FeSiB described as a magnetic nanoglass-like structure  
Journal of Alloys and Compounds **615**, S224-S227 (2014)

Disch S., Hermann R.P., Wetterskog E., Podlesnyak A.A., An K., Hyeon T., Salazar-Alvarez G., Bergström L., Brückel T. Spin excitations in cubic maghemite nanoparticles studied by time-of-flight neutron spectroscopy  
Physical Review B **89**, 064402-1-064402-7 (2014)

Erni R., Abakumov A.M., Rossell M.D., Batuk D., Tsirlin A.A., Néner G., Van Tendeloo G. Nanoscale phase separation in perovskites revisited  
Nature Materials **13**, 216-217 (2014)

Fåk B., Adroja D.T., Enderle M., Böhm M., Lapertot G., Mineev V.P. Anomalous spin response in the non-centrosymmetric metal CePt<sub>3</sub>Si  
Journal of the Physical Society of Japan **83**, 063703-1-063703-4 (2014)

Fennell T., Kenzelmann M., Roessli B., Mutka H., Ollivier J., Ruminy M., Stuhr U., Zaharko O., Bovo L., Cervellino A., Haas M.K., Cava R.J. Magnetoelastic excitations in the pyrochlore spin liquid Tb<sub>2</sub>Ti<sub>2</sub>O<sub>7</sub>  
Physical Review Letters **112**, 017203-1-017203-5 (2014)

Garlatti E., Albring M.A., Baker M.L., Docherty R.J., Mutka H., Guidi T., García Sakai V., Whitehead G.F.S., Pritchard R.G., Timco G.A., Tuna F., Amoretti G., Carretta S., Santini P., Lorusso G., Affronte M., McInnes E.J.L., Collison D., Winpenny R.E.P. A detailed study of the magnetism of chiral {Cr<sub>2</sub>M} rings: An investigation into parametrisation and transferability of parameters  
Journal of the American Chemical Society **136**, 9763-9772 (2014)

Guigue M., Pignol G., Golub R., Petukhov A.K. Universality of spin relaxation for spin-1/2 particles diffusing over magnetic-field inhomogeneities in the adiabatic regime  
Physical Review A **90**, 013407-1-013407-6 (2014)

Henry S., Pipe M., Cottle A., Clarke C., Divakar U., Lynch A. Characterisation of superconducting capillaries for magnetic shielding of twisted-wire pairs in a neutron electric dipole moment experiment  
Nuclear Instruments and Methods in Physics Research A **763**, 155-162 (2014)

Hiess A., Schneidewind A., Stockert O., Fisk Z. Signature of superconductivity in UBe<sub>13</sub> as seen by neutron scattering: Superconducting and magnetic energy scales  
Physical Review B **89**, 235118-1-235118-7 (2014)

Hill A.H., Jacobsen H., Stewart J.R., Jiao F., Jensen N.P., Holm S.L., Mutka H., Seydel T., Harrison A., Lefmann K. Magnetic properties of nano-scale hematite, α-Fe<sub>2</sub>O<sub>3</sub>, studied by time-of-flight inelastic neutron spectroscopy  
Journal of Chemical Physics **140**, 044709-1-044709-8 (2014)

Jang H., Friemel G., Ollivier J., Dukhnenko A.V., Shitsevalova N.Y., Filipov V.B., Keimer B., Inosov D.S. Intense low-energy ferromagnetic fluctuations in the antiferromagnetic heavy-fermion metal CeB<sub>6</sub>  
Nature Materials **13**, 682-687 (2014)

Jones S.P.P., Gaw S.M., Doig K.I., Prabhakaran D., Hétyroy Wheeler E.M., Boothroyd A.T., Lloyd-Hughes J. High-temperature electromagnons in the magnetically induced multiferroic cupric oxide driven by intersublattice exchange  
Nature Communications **5**, 3787-1-3787-7 (2014)

Kadlec F., Goian V., Kadlec C., Kempa M., Vaněk P., Taylor J., Rols S., Prokléška J., Orlita M., Kamba S. Possible coupling between magnons and phonons in multiferroic CaMn<sub>7</sub>O<sub>12</sub>  
Physical Review B **90**, 054307-1-054307 (2014)

Kaneko K., Stockert O., Fåk B., Raymond S., Skoulatos M., Takeuchi T., Ōnuki Y. Magnetic-field-enhanced antiferromagnetism in noncentrosymmetric heavy-fermion superconductor CePt<sub>3</sub>Si  
Physical Review B **89**, 241105-1-241105-5 (2014)

## PUBLICATIONS

- Kunkemöller S., Nugroho A.A., Sidis Y., Braden M. Spin-density-wave ordering in  $\text{Ca}_{0.5}\text{Sr}_{1.5}\text{RuO}_4$  studied by neutron scattering  
*Physical Review B* **89**, 045119-1-045119-6 (2014)
- Lancaster T., Giblin S.R., Allodi G., Bordignon S., Mazzani M., De Renzi R., Freeman P.G., Baker P.J., Pratt F.L., Babkevich P., Blundell S.J., Boothroyd A.T., Möller J.S., Prabhakaran D. Stripe disorder and dynamics in the hole-doped antiferromagnetic insulator  $\text{La}_{5/3}\text{Sr}_{1/3}\text{CoCO}_4$   
*Physical Review B* **89**, 020405-1-020405-6 (2014)
- Merchant P., Normand B., Krämer K.W., Boehm M., McMorrow D.F., Rüegg C. Quantum and classical criticality in a dimerised quantum antiferromagnet  
*Nature Physics* **10**, 373-379 (2014)
- Mirebeau I., Petit S. Magnetic frustration probed by inelastic neutron scattering: Recent examples  
*Journal of Magnetism and Magnetic Materials* **350**, 209-216 (2014)
- Mukhopadhyay S., Gutmann M.J., Jura M., Jochym D.B., Jiménez-Ruiz M., Sturmiolo S., Refson K., Fernandez-Alonso F. Ferroelectric behaviour in solid croconic acid using neutron scattering and first-principles density functional theory  
*Chemical Physics* **427**, 95-100 (2013)
- Pedersen K.S., Sigrist M., Sørensen M.A., Barra A.L., Weyhermüller T., Piligkos S., Thuesen C.A., Vinum M.G., Mutka H., Weihe H., Clérac R., Bendix J.  $[\text{ReF}_6]^{2-}$ : A robust module for the design of molecule-based magnetic materials  
*Angewandte Chemie* **126**, 1375-1378 (2014)
- Pedersen K.S., Sigrist M., Sørensen M.A., Barra A.L., Weyhermüller T., Piligkos S., Thuesen C.A., Vinum M.G., Mutka H., Weihe H., Clérac R., Bendix J.  $[\text{ReF}_6]^{2-}$ : A robust module for the design of molecule-based magnetic materials  
*Angewandte Chemie International Edition* **53**, 1351-1354 (2014)
- Pedersen K.S., Sigrist M., Weihe H., Bond A.D., Thuesen C.A., Simonsen K.P., Birk T., Mutka H., Barra A.L., Bendix J. Magnetic interactions through fluoride: Magnetic and spectroscopic characterisation of discrete, linearly bridged  $[\text{Mn}^{\text{III}}_2(\mu\text{-F})_4(\text{Me}_3\text{tacn})_2](\text{PF}_6)$   
*Inorganic Chemistry* **53**, 5013-5019 (2014)
- Pedersen K.S., Ungur L., Sigrist M., Sundt A., Schau-Magnussen M., Vieru V., Mutka H., Rols S., Weihe H., Waldmann O., Chibotaru L.F., Bendix J., Dreiser J. Modifying the properties of 4f single-ion magnets by peripheral ligand functionalisation  
*Chemical Science* **5**, 1650-1660 (2014)
- Petit S., Robert J., Guitteny S., Bonville P., Decorse C., Ollivier J., Mutka H., Gingras M.J.P., Mirebeau I. Order by disorder or energetic selection of the ground state in the XY pyrochlore antiferromagnet  $\text{Er}_2\text{Ti}_2\text{O}_7$ : An inelastic neutron-scattering study  
*Physical Review B* **90**, 060410-1-060410-5 (2014)
- Prytuliak A., Godlewska E., Mars K., Berthebaud D. Synchrotron study of Ag-doped  $\text{Mg}_2\text{Si}$ : Correlation between properties and structure  
*Journal of Electronic Materials* **43**, 3746-3752 (2014)
- Qureshi N., Lee C.H., Kihou K., Schmalzl K., Steffens P., Braden M. Anisotropy of incommensurate magnetic excitations in slightly overdoped  $\text{Ba}_{0.5}\text{K}_{0.5}\text{Fe}_2\text{As}_2$  probed by polarised inelastic neutron-scattering experiments  
*Physical Review B* **90**, 100502-1-100502-5 (2014)
- Qureshi N., Steffens P., Lamago D., Sidis Y., Sobolev O., Ewings R.A., Harnagea L., Wurmehl S., Büchner B., Braden M. Fine structure of the incommensurate antiferromagnetic fluctuations in single-crystalline  $\text{LiFeAs}$  studied by inelastic neutron-scattering  
*Physical Review B* **90**, 144503-1-144503-8 (2014)
- Saerbeck T. Magnetic exchange phenomena probed by neutron scattering  
*Solid State Physics* **65**, 237-352 (2014)
- Toulouse C., Liu J., Gallais Y., Measson M.A., Sacuto A., Cazayous M., Chaix L., Simonet V., de Brion S., Pinsard-Godart L., Willaert F., Brubach J.B., Roy P., Petit S. Lattice and spin excitations in multiferroic  $h\text{-YMnO}_3$   
*Physical Review B* **89**, 094415-1-094415-8 (2014)
- Uribe-Laverde M.A., Satapathy D.K., Marozau I., Malik V.K., Das S., Sen K., Stahn J., Rühm A., Kim J.H., Keller T., Devishvili A., Toperverg B.P., Bernhard C. Depth profile of the ferromagnetic order in a  $\text{YBa}_2\text{Cu}_3\text{O}_7/\text{La}_{2/3}\text{Ca}_{1/3}$  superlattice on a LSAT substrate: A polarised neutron reflectometry study  
*Physical Review B* **87**, 115105-1-115105-11 (2013)
- Wang C., Zhang R., Wang F., Luo H., Regnault L.P., Dai P., Li Y. Longitudinal spin excitations and magnetic anisotropy in antiferromagnetically ordered  $\text{BaFe}_2\text{As}_2$   
*Physical Review X* **3**, 041036-1-041036-6 (2013)
- Zhang C., Song Y., Regnault L.P., Su Y., Enderle M., Kulda J., Tan G., Sims Z.C., Egami T., Si Q., Dai P. Anisotropic neutron spin resonance in underdoped superconducting  $\text{NaFe}_{1-x}\text{Co}_x\text{As}$   
*Physical Review B* **90**, 140502-1-140502-5 (2014)



## Magnetic Structures

- Álvarez-Alonso P., Gorria P., Cuello G., Orench I., Sánchez Llamazares J.L., Franco V., Reiffers M., Blanco J.A. Optimising the Curie temperature of pseudo-binary  $R_xR'_{2-x}Fe_{17}$  ( $R, R' =$  rare earth) for magnetic refrigeration *Journal of Physics: Conference Series* **549**, 012019-1-012019-7 (2014)
- Álvarez-Alonso P., Sánchez Llamazares J.L., Sánchez-Valdés C.F., Cuello G.J., Franco V., Gorria P., Blanco J.A. On the broadening of the magnetic entropy change due to Curie temperature distribution *Journal of Applied Physics* **115**, 17A929-1-17A929-3 (2014)
- Barthem V.M.T.S., Colin C.V., Mayaffre H., Julien M.H., Givord D. Revealing the properties of  $Mn_2Au$  for antiferromagnetic spintronics *Nature Communications* **4**, 2892-1-2892-7 (2013)
- Batuk M., Batuk D., Tsirlin A.A., Rozova M.G., Antipov E.V., Hadermann J., Van Tendeloo G. Homologous series of layered perovskites  $A_{n+1}BnO_{3n+1}Cl$ : Crystal and magnetic structure of a new oxychloride  $Pb_4BiFe_4O_{11}Cl$  *Inorganic Chemistry* **52**, 2208-2218 (2013)
- Baum M., Leist J., Finger T., Schmalzl K., Hiess A., Regnault L.P., Becker P., Bohaty L., Eckold G., Braden M. Kinetics of the multiferroic switching in  $MnWO_4$  *Physical Review B* **89**, 144406-1-144406-10 (2014)
- Belener K.L.A., Kohlmann H. Reaction pathways of oxide-reduction-diffusion (ORD) synthesis of  $SmCo_5$  and *in situ* study of its hydrogen induced amorphisation (HIA) *Journal of Magnetism and Magnetic Materials* **370**, 134-139 (2014)
- Bhattacharyya A., Khalyavin D.D., Adroja D.T., Strydom A.M., Hillier A.D., Manuel P., Takabatake T., Taylor J.W., Ritter C. Anomalous change of the magnetic moment direction by hole doping in  $CeRu_2Al_{10}$  *Physical Review B* **90**, 174412-1-174412-9 (2014)
- Blasco J., García J., Subías G., Stankiewicz J., Lafuerza S., Rodríguez-Velamazán J.A., Ritter C., García-Muñoz J.L. Effects of A-site disorder in the properties of  $A_2CoMnO_6$  ( $A = La, Tb$ ) *Journal of Physics: Condensed Matter* **26**, 386001-1-386001-11 (2014)
- Brand J., Stunault A., Wurmehl S., Harnagea L., Büchner B., Meven M., Braden M. Spin susceptibility in superconducting  $LiFeAs$  studied by polarised neutron diffraction *Physical Review B* **89**, 045141-1-045141-5 (2014)
- Cameron A.S., White J.S., Holmes A.T., Blackburn E., Forgan E.M., Riyat R., Loew T., Dewhurst C.D., Erb A. High magnetic field studies of the vortex lattice structure in  $YBa_2Cu_3O_7$  *Physical Review B* **90**, 054502-1-054502-7 (2014)
- Carlsson S.J.E., Santos-Cottin D., Lepoittevin C., Strobel P., Nassif V., Suard E., Toulemonde P. Interplay of disorder and antiferromagnetism in  $TlFe_{1.6+\delta}(Se_{1-x}S_x)_2$  probed by neutron scattering *Journal of Physics: Condensed Matter* **26**, 275701-1-275701-10 (2014)
- Cermák P., Javorský P., Kratochvilová M., Pajskr K., Klicpera M., Ouladdiaf B., Lemée-Cailleau M.H., Rodríguez-Carvajal J., Boehm M. Magnetic structures of non-cerium analogues of heavy-fermion  $Ce_2RhIn_8$ : The case of  $Nd_2RhIn_8$ ,  $Dy_2RhIn_8$ , and  $Er_2RhIn_8$  *Physical Review B* **89**, 184409-1-184409-9 (2014)
- Chatterji T., Brown P.J. Field dependence of the magnetic structure of  $TbMn_2O_5$  *Journal of Applied Physics* **116**, 203904-1-203904-6 (2014)
- Chatterji T., Hansen T.C., Kimber S.A.J., Bhattacharya D. Magnetoelastic effects in multiferroic  $HoMnO_3$  *Solid State Communications* **180**, 46-51 (2014)
- Chen W.T., Mizumaki M., Seki H., Senn M.S., Saito T., Kan D., Atfield J.P., Shimakawa Y. A half-metallic A- and B-site-ordered quadruple perovskite oxide  $CaCu_3Fe_2Re_2O_{12}$  with large magnetization and a high transition temperature *Nature Communications* **5**, 3909-1-3909-7 (2014)
- Coomer F.C., Cussen E.J. Structural and magnetic study of order-disorder behavior in the double perovskites  $Ba_2Nd_{1-x}Mn_xMoO_6$  *Inorganic Chemistry* **53**, 746-755 (2014)
- Craco L., Laad M.S., Leoni S. Orbital-selective Mottness in layered iron oxychalcogenides: The case of  $Na_2Fe_2OSe_2$  *Journal of Physics: Condensed Matter* **26**, 145602-1-145602-8 (2014)
- Deutsch M., Makarova O.L., Hansen T.C., Fernandez-Diaz M.T., Sidorov V.A., Tsvyashchenko A.V., Fomicheva L.N., Porcher F., Petit S., Koepfner K., Röbber U.K., Mirebeau I. Two-step pressure-induced collapse of magnetic order in the  $MnGe$  chiral magnet *Physical Review B* **89**, 180407-1-180407-5 (2014)
- Diop L.V.B., Arnold Z., Isnard O., Kamarád J. Magnetic properties of  $LaCo_{12}B_6$  compound as probed by neutron diffraction and by magnetisation study under high pressures *Journal of Alloys and Compounds* **593**, 163-168 (2014)

## PUBLICATIONS

- Díaz-Gallifa P., Fabelo O., Pasán J., Cañadillas-Delgado L., Rodríguez-Carvajal J., Lloret F., Julve M., Ruiz-Pérez C. Synthesis, crystal structure, and magnetic characterisation of the three-dimensional compound  $[\text{Co}_2(\text{cbut})(\text{H}_2\text{O})_3]_n$  ( $\text{H}_4\text{cbut} = 1,2,3,4\text{-cyclobutanetetracarboxylic acid}$ ) *Inorganic Chemistry* **53**, 5674-5683 (2014)
- Dyadkin V., Prša K., Grigoriev S.V., White J.S., Huang P., Rønnow H.M., Magrez A., Dewhurst C.D., Chernyshov D. Chirality of structure and magnetism in the magnetoelectric compound  $\text{Cu}_2\text{OSeO}_3$  *Physical Review B* **89**, 140409-1-140409-5 (2014)
- ElMassalami M., Takeya H., Ouladdiaf B., Gomes A.M., Paiva T., Dos Santos R.R. Evolution of magnetic layers stacking sequence within the magnetic structure of  $\text{Ho}(\text{Co}_x\text{Ni}_{1-x})_2\text{B}_2\text{C}$  *Journal of Magnetism and Magnetic Materials* **372**, 74-78 (2014)
- Enderle M. Neutrons and magnetism *Collection SFN* **13**, 01002-1-01002-23 (2014)
- Garces D., Setevich C.F., Caneiro A., Cuello G.J., Mogni L. Effect of cationic order-disorder on the transport properties of  $\text{LaBaCo}_2\text{O}_{6-\delta}$  and  $\text{La}_{0.5}\text{Ba}_{0.5}\text{CoO}_{3-\delta}$  perovskites *Journal of Applied Crystallography* **47**, 325-334 (2014)
- Gerber S., Bartkowiak M., Gavilano J.L., Ressouche E., Egetenmeyer N., Niedermayer C., Bianchi A.D., Movshovich R., Bauer E.D., Thompson J.D., Kenzelmann M. Switching of magnetic domains reveals spatially inhomogeneous superconductivity *Nature Physics* **10**, 126-129 (2013)
- Ghosh B., Siruguri V., Raychaudhuri A.K., Chatterji T. Effect of size reduction on the structural and magnetic order in  $\text{LaMnO}_{3+\delta}$  ( $\delta \approx 0.03$ ) nanocrystals: A neutron diffraction study *Journal of Physics: Condensed Matter* **26**, 025603-1-025603-9 (2014)
- Gorria P., Fernández-Martínez A., Santos J.D., Pérez M.J., Cuello G.J. Investigating the crystallisation process in a FeCrB metallic glass by combining magnetic and neutron thermo-diffraction experiments *Journal of Physics: Conference Series* **549**, 012018-1-012018-6 (2014)
- Gurusinghe N.N.M., Fones J.C., Marco J.F., Berry F.J., Greaves C. Fluorine insertion into the Ruddlesden-Popper phase  $\text{La}_2\text{BaFe}_2\text{O}_7$ : The structure and magnetic properties of  $\text{La}_2\text{BaFe}_2\text{O}_5\text{F}_4$  *Dalton Transactions* **43**, 2038-2043 (2014)
- Günther A., Bick J.P., Szary P., Honecker D., Dewhurst C.D., Keiderling U., Feoktystov A.V., Tschöpe A., Birringer R., Michels A. Magnetic field dependent small-angle neutron scattering on a Co nanorod array: Evidence for intraparticle spin misalignment *Journal of Applied Crystallography* **47**, 992-998 (2014)
- Lambri O.A., Pérez-Landazábal J.I., Cuello G.J., Gargicevich D., Recarte V., Bonifacich F.G., Giordano E.D., Sánchez Alarcos V. Relation between order degree, damping behaviour and magnetic response in Fe-Si and Fe-Al-Si alloys *Neutron News* **25**, 28-31 (2014)
- Landsgeßel S., Prokës K., Hansen T., Frontzek M. An unexpected gap: Magnetic structures of  $\text{La}_2\text{O}_3(\text{Fe}_{1-x}\text{Mnx})_2\text{Se}_2$  investigated by neutron diffraction and physical property measurements *Acta Materialia* **66**, 232-240 (2014)
- Lefrançois E., Chapon L.C., Simonet V., Lejay P., Khalyavin D., Rayaprol S., Sampathkumaran E.V., Ballou R., Adroja D.T. Magnetic order in the frustrated Ising-like chain compound  $\text{Sr}_3\text{NiIrO}_6$  *Physical Review B* **90**, 014408-1-014408-7 (2014)
- Leithe-Jasper A., Schnelle W., Rosner H., Schweika W., Isnard O. Neutron diffraction and scattering study of the weak ferromagnetism in  $\text{NaFe}_4\text{Sb}_{12}$  skutterudite *Physical Review B* **90**, 144416-1-144416-7 (2014)
- Li H.F., Wildes A., Hou B., Zhang C., Schmitz B., Meuffels P., Roth G., Brückel T. Magnetisation, crystal structure and anisotropic thermal expansion of single-crystal  $\text{SrEr}_2\text{O}_4$  *RSC Advances* **4**, 53602-53607 (2014)
- Li H.F., Zhang A., Senyshyn A., Wildes A., Schmalzl K., Schmidt W., Boehm M., Ressouche E., Hou B.Y., Meuffels P., Roth G., Brückel T. Incommensurate antiferromagnetic order in the manifoldly-frustrated  $\text{SrTb}_2\text{O}_4$  with transition temperature up to 4.28 K *Frontiers in Physics* **2**, 42-1-42-10 (2014)
- Lu X., Tam D.W., Zhang C., Luo H., Wang M., Zhang R., Harriger L.W., Keller T., Keimer B., Regnault L.P., Maier T.A., Dai P. Short-range cluster spin glass near optimal superconductivity in  $\text{BaFe}_{2-x}\text{Ni}_x\text{As}_2$  *Physical Review B* **90**, 024509-1-024509-6 (2014)
- Maruyama S., Anbusathaiah V., Fennell A., Enderle M., Takeuchi I., Ratcliff W.D. Change in the magnetic structure of  $(\text{Bi},\text{Sm})\text{FeO}_3$  thin films at the morphotropic phase boundary probed by neutron diffraction *APL Materials* **2**, 116106-1-116106-7 (2014)
- McCabe E.E., Wills A.S., Chapon L., Manuel P., Evans J.S.O. Structural and magnetic characterisation of iron oxyselenides  $\text{Ce}_2\text{O}_2\text{Fe}_2\text{OSe}_2$  and  $\text{Nd}_2\text{O}_2\text{Fe}_2\text{OSe}_2$  *Physical Review B* **90**, 165111-1-165111-7 (2014)
- Mesbah A., Rabu P., Sibille R., Lebègue S., Mazet T., Malaman B., François M. From hydrated  $\text{Ni}_3(\text{OH})_2(\text{C}_8\text{H}_4\text{O}_4)_2(\text{H}_2\text{O})_4$  to anhydrous  $\text{Ni}_2(\text{OH})_2(\text{C}_8\text{H}_4\text{O}_4)$ : Impact of structural transformations on magnetic properties *Inorganic Chemistry* **53**, 872-881 (2014)

- Morisaki-Ishii R., Kawano-Furukawa H., Cameron A.S., Lemberger L., Blackburn E., Holmes A.T., Forgan E.M., DeBeer-Schmitt L.M., Littrell K., Nakajima M., Kihou K., Lee C.H., Iyo A., Eisaki H., Uchida S., White J.S., Dewhurst C.D., Gavalano J.L., Zolliker M. Vortex lattice structure in  $\text{BaFe}_2(\text{As}_{0.67}\text{P}_{0.33})_2$  via small-angle neutron scattering *Physical Review B* **90**, 125116-1-125116-9 (2014)
- Morozkin A.V., Yuan F., Mozharivskiy Y., Isnard O. Magnetic order of  $\text{YNi}_4\text{Si}$ -type  $\text{TbNi}_4\text{Si}$  *Journal of Magnetism and Magnetic Materials* **368**, 121-125 (2014)
- Nair H.S., Pradheesh R., Xiao Y., Cherian D., Elizabeth S., Hansen T.C., Chatterji T., Brückel T. Magnetisation-steps in  $\text{Y}_2\text{CoMnO}_6$  double perovskite: The role of antisite disorder *Journal of Applied Physics* **116**, 123907-1-123907-7 (2014)
- Nandi S., Jin W.T., Xiao Y., Su Y., Price S., Schmidt W., Schmalzl K., Chatterji T., Jeevan H.S., Gegenwart P., Brückel T. Magnetic structure of the  $\text{Eu}^{2+}$  moments in superconducting  $\text{EuFe}_2(\text{As}_{1-x}\text{P}_x)_2$  with  $x = 0.19$  *Physical Review B* **90**, 094407-1-094407-8 (2014)
- Nandi S., Xiao Y., Su Y., Chapon L.C., Chatterji T., Jin W.T., Price S., Wolf T., Brown P.J., Brückel T. Magnetisation distribution and orbital moment in the nonsuperconducting chalcogenide compound  $\text{K}_{0.8}\text{Fe}_{1.6}\text{Se}_2$  *Physical Review B* **88**, 184413-1-184413-7 (2013)
- Nilsen G.J., Okamoto Y., Ishikawa H., Simonet V., Colin C.V., Cano A., Chapon L.C., Hansen T., Mutka H., Hiroi Z. Helical order and multiferroicity in the  $S = \frac{1}{2}$  quasi-kagome system  $\text{KCu}_3\text{As}_2\text{O}_7(\text{OD})_3$  *Physical Review B* **89**, 140412-1-140412-5 (2014)
- Orlandi F., Righi L., Ritter C., Pernechele C., Solzi M., Cabassi R., Bolzoni F., Calestani G. Superspace application on magnetic structure analysis of the  $\text{Pb}_2\text{MnWO}_6$  double perovskite system *Journal of Materials Chemistry C* **2**, 9215-9223 (2014)
- Paddison J.A.M., Agrestini S., Lees M.R., Fleck C.L., Deen P.P., Goodwin A.L., Stewart J.R., Petrenko O.A. Spin correlations in  $\text{Ca}_3\text{Co}_2\text{O}_6$ : Polarised-neutron diffraction and Monte Carlo study *Physical Review B* **90**, 014411-1-014411-10 (2014)
- Padilla-Pantoja J., Barón-González A.J., Bozzo B., Blasco J., Ritter C., Herrero-Martín J., García-Muñoz J.L. Role of Pr cations and the low temperature transition in  $\text{Pr}_{0.50}\text{Sr}_{0.50}\text{CoO}_3$ : A comparison to  $\text{Pr}_{0.50}\text{Ca}_{0.50}\text{CoO}_3$  *Physica B* **455**, 56-59 (2014)
- Padilla-Pantoja J., Herrero-Martín J., Torrelles X., Bozzo B., Blasco J., Ritter C., García-Muñoz J.L. The low temperature magnetostructural transition in  $\text{Pr}_{0.50}\text{Sr}_{0.50}\text{CoO}_3$ : Bulk versus thin film behavior *Journal of Applied Physics* **115**, 17D721-1-17D721-3 (2014)
- Pagliari L., Dapiaggi M., Maglia F., Sarkar T., Raychaudhuri A.K., Chatterji T., Carpenter M.A. Strain heterogeneity and magnetoelastic behaviour of nanocrystalline half-doped La, Ca manganite,  $\text{La}_{0.5}\text{Ca}_{0.5}\text{MnO}_3$  *Journal of Physics: Condensed Matter* **26**, 435303-1-435303-13 (2014)
- Patra M., Majumdar S., Giri S., Xiao Y., Chatterji T. Magnetic, magnetocaloric and magnetoresistive properties of cubic laves phase  $\text{HoAl}_2$  single crystal *Journal of Physics: Condensed Matter* **26**, 046004-1-046004-7 (2014)
- Prokös K., Petříček V., Ressouche E., Hartwig S., Ouladdiaf B., Mydosh J.A., Hoffmann R.D., Huang Y.K., Pöttgen R. (3 + 1)-dimensional crystal and antiferromagnetic structures in  $\text{CeRuSn}$  *Journal of Physics: Condensed Matter* **26**, 122201-1-122201-6 (2014)
- Rayaprol S., Siruguri V., Hoser A., Ritter C., Sampathkumaran E.V. Microscopic evidence for magnetic-phase coexistence in the intermetallic compound  $\text{Nd}_7\text{Rh}_3$  *Physical Review B* **90**, 134417-1-134417-7 (2014)
- Ressouche E. Reminder: Magnetic structures description and determination by neutron diffraction *Collection SFN* **13**, 02001-1-02001-22 (2014)
- Reynaud M., Rodríguez-Carvajal J., Chotard J.N., Tarascon J.M., Rouse G. Magnetic structure and properties of orthorhombic  $\text{Li}_2\text{Ni}(\text{SO}_4)_2$ : A possible magnetoelectric material *Physical Review B* **89**, 104419-1-104419-9 (2014)
- Ritter C., Dhar S.K., Kulkarni R., Provino A., Paudyal D., Manfrinetti P., Gschneidner K.A. Electronically- and crystal-structure-driven magnetic structures and physical properties of  $\text{RScSb}$  (R = rare earth) compounds: A neutron diffraction, magnetisation and heat capacity study *Journal of Physics: Condensed Matter* **26**, 366001-1-366001-13 (2014)
- Rodríguez-Velamazán J.A., Fabelo O., Beavers C.M., Natividad E., Evangelisti M., Roubeau O. A multifunctional magnetic material under pressure *Chemistry: A European Journal* **20**, 7956-7961 (2014)
- Rouse G., Rodríguez-Carvajal J., Wurm C., Masquelier C. Spiral magnetic structure in the iron diarsenate  $\text{LiFeAs}_2\text{O}_7$ : A neutron diffraction study *Physical Review B* **88**, 214433-1-214433-9 (2013)
- Saito T., Toyoda M., Ritter C., Zhang S., Oguchi T., Atfield J.P., Shimakawa Y. Symmetry-breaking  $60^\circ$ -spin order in the A-site-ordered perovskite  $\text{LaMn}_3\text{V}_4\text{O}_{12}$  *Physical Review B* **90**, 214405-1-214405-6 (2014)

## PUBLICATIONS

- Saito T., Yamada R., Ritter C., Senn M.S., Attfield J.P., Shimakawa Y. Control of L-type ferrimagnetism by the Ce/vacancy ordering in the A-site-ordered perovskite  $\text{Ce}_{1/2}\text{Cu}_3\text{Ti}_4\text{O}_{12}$  *Inorganic Chemistry* **53**, 1578-1584 (2014)
- Sazonov A.P., Gukasov A., Cao H.B., Bonville P., Ressouche E., Decorse C., Mirebeau I. Magnetic structure in the spin liquid  $\text{Tb}_2\text{Ti}_2\text{O}_7$  induced by a [111] magnetic field: Search for a magnetization plateau *Physical Review B* **88**, 184428-1-184428-10 (2013)
- Schobinger-Papamantellos P., Buschow K.H.J., Rodríguez-Carvajal J. Double symmetry breaking in  $\text{TmFe}_4\text{Ge}_2$  compared to  $\text{RFe}_4\text{Ge}_2$  (R = Y, Lu, Er, Ho, Dy) magnetic behaviour *Journal of Magnetism and Magnetic Materials* **355**, 104-120 (2014)
- Schobinger-Papamantellos P., Rodríguez-Carvajal J., Buschow K.H.J. Magnetic ordering of  $\text{ScMn}_6\text{Ge}_6$  by neutron diffraction *Journal of Magnetism and Magnetic Materials* **369**, 243-248 (2014)
- Sibille R., Lhotel E., Mazet T., Malaman B., Ritter C., Ban V., François M. Magnetic structure and dynamics of a strongly one-dimensional cobalt<sup>II</sup> metal-organic framework *Physical Review B* **89**, 104413-1-104413-12 (2014)
- Sikolenko V.V., Efimov V.V., Schorr S., Ritter C., Troyanchuk I.O. Neutron diffraction studies of the structure of substituted complex cobalt oxides *Physics of the Solid State* **56**, 77-80 (2014)
- Singh S., Muthu S.E., Senyshyn A., Rajput P., Suard E., Arumugam S., Barman S.R. Inverse magnetocaloric effect in  $\text{Mn}_2\text{NiGa}$  and  $\text{Mn}_{1.75}\text{Ni}_{1.25}\text{Ga}$  magnetic shape memory alloys *Applied Physics Letters* **104**, 051905-1-051905-5 (2014)
- Takatsu H., Néner G., Kadowaki H., Yoshizawa H., Enderle M., Yonezawa S., Maeno Y., Kim J., Tsuji N., Takata M., Zhao Y., Green M., Broholm C. Magnetic structure of the conductive triangular-lattice antiferromagnet  $\text{PdCrO}_2$  *Physical Review B* **89**, 104408-1-104408-12 (2014)
- Tao L., Neilson J.R., Melot B.C., McQueen T.M., Masquelier C., Rouse G. Magnetic structures of  $\text{LiMBO}_3$  (M = Mn, Fe, Co) lithiated transition metal borates *Inorganic Chemistry* **52**, 11966-11974 (2013)
- Tencé S., Isnard O., Wrubl F., Manfrinetti P. A neutron diffraction study of the  $\text{R}_{15}\text{Ge}_9\text{C}$  compounds (R = Ce, Pr, Nd) *Journal of Alloys and Compounds* **594**, 148-152 (2014)
- Tereshina E.A., Isnard O., Smekhova A., Andreev A.V., Rogalev A., Khmelevskiy S. Experimental and theoretical study of magnetic ordering and local atomic polarisation in Ru-substituted  $\text{Lu}_2\text{Fe}_{17}$  *Physical Review B* **89**, 094420-1-094420-10 (2014)
- Thammajak N., Battle P.D., Brown C., Higgon K., Stansfield R. Structural chemistry and magnetic properties of  $\text{Nd}_{18}\text{Li}_8\text{Fe}_4\text{M}'\text{O}_{39}$  (M' = Al, Ga) and  $\text{La}_{18}\text{Li}_8\text{Fe}_{4.5}\text{In}_{0.5}\text{O}_{39}$  *Journal of Solid State Chemistry* **209**, 120-126 (2014)
- Thomson R.I., Chatterji T., Howard C.J., Palstra T.T.M., Carpenter M.A. Elastic anomalies associated with structural and magnetic phase transitions in single crystal hexagonal  $\text{YMnO}_3$  *Journal of Physics: Condensed Matter* **26**, 045901-1-045901-9 (2014)
- Urcelay-Olabarria I., Ressouche E., Mukhin A.A., Ivanov V.Y., Kadomtseva A.M., Popov Y.F., Vorob'ev G.P., Balbashov A.M., García-Muñoz J.L., Skumryev V. X phase of  $\text{MnWO}_4$  *Physical Review B* **90**, 024408-1-024408-5 (2014)
- Vališka M., Pospíšil J., Néner G., Stunault A., Prokeš K., Sechovský V. Magnetism in  $\text{UCo}_{0.88}\text{Ru}_{0.12}\text{Ge}$  studied by polarised neutrons *Acta Physica Polonica A* **126**, 330-331 (2014)
- Vecchini C., Bombardi A., Chapon L.C., Lee N., Radaelli P.G., Cheong S.W. Magnetic phase diagram and ordered ground state of  $\text{GdMn}_2\text{O}_5$  multiferroic studied by X-ray magnetic scattering *Journal of Physics: Conference Series* **519**, 012004-1-012004-9 (2014)
- White J.S., Bowell C.J., Cameron A.S., Heslop R.W., Mesot J., Gavilano J.L., Strässle S., Mächler L., Khasanov R., Dewhurst C.D., Karpinski J., Forgan E.M. Magnetic field dependence of the basal-plane superconducting anisotropy in  $\text{YBa}_2\text{Cu}_3\text{O}_8$  from small-angle neutron-scattering measurements of the vortex lattice *Physical Review B* **89**, 024501-1-024501-7 (2014)
- Zhang Q., Singh K., Simon C., Tung L.D., Balakrishnan G., Hardy V. Impact of the various spin- and orbital-ordering processes on the multiferroic properties of orthovanadate  $\text{DyVO}_3$  *Physical Review B* **90**, 024418-1-024418-9 (2014)



## Materials Science and Engineering

Agostini G., Piovano A., Bertinetti L., Pellegrini R., Leofanti G., Groppo E., Lamberti C. Effect of different face centered cubic nanoparticle distributions on particle size and surface area determination: A theoretical study  
Journal of Physical Chemistry C **118**, 4085-4094 (2014)

Atanasov V., Bürger M., Lyonard S., Porcar L., Kerres J. Sulfonated poly(pentafluorostyrene): Synthesis & characterisation  
Solid State Ionics **252**, 75-83 (2013)

Bahadur J., Prakash J., Sen D., Mazumder S., Sastry P. U., Paul B., Chakravarty J.K., Lemmel H. A facile fabrication of a uniform and homogeneous CNT-TiO<sub>2</sub> composite: A microscopic and scattering investigation  
RSC Advances **4**, 13231-13240 (2014)

Balima F., Le Floch S., San-Miguel A., Lindner P., Brület A., Duclaux L., Pischedda V. Shear effects on expanded graphite under uniaxial pressure: An *in situ* small-angle neutron scattering study  
Carbon **74**, 54-62 (2014)

Bergner F., Ulbricht A., Lindner P., Keiderling U., Malerba L. Post-irradiation annealing behavior of neutron-irradiated FeCu, FeMnNi and FeMnNiCu model alloys investigated by means of small-angle neutron scattering  
Journal of Nuclear Materials **454**, 22-27 (2014)

Bousige C., Rols S., Paineau E., Rouzière S., Mocuta C., Kataura H., Launois P. In situ X-ray diffraction observation of two-step fullerene coalescence in carbon peapods  
Europhysics Letters **103**, 66002-1-66002-6 (2013)

Carradò A., Palkowski H. Interface and in bulk residual stress analysis in biomedical systems by non-destructive techniques  
Surface and Coatings Technology **243**, 10-14 (2014)

Carretero-Genevriero A., Gich M., Picas L., Gazquez J., Drisko G.L., Boissière C., Grosso D., Rodríguez-Carvajal J., Sanchez C. Soft-chemistry-based routes to epitaxial  $\alpha$ -quartz thin films with tunable textures  
Science **340**, 827-831 (2013)

Carretero-Genevriero A., Oro-Sole J., Gazquez J., Magén C., Miranda L., Puig T., Obradors X., Ferain E., Sanchez C., Rodríguez-Carvajal J., Mestres N. Direct monolithic integration of vertical single crystalline octahedral molecular sieve nanowires on silicon  
Chemistry of Materials **26**, 1019-1028 (2014)

Cioffi F., Hidalgo J.I., Fernández R., Pirling T., Fernández B., Gesto D., Puente-Orench I., Rey P., González-Doncel G. Analysis of the unstressed lattice spacing,  $d_0$ , for the determination of the residual stress in a friction stir welded plate of an age-hardenable aluminum alloy – Use of equilibrium conditions and a genetic algorithm  
Acta Materialia **74**, 189-199 (2014)

Das A., Mazumder S., Sen D., Yalmali V., Shah J.G., Ghosh A., Sahu A.K., Wattal P.K. Small-angle neutron scattering as a probe to decide the maximum limit of chemical waste immobilisation in a cement matrix  
Journal of Applied Crystallography **47**, 421-429 (2014)

Drezet J.M., Mireux B., Szaraz Z., Pirling T. Determination of coherency and rigidity temperatures in Al-Cu alloys using *in situ* neutron diffraction during casting  
JOM **66**, 1425-1430 (2014)

Drezet J.M., Mireux B., Szaraz Z., Pirling T. *In situ* neutron diffraction during casting: Determination of rigidity point in grain refined Al-Cu alloys  
Materials **7**, 1165-1172 (2014)

Drezet J.M., Pirling T. Influence of a wiper on residual stresses in AA7050 rolling plate ingots  
Journal of Materials Processing Technology **214**, 1372-1378 (2014)

Epp J., Pirling T., Hirsch T. Non-destructive residual stress analysis of induction hardened components by neutron and X-ray diffraction  
Materials Science Forum **768-769**, 420-427 (2013)

Farbos B., Weisbecker P., Fischer H.E., Da Costa J.P., Lalanne M., Chollon G., Germain C., Vignoles G.L., Leyssale J.M. Nanoscale structure and texture of highly anisotropic pyrocarbons revisited with transmission electron microscopy, image processing, neutron diffraction and atomistic modeling  
Carbon **80**, 472-489 (2014)

Farmahini A.H., Shahtalebi A., Jobic H., Bhatia S.K. Influence of structural heterogeneity on diffusion of CH<sub>4</sub> and CO<sub>2</sub> in silicon carbide-derived nanoporous carbon  
Journal of Physical Chemistry C **118**, 11784-11798 (2014)

Giglio F., Pontiroli D., Gaboardi M., Aramini M., Cavallari C., Brunelli M., Galinetto P., Milanese C., Riccò M. Li<sub>12</sub>C<sub>60</sub>: A lithium clusters intercalated fullerene  
Chemical Physics Letters **609**, 155-160 (2014)

## PUBLICATIONS

- Hubert F., Bihannic I., Prêt D., Tertre E., Nauleau B., Pelletier M., Demé B., Ferrage E. Investigating the anisotropic features of particle orientation in synthetic swelling clay porous media  
*Clays and Clay Minerals* **61**, 397-415 (2013)
- James M.N., Newby M., Doubell P., Hattingh D.G., Serasli K., Smith D.J. Weld residual stresses near the bimetallic interface in clad RPV steel: A comparison between deep-hole drilling and neutron diffraction data  
*Nuclear Engineering and Design* **274**, 56-65 (2014)
- Jazaeri H., Bouchard P.J., Hutchings M., Lindner P. Study of creep cavitation in stainless steel weldment  
*Materials Science and Technology* **30**, 38-42 (2014)
- Kapadia P., Davies C.M., Pirling T., Dean D.W., Nikbin K.M. Neutron diffraction residual stress measurements in electron beam welded compact tension specimens  
*Materials Science Forum* **777**, 99-104 (2014)
- Kitchen H.J., Vallance S.R., Kennedy J.L., Tapia-Ruiz N., Carassiti L., Harrison A., Whittaker A.G., Drysdale T.D., Kingman S.W., Gregory D.H. Modern microwave methods in solid-state inorganic materials chemistry: From fundamentals to manufacturing  
*Chemical Reviews* **114**, 1170-1206 (2014)
- László K., Demé B., Czakkel O., Geissler E. Incompatible liquids in confined conditions  
*Journal of Physical Chemistry C* **118**, 23723-23727 (2014)
- Manzoni A.M., Denquin A., Vermaut P., Puente-Orench I., Prima F., Portier R.A. Shape-memory deformation mechanisms of Ru-Nb and Ru-Ta shape-memory alloys with transformation temperatures  
*Intermetallics* **52**, 57-63 (2014)
- Mitchell E., Beaucour J., Capria E., Klunder R., Lafford T., Royer J.C., Segura-Ruiz J. The ESRF: A Synchrotron in Europe's Silicon Valley  
*Synchrotron Radiation News* **27**, 15-18 (2014)
- Morozkin A.V., Svitlyk V., Mozharivskiy Y., Isnard O. Magnetic order of the  $\text{La}_3\text{NiGe}_2$ -type  $\text{Tb}_3\text{NiSi}_2$   
*Journal of Magnetism and Magnetic Materials* **349**, 201-207 (2014)
- Morozkin A.V., Yao J., Yuan F., Mozharivskiy Y., Isnard O. Magnetic order of the  $\text{La}_3\text{NiGe}_2$ -type  $\text{Ho}_3\text{NiGe}_2$   
*Journal of Magnetism and Magnetic Materials* **360**, 200-204 (2014)
- Palkowski H., Brück S., Pirling T., Carradó A. Investigation on the residual stress state of drawn tubes by numerical simulation and neutron diffraction analysis  
*Materials* **6**, 5118-5130 (2013)
- Patapy C., Gouraud F., Huger M., Guinebretière R., Ouladdiaf B., Chateigner D., Chotard T. Investigation by neutron diffraction of texture induced by the cooling process of zirconia refractories  
*Journal of the European Ceramic Society* **34**, 4043-4052 (2014)
- Poncé S., Antonius G., Boulanger P., Cannuccia E., Marini A., Côté M., Gonze X. Verification of first-principles codes: Comparison of total energies, phonon frequencies, electron-phonon coupling and zero-point motion correction to the gap between ABINIT and QE/Yambo  
*Computational Materials Science* **83**, 341-348 (2014)
- Porcar L., Courtois P., Crouigneau G., Debray J., Bourgault D. Irreversibility of the martensitic transformation in Ni-Mn-In single crystal studied by resistivity under pressure and *in situ* optical observations  
*Applied Physics Letters* **105**, 151907-1-151907-4 (2014)
- Raghuwanshi V.S., Harizanova R., Haas S., Tatchev D., Gugov I., Dewhurst C., Rüssel C., Hoell A. Magnetic nanocrystals embedded in silicate glasses studied by polarised SANS  
*Journal of Non-Crystalline Solids* **385**, 24-29 (2014)
- Reynaud M., Rouse G., Abakumov A.M., Sougrati M.T., Van Tendeloo G., Chotard J.N., Tarascon J.M. Design of new electrode materials for Li-ion and Na-ion batteries from the bloedite mineral  $\text{Na}_2\text{Mg}(\text{SO}_4)_2 \cdot 4\text{H}_2\text{O}$   
*Journal of Materials Chemistry A* **2**, 2671-2680 (2014)
- Rozas F., Bengtsson N., Fabelo O., Puente I., Castellote M. Optimum calcination temperature in the synthesis of a N-C-S co-doped  $\text{TiO}_2$  photocatalyst, as monitored by neutron diffraction  
*Journal of Physics: Conference Series* **549**, 012026-1-012026-5 (2014)
- Senyshyn A., Mühlbauer M.J., Dolotko O., Hofmann M., Pirling T., Ehrenberg H. Spatially resolved *in operando* neutron-scattering studies on Li-ion batteries  
*Journal of Power Sources* **245**, 678-683 (2014)
- Shahtalebi A., Farmahini A.H., Shukla P., Bhatia S.K. Slow diffusion of methane in ultra-micropores of silicon carbide-derived carbon  
*Carbon* **77**, 560-576 (2014)

---

## Nuclear and Particle Physics

---

Tapasztó O., Lemmel H., Markó M., Balázi K., Balázi C., Tapasztó L. The influence of sintering on the dispersion of carbon nanotubes in ceramic matrix composites  
*Chemical Physics Letters* **614**, 148-150 (2014)

Tealdi C., Chiodelli G., Pin S., Malavasi L., Flor G. Ionic conductivity in melilite-type silicates  
*Journal of Materials Chemistry A* **2**, 907-910 (2014)

Terzi S., Daudin R., Villanova J., Srirangam P., Lhuissier P., Salvo L., Boller E., Schweins R., Lindner P., Blandin J.J., Lee P., Lemmel H. X-ray tomography and small-angle neutron scattering characterisation of nano-composites: Static and *in situ* experiments  
In "Light Metals 2014" Grandfield J. Ed. (2014, Wiley) pp. 1389-1393

Zacher D., Nayuk R., Schweins R., Fischer R.A., Huber K. Monitoring the coordination modulator shell at MOF nanocrystals  
*Crystal Growth & Design* **14**, 4859-4863 (2014)

Zalden P., Siegert K.S., Rols S., Fischer H.E., Schlich F., Hu T., Wuttig M. Specific heat of  $(\text{GeTe})_x(\text{Sb}_2\text{Te}_3)_{1-x}$  phase-change materials: The impact of disorder and anharmonicity  
*Chemistry of Materials* **26**, 2307-2312 (2014)

Zanini L., Köster U., David J.C., Tall Y., Andersson M., Berg K., Cormon S., Fallot M., Foucher Y., Fränberg H., Gröschel F., Guertin A., Kirchner T., Leray S., Manfrin E., Noah E., Ravn H., Stora T., Thiollière N., Wohlmuther M. Measurement of volatile radionuclides production and release yields followed by a post-irradiation analysis of a Pb/Bi filled Ta target at ISOLDE  
*Nuclear Data Sheets* **119**, 292-295 (2014)

Zucali M., Fontana E., Panseri M., Tartarotti P., Capelli S., Ouladdiaf B. Submarine lava-flow direction revealed by neutron diffraction analysis in mineral lattice orientation  
*Geochemistry, Geophysics, Geosystems* **15**, 765-780 (2014)

Zucali M., Vho A., Chateigner D., Lutterotti L., Ouladdiaf B. Microstructures and LPO as indicators of strain partition in metamorphic tectonites: The example of the Eclogite Micaschists Complex (Sesia-Lanzo Zone, Austroalpine domain, Western Alps, Italy)  
*Rendiconti Online della Società Geologica Italiana* **29**, 202-205 (2013)

Zucali M., Voltolini M., Ouladdiaf B., Mancini L., Chateigner D. The 3D quantitative lattice and shape preferred orientation of a mylonitised metagranite from Monte Rosa (Western Alps): Combining neutron diffraction texture analysis and synchrotron X-ray microtomography  
*Journal of Structural Geology* **63**, 91-105 (2014)

Afach S., Baker C.A., Ban G., Bison G., Bodek K., Burghoff M., Chowdhuri Z., Daum M., Fertl M., Franke B., Geltenbort P., Green K., Van der Grinten M.G.D., Grujic Z., Harris P.G., Heil W., H elaine V., Henneck R., Horras M., Iaydjiev P., Ivanov S.N., Kasprzak M., Kermaidic Y., Kirch K., Knecht A., Koch H.C., Krempel J., Kuzniak M., Lauss B., Lefort T., Lemi ere Y., Mtchedlishvili A., Naviliat-Cuncic O., Pendlebury J.M., Perkowski M., Pierre E., Piegsa F.M., Pignol G., Prashanth P.N., Qu em ener G., Rebreyend D., Ries D., Roccia S., Schmidt-Wellenburg P., Schnabel A., Severijns N., Shiers D., Smith K.F., Voigt J., Weis A., Wyszynski G., Zejma J., Zenner J., Zsigmond G. A measurement of the neutron to  $^{199}\text{Hg}$  magnetic moment ratio  
*Physics Letters B* **739**, 128-132 (2014)

Baker C.A., Chibane Y., Chouder M., Geltenbort P., Green K., Harris P.G., Heckel B.R., Iaydjiev P., Ivanov S.N., Kilvington I., Lamoreaux S.K., May D.J., Pendlebury J.M., Richardson J.D., Shiers D.B., Smith K.F., Van der Grinten M. Apparatus for measurement of the electric dipole moment of the neutron using a cohabiting atomic-mercury magnetometer  
*Nuclear Instruments and Methods in Physics Research A* **736**, 184-203 (2014)

Blanc A., Chebboubi A., Faust H., Jentschel M., Kessedjian G., K oster U., Materna T., Panebianco S., Sage C., Urban W. Fission product prompt  $\gamma$ -ray spectrometer: Development of an instrumented gas-filled magnetic spectrometer at the ILL  
*Nuclear Instruments and Methods in Physics Research B* **317**, 333-337 (2013)

Casperson R.J., Burke J.T., Scielzo N.D., Escher J.E., McCleskey E., McCleskey M., Saastamoinen A., Spiridon A., Ratkiewicz A., Blanc A., Kurokawa M., Pizzone R.G. Measurement of the  $^{240}\text{Am}(n,f)$  cross section using the surrogate-ratio method  
*Physical Review C* **90**, 034601-1-034601-9 (2014)

de France G., Blanc A., Drouet F., Jentschel M., K oster U., Mutti P., R egis J.M., Simpson G., Soldner T., Stezowski O., Ur C.A., Urban W., Vancrayenest A. Spectroscopy of neutron-rich nuclei using cold neutron induced fission of actinide targets at the ILL: the EXILL campaign  
*EPJ Web of Conferences* **66**, 02010-1-02010-4 (2014)

Dubbers D., Raffelt L., M arkisch B., Friedl F., Abele H. The point spread function of electrons in a magnetic field, and the decay of the free neutron  
*Nuclear Instruments and Methods in Physics Research A* **763**, 112-119 (2014)

Dufour G., Debu P., Lambrecht A., Nesvizhevsky V.V., Reynaud S., Voronin A.Y. Shaping the distribution of vertical velocities of antihydrogen in GBAR  
*European Physical Journal C* **74**, 2731-1-2731-10 (2014)

## PUBLICATIONS

- Faust H., Chebboubi A., Kessedjian G., Sage C., Köster U., Blanc A. Principles of a gas filled magnetic spectrometer for fission studies EPJ Web of Conferences **62**, 05004-1-05004-6 (2013)
- Geppert H., Denkmayr T., Sponar S., Lemmel H., Hasegawa Y. Improvement of the polarised neutron interferometer setup demonstrating violation of a Bell-like inequality Nuclear Instruments and Methods in Physics Research A **763**, 417-423 (2014)
- Ghys L., Andreyev A.N., Huyse M., Van Duppen P., Sels S., Andel B., Antalic S., Barzakh A., Capponi L., Cocolios T.E., Derckx X., De Witte H., Elseviers J., Fedorov D.V., Fedosseev V.N., Hessberger F.P., Kalaninová Z., Köster U., Lane J.F.W., Liberati V., Lynch K.M., Marsh B.A., Mitsuoka S., Möller P., Nagame Y., Nishio K., Ota S., Pauwels D., Page R.D., Popescu L., Radulov D., Rajabali M.M., Randrup J., Rapisarda E., Rothe S., Sandhu K., Seliverstov M.D., Sjödin A.M., Truesdale V.L., Van Beveren C., Van den Bergh P., Wakabayashi Y., Warda M. Evolution of fission-fragment mass distributions in the neutron-deficient lead region Physical Review C **90**, 041301-1-041301-6 (2014)
- Gledenov Y.M., Nesvizhevsky V.V., Sedyshev P.V., Shul'gina E.V., Vesna V.A. Search for *P*-ODD asymmetry in the radiative cross-section of the interaction of neutrons with lead nuclei Physics of Atomic Nuclei **77**, 316-320 (2014)
- Harris P.G., Pendlebury J.M., Devenish N.E. Gravitationally enhanced depolarization of ultracold neutrons in magnetic-field gradients Physical Review D **89**, 016011-1-016011-5 (2014)
- Hasegawa Y. Investigations of fundamental phenomena in quantum mechanics with neutrons Journal of Physics: Conference Series **504**, 012025-1-012025-13 (2014)
- Ichikawa G., Komamiya S., Kamiya Y., Minami Y., Tani M., Geltenbort P., Yamamura K., Nagano M., Sanuki T., Kawasaki S., Hino M., Kitaguchi M. Observation of the spatial distribution of gravitationally bound quantum states of ultracold neutrons and its derivation using the wigner function Physical Review Letters **112**, 071101-1-071101-5 (2014)
- Ignatovich V.K., Nesvizhevsky V.V. Reflection of slow neutrons from nanorod powder Atomic Energy **116**, 132-143 (2014)
- Indelicato P., Chardin G., Grandemange P., Lunney D., Manea V., Badertscher A., Crivelli P., Curioni A., Marchionni A., Rossi B., Rubbia A., Nesvizhevsky V., Brook-Roberge D., Comini P., Debu P., Dupré P., Liskay L., Mansoulié B., Perez P., Rey J.M., Reymond B., Ruiz N., Sacquin Y., Vallage B., Biraben F., Clade P., Douillet A., Dufour G., Guellati S., Hilico L., Lambrecht A., Guerout R., Karr J.P., Nez F., Reynaud S., Szabo C.I., Tran V.Q., Trapateau J., Mohri A., Yamazaki Y., Charlton M., Eriksson S., Madsen N., Van der Werf D.P., Kuroda N., Torii H., Nagashima Y., Schmidt-Kaler F., Walz J., Wolf S., Hervieux P.A., Manfredi G., Voronin A., Froelich P., Wronka S., Staszczak M. The Gbar project, or how does antimatter fall? Hyperfine Interactions **228**, 141-150 (2014)
- Jenke T., Cronenberg G., Burgdörfer J., Chizhova L.A., Geltenbort P., Ivanov A.N., Lauer T., Lins T., Rotter S., Saul H., Schmidt U., Abele H. Gravity resonance spectroscopy constrains dark energy and dark matter scenarios Physical Review Letters **112**, 151105-1-151105-5 (2014)
- Jentschel M., Sengele L., Curien D., Dudek J., Haas F. The negative parity bands in <sup>156</sup>Gd Physica Scripta **89**, 054017-1-054017-6 (2014)
- Jungclaus A., Simpson G.S., Gey G., Taprogge J., Nishimura S., Doornenbal P., Lorusso G., Söderström P.A., Sumikama T., Xu Z., Baba H., Browne F., Fukuda N., Inabe N., Isobe T., Jung H.S., Kameda D., Kim G.D., Kim Y.K., Kojouharov I., Kubo T., Kurz N., Kwon Y.K., Li Z., Sakurai H., Schaffner H., Suzuki H., Takeda H., Vajta Z., Watanabe H., Wu J., Yagi A., Yoshinaga K., Bonig S., Daugas J.M., Drouet F., Gernhäuser R., Ilieva S., Kröll T., Montaner-Piza A., Moschner K., Mucher D., Nishibata H., Orlandi R., Steiger K., Wendt A. Isomer and beta decay spectroscopy in the <sup>132</sup>Sn region with EURICA EPJ Web of Conferences **66**, 02040-1-02040-4 (2014)
- Jungclaus A., Taprogge J., Simpson G.S., Gey G., Nishimura S., Doornenbal P., Lorusso G., Söderström P.A., Sumikama T., Xu Z., Baba H., Browne F., Fukuda N., Inabe N., Isobe T., Jung H.S., Kameda D., Kim G.D., Kim Y.K., Kojouharov I., Kubo T., Kurz N., Kwon Y.K., Li Z., Sakurai H., Schaffner H., Suzuki H., Takeda H., Vajta Z., Watanabe H., Wu J., Yagi A., Yoshinaga K., Bonig S., Daugas J.M., Drouet F., Gernhäuser R., Ilieva S., Kröll T., Montaner-Piza A., Moschner K., Mucher D., Nishibata H., Orlandi R., Steiger K., Wendt A. Beta decay and isomer spectroscopy in the <sup>132</sup>Sn region: New results from EURICA Journal of Physics: Conference Series **533**, 012045-1-012045-4 (2014)
- Klauser C., Abele H., Soldner T. Beam line parameters for PERC at the ESS Physics Procedia **51**, 46-49 (2014)
- Klepp J., Sponar S., Hasegawa Y. Fundamental phenomena of quantum mechanics explored with neutron interferometers Progress of Theoretical and Experimental Physics **2014**, 082A01-1-082A01-61 (2014)

- Konstantinopoulos T., Astier A., Petrache C., Abudra A., Bontemps R., Deloncle I., Kaim S., Leguillon R., Porquet M.G., Zerrouki T., Grente L., Salsac M.D., Zielinska M., France G. de, Janas Z., Karny M., Korgul A., Ramdhane M., Gey G., Simpson G., Vancraeynest A., Blanc A., Jentschel M., Köster U., Mutti P., Soldner T., Urban W., Duchene G., Lozeva R., Ibrahim F., Gargano A., Covello A., Mengoni D., Ur C.A., Sferrazza M., Melon B.  $\gamma$ -ray spectroscopy of fission fragments from the cold neutron  $^{235}\text{U}$  induced fission with EXILL EPJ Web of Conferences **62**, 01006-1-01006-4 (2013)
- Kreim S., Atanasov D., Beck D., Blaum K., Böhm C., Borgmann C., Breitenfeldt M., Cocolios T.E., Fink D., George S., Herlert A., Kellerbauer A., Köster U., Kowalska M., Lunney D., Manea V., Minaya Ramirez E., Naimi S., Neidherr D., Nicol T., Recent exploits of the ISOLTRAP mass spectrometer Nuclear Instruments and Methods in Physics Research B **317**, 492-500 (2013)
- Kulin G.V., Strepetov A.N., Frank A.I., Geltenbort P., Goryunov S.V., Jentschel M., Kustov D.V. New experimental test of dispersion law for very slow neutrons Physics Letters A **378**, 2553-2556 (2014)
- Kurpeta J., Jokinen A., Penttilä H., Płochocki A., Rissanen J., Urban W., Äystö J. Trap-assisted studies of odd, neutron-rich isotopes from Tc to Pd Hyperfine Interactions **223**, 175-184 (2014)
- Liča R., Mărginean N., Ghiță D.G., Mach H., Fraile L.M., Simpson G.S., Aprahamian A., Bernards C., Briz J.A., Bucher B., Chiara C.J., Dlouhý Z., Gheorghe I., Hoff P., Jolie J., Köster U., Kurcewicz W., Mărginean R., Olaizola B., Pazyi V., Régis J.M., Rudigier M., Sava T., Stanoiu M., Stroe L., Walters W.B. Low-lying isomeric states in  $^{80}\text{Ga}$  from the  $\beta$  decay of  $^{80}\text{Zn}$  Physical Review C **90**, 014320-1-014320-7 (2014)
- Lychagin E.V., Muzychka A.Y., Nesvizhevsky V.V. Nano-structured reflectors for slow neutrons In "New Developments in Low-Energy Physics Research" Zoeng T. et al. Eds. (2013, Nova Science Publishers) pp. 1-12
- Marsh B.A., Andel B., Andreyev A.N., Antalic S., Atanasov D., Barzakh A.E., Bastin B., Borgmann C., Capponi L., Cocolios T.E., Day Goodacre T., Dehairs M., Derckx X., De Witte H., Fedorov D.V., Fedosseev V.N., Focker G.J., Fink D.A., Flanagan K.T., Franchoo S., Ghys L., Huyse M., Imai N., Kalaninova Z., Köster U., Kreim S., Kesteloot N., Kudryavtsev Yu., Lane J., Lecesne N., Liberati V., Lunney D., Lynch K.M., Manea V., Molkanov P.L., Nicol T., Pauwels D., Popescu L., Radulov D., Rapisarda E., Rosenbusch M., Rossel R.E., Rothe S., Schweikhard L., Seliverstov M.D., Sels S., Sjödin A.M., Truesdale V., Van Beveren C., Van Duppen P., Wendt K., Wienholtz F., Wolf R.N., Zemlyanoy S.G. New developments of the in-source spectroscopy method at RILIS/ISOLDE Nuclear Instruments and Methods in Physics Research B **317**, 550-556 (2013)
- Martin F., Sage C., Kessedjian G., Sérot O., Amouroux C., Bacri C.O., Bidaud A., Billebaud A., Capellan N., Chabod S., Doligez X., Faust H., Köster U., Letourneau A., Materna T., Mathieu L., Méplan O., Panebianco S. Measurements of the mass and isotopic yields of the  $^{233}\text{U}(n_{th},f)$  reaction by the Lohengrin spectrometer Nuclear Data Sheets **119**, 328-330 (2014)
- Murray E., Smith A.G., Pollitt A.J., Matarranz J., Tsekhanovich I., Soldner T., Koster U., Biswas D.C. Measurement of gamma energy distributions and multiplicities using STEFF Nuclear Data Sheets **119**, 217-220 (2014)
- Muto S., Stone N.J., Bingham C.R., Stone J.R., Walker P.M., Audi G., Gaulard C., Köster U., Nikolov J., Nishimura K., Ohtsubo T., Podolyak Z., Risegari L., Veskovic M., Simpson G.S., Walters W.B. Magnetic properties of  $^{177}\text{Hf}$  and  $^{180}\text{Hf}$  in the strong-coupling deformed model Physical Review C **89**, 044309-1-044309-8 (2014)
- Nesvizhevsky V.V. Application of sapphire in low-energy neutron physics In "New Developments in Low-Energy Physics Research" Zoeng T. et al. Eds. (2013, Nova Science Publishers) pp. 183-188
- Piegsa F.M., Ferli M., Ivanov S.N., Kreuz M., Leung K.K.H., Schmidt-Wellenburg P., Soldner T., Zimmer O. New source for ultracold neutrons at the Institut Laue-Langevin Physical Review C **90**, 015501-1-015501-10 (2014)
- Régis J.M., Simpson G.S., Blanc A., de France G., Jentschel M., Köster U., Mutti P., Pazyi V., Saed-Samii N., Soldner T., Ur C.A., Urban W., Bruce A.M., Drouet F., Fraile L.M., Ilieva S., Jolie J., Kortén W., Kröll T., Lalkovski S., Mach H., Mărginean N., Pascovici G., Podolyak Z., Regan P.H., Roberts O.J., Smith J.F., Townsley C., Vancraeynest A., Warr N. Germanium-gated  $\gamma$ - $\gamma$  fast timing of excited states in fission fragments using the EXILL&FATIMA spectrometer Nuclear Instruments and Methods in Physics Research A **763**, 210-220 (2014)
- Salvat D.J., Adamek E.R., Barlow D., Bowman J.D., Broussard L.J., Callahan N.B., Clayton S.M., Cude-Woods C., Currie S., Dees E.B., Fox W., Geltenbort P., Hickerson K.P., Holley A.T., Liu C.Y., Makela M., Medina J., Morley D.J., Morris C.L., Penttilä S.I., Ramsey J., Saunders A., Seestrom S.J., Sharapov E.I., Sjøe S.K.L., Slaughter B.A., Vanderwerp J., VornDick B., Walstrom P.L., Wang Z., Womack T.L., Young A.R. Storage of ultracold neutrons in the magneto-gravitational trap of the UCNT experiment Physical Review C **89**, 052501-1-052501-6 (2014)



## PUBLICATIONS

- Seliverstov M.D., Cocolios T.E., Dexters W., Andreyev A.N., Antalic S., Barzakh A.E., Bastin B., Büscher J., Darby I.G., Fedorov D.V., Fedosseev V.N., Flanagan K.T., Franchoo S., Huber G., Huyse M., Keupers M., Köster U., Kudryavtsev Y., Marsh B.A., Molkanov P.L., Page R.D., Sjödin A.M., Stefan I., Van Duppen P., Venhart M., Zemlyanov S.G.  
Electromagnetic moments of odd- $A^{193,203,211}\text{Po}$  isotopes  
*Physical Review C* **89**, 034323-1-034323-10 (2014)
- Serebrov A.P., Geltenbort P., Zhrebtsov O.M., Sbitnev S.V., Varlamov V.E., Vassiljev A.V., Lasakov M.S., Krasnoschekova I.A., Ivanov S.N., Pushin D. Experimental search for long-range forces in neutron scattering via a gravitational spectrometer  
*Physical Review C* **89**, 044002-1-044002-11 (2014)
- Serebrov A.P., Kolomenskiy E.A., Pirozhkov A.N., Krasnoschekova I.A., Vassiljev A.V., Polushkin A.O., Lasakov M.S., Fomin A.K., Shoka I.V., Solovey V.A., Zhrebtsov O.M., Geltenbort P., Ivanov S.N., Zimmer O., Alexandrov E.B., Dmitriev S.P.  
New measurements of the neutron electric dipole moment  
*JETP Letters* **99**, 4-8 (2014)
- Serot O., Amouroux C., Bidaud A., Capellan N., Chabod S., Ebran A., Faust H., Kessedjian G., Köster U., Letourneau A., Litaize O., Martin F., Materna T., Mathieu L., Panebianco S., Regis J.M., Rudigier M., Sage C., Urban W. Recent results from Lohengrin on fission yields and related decay properties  
*Nuclear Data Sheets* **119**, 320-323 (2014)
- Simpson G.S., Gey G., Jungclaus A., Taprogge J., Nishimura S., Sieja K., Doornenbal P., Lorusso G., Söderström P.A., Sumikama T., Xu Z.Y., Baba H., Browne F., Fukuda N., Inabe N., Isobe T., Jung H.S., Kameda D., Kim G.D., Kim Y.K., Kojouharov I., Kubo T., Kurz N., Kwon Y.K., Li Z., Sakurai H., Schaffner H., Shimizu Y., Suzuki H., Takeda H., Vajta Z., Watanabe H., Wu J., Yagi A., Yoshinaga K., Bonig S., Daugas J.M., Drouet F., Gernhäuser R., Ilieva S., Kröll T., Montaner-Piza A., Moschner K., Mucher D., Naidja H., Nishibata H., Nowacki F., Odahara A., Orlandi R., Steiger K., Wendt A.  
Yrast  $6^+$  seniority isomers of  $^{136,138}\text{Sn}$   
*Physical Review Letters* **113**, 132502-1-132502-6 (2014)
- Soti G., Wauters F., Breitenfeldt M., Finlay P., Herzog P., Knecht A., Köster U., Kraev I.S., Porobic T., Prashanth P.N., Towner I.S., Tramm C., Zákoucký D., Severijns N. Measurement of the  $\beta$ -asymmetry parameter of  $^{67}\text{Cu}$  in search for tensor-type currents in the weak interaction  
*Physical Review C* **90**, 035502-1-035502-15 (2014)
- Steyerl A., Kaufman C., Müller G., Malik S.S., Desai A.M., Golub R. Calculation of geometric phases in electric dipole searches with trapped spin-1/2 particles based on direct solution of the Schrödinger equation  
*Physical Review A* **89**, 052129-1-052129-10 (2014)
- Taprogge J., Jungclaus A., Grawe H., Nishimura S., Doornenbal P., Lorusso G., Simpson G.S., Söderström P.A., Sumikama T., Xu Z.Y., Baba H., Browne F., Fukuda N., Gernhäuser R., Gey G., Inabe N., Isobe T., Jung H.S., Kameda D., Kim G.D., Kim Y.K., Kojouharov I., Kubo T., Kurz N., Kwon Y.K., Li Z., Sakurai H., Schaffner H., Steiger K., Suzuki H., Takeda H., Vajta Z., Watanabe H., Wu J., Yagi A., Yoshinaga K., Benzoni G., Bonig S., Chae K.Y., Coraggio L., Covello A., Daugas J.M., Drouet F., Gadea A., Gargano A., Ilieva S., Kondev F.G., Kröll T., Lane G.J., Montaner-Piza A., Moschner K., Mucher D., Naqvi F., Niikura M., Nishibata H., Odahara A., Orlandi R., Patel Z., Podolyak Z., Wendt A.  $1p_{3/2}$  proton-hole state in  $^{132}\text{Sn}$  and the shell structure along  $N = 82$   
*Physical Review Letters* **112**, 132501-1-132501-6 (2014)
- Taprogge J., Jungclaus A., Grawe H., Nishimura S., Xu Z.Y., Doornenbal P., Lorusso G., Nácher E., Simpson G.S., Söderström P.A., Sumikama T., Baba H., Browne F., Fukuda N., Gernhäuser R., Gey G., Inabe N., Isobe T., Jung H.S., Kameda D., Kim G.D., Kim Y.K., Kojouharov I., Kubo T., Kurz N., Kwon Y.K., Li Z., Sakurai H., Schaffner H., Steiger K., Suzuki H., Takeda H., Vajta Z., Watanabe H., Wu J., Yagi A., Yoshinaga K., Benzoni G., Bonig S., Chae K.Y., Coraggio L., Covello A., Daugas J.M., Drouet F., Gadea A., Gargano A., Ilieva S., Kondev F.G., Kröll T., Lane G.J., Montaner-Piza A., Moschner K., Mucher D., Naqvi F., Niikura M., Nishibata H., Odahara A., Orlandi R., Patel Z., Podolyak Z., Wendt A. Identification of a millisecond isomeric state in  $^{129}\text{Cd}_{81}$  via the detection of internal conversion and Compton electrons  
*Physics Letters B* **738**, 223-227 (2014)
- Voronin A.Y., Nesvizhevsky V.V., Dalkarov O.D., Kupriyanova E.A., Froelich P.  
Resonance spectroscopy of gravitational states of antihydrogen  
*Hyperfine Interactions* **228**, 133-139 (2014)
- Young A.R., Clayton S., Filippone B.W., Geltenbort P., Ito T.M., Liu C.Y., Makela M., Morris C.L., Plaster B., Saunders A., Seestrom S.J., Vogelaar R.B. Beta decay measurements with ultracold neutrons: A review of recent measurements and the research program at Los Alamos National Laboratory  
*Journal of Physics G* **41**, 114007-1-114007-72 (2014)
- Zimmer O. Superfluid-helium ultracold neutron sources: Concepts for the European Spallation Source?  
*Physics Procedia* **51**, 85-88 (2014)

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## Soft Matter

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- Abbott S.B., de Vos W.M., Mears L.L.E., Barker R., Richardson R.M., Prescott S.W. Hydration of odd-even terminated polyelectrolyte multilayers under mechanical confinement  
*Macromolecules* **47**, 3263-3273 (2014)
- Ábrahám Á., Kardos A., Mezei A., Campbell R.A., Varga I. Effects of ionic strength on the surface tension and nonequilibrium interfacial characteristics of poly(sodium styrenesulfonate)/dodecyltrimethylammonium bromide mixtures  
*Langmuir* **30**, 4970-4979 (2014)
- Alexander S., Smith G.N., James C., Rogers S.E., Guittard F., Sagisaka M., Eastoe J. Low-surface energy surfactants with branched hydrocarbon architectures  
*Langmuir* **30**, 3413-3421 (2014)
- Ang J.C., Henderson M.J., Campbell R.A., Lin J.M., Yaron P.N., Nelson A., Faunce T., White J.W. Human serum albumin binding to silica nanoparticles – Effect of protein fatty acid ligand  
*Physical Chemistry Chemical Physics* **16**, 10157-10168 (2014)
- Appel M., Frick B., Ivanov A., Elbert J., Rehahn M., Gallei M., Spehr T.L., Stühn B. Vibrational spectra of ferrocene, ferrocene-containing polymers and their oxidised compounds  
*Journal of Physics: Conference Series* **554**, 012008-1-012008-8 (2014)
- Arbe A. Nanophase separation and exotic dynamic behavior in comb-like polymers  
*Journal of the Physical Society of Japan* **82**, SA015-1-SA015-14 (2013)
- Armstrong C.L., Häußler W., Seydel T., Katsaras J., Rheinstädter M.C. Nanosecond lipid dynamics in membranes containing cholesterol  
*Soft Matter* **10**, 2600-2611 (2014)
- Bergström L.M., Grillo I. Correlation between the geometrical shape and growth behaviour of surfactant micelles investigated with small-angle neutron scattering  
*Soft Matter* **10**, 9362-9372 (2014)
- Bergström L.M., Skoglund S., Edwards K., Eriksson J., Grillo I. Spontaneous transformations between surfactant bilayers of different topologies observed in mixtures of sodium octyl sulfate and hexadecyltrimethylammonium bromide  
*Langmuir* **30**, 3928-3938 (2014)
- Bergström L.M., Skoglund S., Edwards K., Eriksson J., Grillo I. Self-assembly in mixtures of an anionic and a cationic surfactant: A comparison between small-angle neutron scattering and cryo-transmission electron microscopy  
*Langmuir* **29**, 11834-11848 (2013)
- Berts I., Ossipov D., Fragneto G., Frisk A., Rennie A.R. Polymeric smart coating strategy for titanium implants  
*Advanced Engineering Materials* **16**, 1340-1350 (2014)
- Boulogne F., Pauchard L., Giorgiutti-Dauphiné F., Botet R., Schweins R., Sztucki M., Li J., Cabane B., Goehring L. Structural anisotropy of directionally dried colloids  
*Europhysics Letters* **105**, 38005-p1-38005-p6 (2014)
- Brás A.R., Gooßen S., Krutyeva M., Radulescu A., Farago B., Allgaier J., Pyckhout-Hintzen W., Wischniewski A., Richter D. Compact structure and non-Gaussian dynamics of ring polymer melts  
*Soft Matter* **10**, 3649-3655 (2014)
- Browning K.L., Griffin L.R., Gutfreund P., Barker R.D., Clifton L.A., Hughes A., Clarke S.M. Specular neutron reflection at the mica/water interface – Irreversible adsorption of a cationic dichain surfactant  
*Journal of Applied Crystallography* **47**, 1638-1646 (2014)
- Brüning B.A., Prévost S., Stehle R., Steitz R., Falus P., Farago B., Hellweg T. Bilayer undulation dynamics in unilamellar phospholipid vesicles: Effect of temperature, cholesterol and trehalose  
*Biochimica et Biophysica Acta* **1838**, 2412-2419 (2014)
- Campana M., Webster J.R.P., Zarbakhsh A. Structural studies of nonionic dodecanol ethoxylates at the oil-water interface: Effect of increasing head group size  
*Langmuir* **30**, 10241-10247 (2014)
- Campbell R.A., Watkins E.B., Jagalski V., Åkesson-Runnsjö A., Cárdenas M. Key factors regulating the mass delivery of macromolecules to model cell membranes: Gravity and electrostatics  
*ACS Macro Letters* **3**, 121-125 (2014)
- Campbell R.A., Yanez Arteta M., Angus-Smyth A., Nylander T., Noskov B.A., Varga I. Direct impact of non-equilibrium aggregates on the structure and morphology of PdAdmac/SDS layers at the air/water interface  
*Langmuir* **30**, 8664-8674 (2014)
- Chiappisi L., Prévost S., Gradzielski M. Form factor of cylindrical superstructures composed of globular particles  
*Journal of Applied Crystallography* **47**, 827-834 (2014)
- Chiappisi L., Prévost S., Grillo I., Gradzielski M. Chitosan/alkylethoxy carboxylates: A surprising variety of structures  
*Langmuir* **30**, 1778-1787 (2014)
- Chrissopoulou K., Fotiadou S., Androulaki K., Tanis I., Karatasos K., Prevosto D., Labardi M., Frick B., Anastasiadis S.H. Dynamics of dendritic polymers in the bulk and under confinement  
*AIP Conference Proceedings* **1599**, 250-253 (2014)

## PUBLICATIONS

- Cowsill B.J., Zhao X., Waigh T.A., Eapen S., Davies R., Laux V., Haertlein M., Forsyth V.T., Lu J.R. Interfacial structure of immobilized antibodies and perdeuterated HSA in model pregnancy tests measured with neutron reflectivity  
*Langmuir* **30**, 5880-5887 (2014)
- Cupane A., Fomina M., Piazza I., Peters J., Schirò G. Experimental evidence for a liquid-liquid crossover in deeply cooled confined water  
*Physical Review Letters* **113**, 215701-1-215701-5 (2014)
- Cupane A., Fomina M., Schirò G. The boson peak of deeply cooled confined water reveals the existence of a low-temperature liquid-liquid crossover  
*Journal of Chemical Physics* **141**, 18C510-1-18C510-7 (2014)
- Dattani R., Michels R., Nedoma A.J., Schweins R., Westacott P., Huber K., Cabral J.T. Conformation and interactions of polystyrene and fullerenes in dilute to semidilute solutions  
*Macromolecules* **47**, 6113-6120 (2014)
- de Ghellinck A., Schaller H., Laux V., Haertlein M., Sferrazza M., Maréchal E., Wacklin H., Jouhet J., Fragneto G. Production and analysis of perdeuterated lipids from *Pichia pastoris* cells  
*PLoS One* **9**, e92999-1-e92999-9 (2014)
- Dyakonova M.A., Stavrouli N., Popescu M.T., Kyriakos K., Grillo I., Philipp M., Jaksch S., Tsitsilianis C., Papadakis C.M. Physical hydrogels via charge driven self-organisation of a triblock polyampholyte – rheological and structural investigations  
*Macromolecules* **47**, 7561-7572 (2014)
- Eberle A.P.R., Martys N., Porcar L., Kline S.R., George W.L., Kim J.M., Butler P.D., Wagner N.J. Shear viscosity and structural scalings in model adhesive hard-sphere gels  
*Physical Review E* **89**, 050302-1-050302-5 (2014)
- Elgammal M., Prévost S., Schweins R., Schneider R., Gradzielski M. "Nanosized latexes for textile printing applications obtained by miniemulsion polymerisation"  
*Colloid and Polymer Science* **292**, 1487-1500 (2014)
- Exner A., Rosenfeldt S., Fischer S., Lindner P., Förster S. Defect accommodation in nanostructured soft crystals  
*Nanoscale* **6**, 1635-1645 (2014)
- Foglia F., Fragneto G., Clifton L.A., Lawrence M.J., Barlow D.J. Interaction of amphotericin B with lipid monolayers  
*Langmuir* **30**, 9147-9156 (2014)
- Garg S., Castro-Roman F., Porcar L., Butler P., Bautista P.J., Krzyzanowski N., Perez-Salas U. Cholesterol solubility limit in lipid membranes probed by small-angle neutron-scattering and MD simulations  
*Soft Matter* **10**, 9313-9317 (2014)
- Gentile L., Behrens M.A., Porcar L., Butler P., Wagner N.J., Olsson U. Multilamellar vesicle formation from a planar lamellar phase under shear flow  
*Langmuir* **30**, 8316-8325 (2014)
- Gerelli Y., de Ghellinck A., Jouhet J., Laux V., Haertlein M., Fragneto G. Multi-lamellar organisation of fully deuterated lipid extracts of yeast membranes  
*Acta Crystallographica D* **70**, 3167-3176 (2014)
- Goodwin D.J., Sepassi S., King S.M., Holland S.J., Martini L.G., Lawrence M.J. Characterization of polymer adsorption onto drug nanoparticles using depletion measurements and small-angle neutron scattering  
*Molecular Pharmaceutics* **10**, 4146-4158 (2013)
- Gooßen S., Brás A.R., Krutyeva M., Sharp M., Falus P., Feoktystov A., Gasser U., Pyckhout-Hintzen W., Wischniewski A., Richter D. Molecular scale dynamics of large ring polymers  
*Physical Review Letters* **113**, 168302-1-168302-5 (2014)
- Gurnon A.K., López-Bárron C.R., Wasbrough M.J., Porcar L., Wagner N.J. Spatially resolved concentration and segmental flow alignment in a shear-banding solution of polymerlike micelles  
*ACS Macro Letters* **3**, 276-280 (2014)
- Gurnon A.K., López-Bárron C.R., Eberle A.P.R., Porcar L., Wagner N.J. Spatiotemporal stress and structure evolution in dynamically sheared polymerlike micellar solutions  
*Soft Matter* **10**, 2889-2898 (2014)
- Helsing M.S., Kwaambwa H.M., Nermark F.M., Nkoane B.B.M., Jackson A.J., Wasbrough M.J., Berts I., Porcar L., Rennie A.R. Structure of flocs of latex particles formed by addition of protein from Moringa seeds  
*Colloids and Surfaces A* **460**, 460-467 (2014)
- Hertle Y., Zeiser M., Fouquet P., Maccarini M., Hellweg T. The internal network dynamics of poly(NIPAM) based copolymer micro- and macrogels: A comparative neutron spin-echo study  
*Zeitschrift für Physikalische Chemie* **228**, 1053-1075 (2014)
- Hoffmann I. Neutrons for the study of dynamics in soft matter systems  
*Colloid and Polymer Science* **292**, 2053-2069 (2014)
- Hoffmann I., de Molina P.M., Farago B., Falus P., Herfurth C., Laschewsky A., Gradzielski M. Dynamics of microemulsions bridged with hydrophobically end-capped star polymers studied by neutron spin-echo  
*Journal of Chemical Physics* **140**, 034902-1-034902-9 (2014)

- Hoffmann I., Michel R., Sharp M., Holderer O., Appavou M.S., Polzer F., Farago B., Gradzielski M. Softening of phospholipid membranes by the adhesion of silica nanoparticles – as seen by neutron spin-echo (NSE)  
*Nanoscale* **6**, 6945-6952 (2014)
- Holderer O., Frielinghaus H., Monkenbusch M., Klostermann M., Sottmann T., Richter D. Experimental determination of bending rigidity and saddle splay modulus in bicontinuous microemulsions  
*Soft Matter* **9**, 2308-2313 (2013)
- Hollamby M.J., Korny M., Bomans P.H.H., Sommerdijk N.A.J.M., Saeki A., Seki S., Minamikawa H., Grillo I., Pauw B.R., Brown P., Eastoe J., Möhwald H., Nakanishi T. Directed assembly of optoelectronically active alkyl- $\pi$ -conjugated molecules by adding *n*-alkanes or  $\pi$ -conjugated species  
*Nature Chemistry* **6**, 690-696 (2014)
- Holt C., Lenton S., Nylander T., Sørensen E.S., Teixeira S.C.M. Mineralisation of soft and hard tissues and the stability of biofluids  
*Journal of Structural Biology* **185**, 383-396 (2014)
- Hopkins Hatzopoulos M., James C., Rogers S., Grillo I., Dowding P.J., Eastoe J. Effects of small ionic amphiphilic additives on reverse microemulsion morphology  
*Journal of Colloid and Interface Science* **421**, 56-63 (2014)
- Hurcom J., Paul A., Heenan R.K., Davies A., Woodman N., Schweins R., Griffiths P.C. The interfacial structure of polymeric surfactant stabilised air-in-water foams  
*Soft Matter* **10**, 3003-3008 (2014)
- Jaksch S., Schulz A., Kyriakos K., Zhang J., Grillo I., Pipich V., Jordan R., Papadakis C.M. The collapse and aggregation of thermoresponsive poly(2-oxazoline) gradient copolymers: A time-resolved SANS study  
*Colloid and Polymer Science* **292**, 2413-2425 (2014)
- Jordan E., Roosen-Runge F., Leibfarth S., Zhang F., Sztucki M., Hildebrandt A., Kohlbacher O., Schreiber F. Competing salt effects on phase behaviour of protein solutions: Tailoring of protein interaction by the binding of multivalent ions and charge screening  
*Journal of Physical Chemistry B* **118**, 11365-11374 (2014)
- Kamata Y., Parnell A.J., Gutfreund P., Skoda M.W.A., Dennison A.J.C., Barker R., Mai S., Howse J.R., Ryan A.J., Torikai N., Kawaguchi M., Jones R.A.L. Hydration and ordering of lamellar block copolymer films under controlled water vapor  
*Macromolecules* **47**, 8682-8690 (2014)
- Kanduč M., Schneck E., Netz R.R. Attraction between hydrated hydrophilic surfaces  
*Chemical Physics Letters* **610-611**, 375-380 (2014)
- Khan A.N., Nguyen T.T.T., Dobircau L., Schmutz M., Mesini P.J., Guenet J.M. Investigation of the interactions involved in the formation of nanotubes from organogelators  
*Langmuir* **29**, 16127-16134 (2013)
- Khodadadi S., Clark N.J., McAuley A., Cristiglio V., Curtis J.E., Shalaev E.Y., Krueger S. Influence of sorbitol on protein crowding in solution and freeze-concentrated phases  
*Soft Matter* **10**, 4056-4060 (2014)
- Kienle D.F., de Souza J.V., Watkins E.B., Kuhl T.L. Thickness and refractive index of DPPC and DPPE monolayers by multiple-beam interferometry  
*Analytical and Bioanalytical Chemistry* **406**, 4725-4733 (2014)
- Kityk A.V., Busch M., Rau D., Calus S., Cerclier C.V., Lefort R., Morineau D., Grelet E., Krause C., Schönhals A., Frick B., Huber P. Thermotropic orientational order of discotic liquid crystals in nanochannels: An optical polarimetry study and a Landau-de Gennes analysis  
*Soft Matter* **10**, 4522-4534 (2014)
- Kossi A., Persello J., Cabane B. Acetylacetone stimulus effect on electrorheological properties of TiO<sub>2</sub> aggregated nanoparticles  
*Journal of Materials Science* **49**, 811-818 (2014)
- Kundu S.K., Gupta S., Stellbrink J., Willner L., Richter D. Relating structure and flow of soft colloids  
*European Physical Journal Special Topics* **222**, 2757-2772 (2013)
- Kuttich B., Falus P., Grillo I., Stühn B. Form fluctuations of polymer loaded spherical microemulsions studied by neutron scattering and dielectric spectroscopy  
*Journal of Chemical Physics* **141**, 084903-1-084903-10 (2014)
- Laschewsky A., Müller-Buschbaum P., Papadakis C.M. Thermoresponsive amphiphilic di- and triblock copolymers based on poly(N-isopropylacrylamide) and poly(methoxy diethylene glycol acrylate): Aggregation and hydrogel formation in bulk solution and in thin films  
*Progress in Colloid and Polymer Science* **140**, 15-34 (2013)
- Laupheimer M., Sottmann T., Schweins R., Stubenrauch C. Studying orthogonal self-assembled systems: Microstructure of gelled bicontinuous microemulsions  
*Soft Matter* **10**, 8744-8757 (2014)
- Li X., Porcar L., Sánchez-Díaz L.E., Do C., Liu Y., Kim T.H., Smith G.S., Hamilton W.A., Hong K., Chen W.R. Influence of molecular solvation on the conformation of star polymers  
*ACS Macro Letters* **3**, 458-461 (2014)

## PUBLICATIONS

- Li X., Sánchez-Díaz L.E., Wu B., Hamilton W.A., Falus P., Porcar L., Liu Y., Do C., Faraone A., Smith G.S., Egami T., Chen W.R. Dynamical threshold of diluteness of soft colloids ACS Macro Letters **3**, 1271-1275 (2014)
- Lind T.K., Cárdenas M., Wacklin H.P. Formation of supported lipid bilayers by vesicle fusion: Effect of deposition temperature Langmuir **30**, 7259-7263 (2014)
- López-Barrón C.R., Gurnon A.K., Eberle A.P.R., Porcar L., Wagner N.J. Microstructural evolution of a model, shearbanding micellar solution during shear startup and cessation Physical Review E **89**, 042301-1-042301-11 (2014)
- Iyadinskaya V.V., Bykov A.G., Campbell R.A., Varga I., Lin S.Y., Loglio G., Miller R., Noskov B.A. Dynamic surface elasticity of mixed poly(diallyldimethylammonium chloride)/sodium dodecyl sulfate/NaCl solutions Colloids and Surfaces A **460**, 3-10 (2014)
- Maccarrone S., Scherzinger C., Holderer O., Lindner P., Sharp M., Richtering W., Richter D. Cononsolvency effects on the structure and dynamics of microgels Macromolecules **47**, 5982-5988 (2014)
- Maslovskis A., Guilbaud J.B., Grillo I., Hodson N., Miller A.F., Saiani A. Self-assembling peptide/thermo-responsive polymer composite hydrogels: Effect of peptide-polymer interactions on hydrogel properties Langmuir **30**, 10471-10480 (2014)
- Mehan S., Kumar S., Aswal V.K. Observation of two different fractal structures in nanoparticle, protein and surfactant complexes AIP Conference Proceedings **1591**, 167-169 (2014)
- Moglianetti M., Ong Q.K., Reguera J., Harkness K.M., Marnett M., Radulescu A., Kohlbrecher J., Jud C., Svergun D.I., Stellacci F. Scanning tunneling microscopy and small-angle neutron-scattering study of mixed monolayer protected gold nanoparticles in organic solvents Chemical Science **5**, 1232-1240 (2014)
- Ndao M., Lefort R., Cerclier C.V., Busselez R., Morineau D., Frick B., Ollivier J., Kityk A.V., Huber P. Molecular dynamics of pyrene based discotic liquid crystals confined in nanopores probed by incoherent quasielastic neutron scattering RSC Advances **4**, 59358-59369 (2014)
- Nguyen R., Jouault N., Zanirati S., Rawiso M., Allouche L., Fuks G., Buhler E., Giuseppone N. Core-shell inversion by pH modulation in dynamic covalent micelles Soft Matter **10**, 3926-3937 (2014)
- Pfrang C., Sebastiani F., Lucas C.O.M., King M.D., Hoare I.D., Chang D., Campbell R.A. Ozonolysis of methyl oleate monolayers at the air-water interface: Oxidation kinetics, reaction products and atmospheric implications Physical Chemistry Chemical Physics **16**, 13220-13228 (2014)
- Pieraccini S., Terzidis M.A., Baldassarri E.J., Fragneto G., Mariani P., Masiero S., Chatgililoglu C. A lipophilic "fully-anti" dodecamer from a (5'S)-5',8-cyclo-2'-deoxyguanosine Chemical Communications **50**, 10722-10725 (2014)
- Pottage M.J., Kusuma T., Grillo I., Garvey C.J., Stickland A.D., Tabor R.F. Fluorinated lamellar phases: Structural characterisation and use as templates for highly ordered silica materials Soft Matter **10**, 4902-4912 (2014)
- Rahman S., Santra C., Kumar R., Bahadur J., Sultana A., Schweins R., Sen D., Maity S., Mazumdar S., Chowdhury B. Highly active Ga promoted Co-HMS-X catalyst towards styrene epoxidation reaction using molecular O<sub>2</sub> Applied Catalysis A: General **482**, 61-68 (2014)
- Roosen-Runge F., Zhang F., Schreiber F., Roth R. Ion-activated attractive patches as a mechanism for controlled protein interactions Scientific Reports **4**, 7016-1-7016-5 (2014)
- Ruta B., Czakkel O., Chushkin Y., Pignon F., Nervo R., Zontone F., Rinaudo M. Silica nanoparticles as tracers of the gelation dynamics of a natural biopolymer physical gel Soft Matter **10**, 4547-4554 (2014)
- Sawada D., Ogawa Y., Kimura S., Nishiyama Y., Langan P., Wada M. Solid-solvent molecular interactions observed in crystal structures of  $\beta$ -chitin complexes Cellulose **21**, 1007-1014 (2014)
- Sierra-Martin B., Retama J.R., Laurenti M., Fernández Barbero A., López-Cabarcos E. Structure and polymer dynamics within PNIPAM-based microgel particles Advances in Colloid and Interface Science **205**, 113-123 (2014)
- Smith G.N., Alexander S., Brown P., Gillespie D.A.J., Grillo I., Heenan R.K., James C., Kemp R., Rogers S.E., Eastoe J. Interaction between surfactants and colloidal latexes in nonpolar solvents studied using contrast-variation small-angle neutron scattering Langmuir **30**, 3422-3431 (2014)
- Soraruf D., Roosen-Runge F., Grimaldo M., Zanini F., Schweins R., Seydel T., Zhang F., Roth R., Oettel M., Schreiber F. Protein cluster formation in aqueous solution in the presence of multivalent metal ions – a light scattering study Soft Matter **10**, 894-902 (2014)



- Stals P.J.M., Gillissen M.A.J., Paffen T.F.E., De Greef T.F.A., Lindner P., Meijer E.W., Palmans A.R.A., Voets I.K. Folding polymers with pendant hydrogen bonding motifs in water: The effect of polymer length and concentration on the shape and size of single-chain polymeric nanoparticles  
*Macromolecules* **47**, 2947-2954 (2014)
- Stocker I.N., Miller K.L., Welbourn R.J.L., Clarke S.M., Collins I.R., Kinane C., Gutfreund P. Adsorption of Aerosol-OT at the calcite/water interface – Comparison of the sodium and calcium salts  
*Journal of Colloid and Interface Science* **418**, 140-146 (2014)
- Tresset G., Tatou M., Le Coeur C., Zeghal M., Bailleux V., Lecchi A., Brach K., Klekotko M., Porcar L. Weighing polyelectrolytes packaged in virus-like particles  
*Physical Review Letters* **113**, 128305-1-128305-5 (2014)
- Valle-Obrero J., Wildes A.R., Theodorakopoulos N., Cuesta-López S., Garden J.L., Danilkin S., Peyrard M. Thermal denaturation of A-DNA  
*New Journal of Physics* **16**, 113017-1-113017-14 (2014)
- Vogt K., Siebenbürger M., Clemens D., Rabe C., Lindner P., Russina M., Fromme M., Meizei F., Ballauff M. A new time-of-flight small-angle scattering instrument at the Helmholtz-Zentrum Berlin: V16/VSANS  
*Journal of Applied Crystallography* **47**, 237-244 (2014)
- Wandersman E., Cébers A., Dubois E., Mériquet G., Robert A., Perzynski R. The cage elasticity and under-field structure of concentrated magnetic colloids probed by small-angle X-ray scattering  
*Soft Matter* **9**, 11480-11489 (2013)
- Wang Y., Qin W., Qiu D. Small-angle neutron scattering study of cyclic poly(ethylene glycol) adsorption on colloidal particles  
*Langmuir* **30**, 5170-5175 (2014)
- Watkins E.B., Miller C.E., Liao W.P., Kuhl T.L. Equilibrium or quenched: Fundamental differences between lipid monolayers, supported bilayers, and membranes  
*ACS Nano* **8**, 3181-3191 (2014)
- Wellert S., Hertle Y., Richter M., Medebach M., Magerl D., Wang W., Demé B., Radulescu A., Müller-Buschbaum P., Hellweg T., von Klitzing R. Inner structure of adsorbed ionic microgel particles  
*Langmuir* **30**, 7168-7176 (2014)
- Wolff N., Gerth S., Gutfreund P., Wolff M. Temperature dependent cubic and hexagonal close packing in micellar structures  
*Soft Matter* **10**, 8420-8426 (2014)
- Wong H.C., Li Z., Tan C.H., Zhong H., Huang Z., Bronstein H., McCulloch I., Cabral J.T., Durrant J.R. Morphological stability and performance of polymer-fullerene solar cells under thermal stress: The impact of photoinduced PC<sub>60</sub>BM oligomerisation  
*ACS Nano* **8**, 1297-1308 (2014)
- Xu H., Penfold J., Thomas R.K., Petkov J.T., Tucker I., Grillo I., Terry A. Impact of AlCl<sub>3</sub> on the self-assembly of the anionic surfactant sodium polyethylene glycol monoalkyl ether sulfate in aqueous solution  
*Langmuir* **29**, 13359-13366 (2013)
- Xu H., Penfold J., Thomas R.K., Petkov J.T., Tucker I., Webster J.P.R. The formation of surface multilayers at the air-water interface from sodium polyethylene glycol monoalkyl ether sulfate/AlCl<sub>3</sub> solutions: The role of the size of the polyethylene oxide group  
*Langmuir* **29**, 11656-11666 (2013)
- Xu H., Penfold J., Thomas R.K., Petkov J.T., Tucker I., Webster J.P.R., Grillo I., Terry A. Ion-specific effects in trivalent counterion induced surface and solution self-assembly of the anionic surfactant sodium polyethylene glycol monododecyl ether sulfate  
*Langmuir* **30**, 4694-4702 (2014)
- Yanez Arteta M., Berti D., Montis C., Campbell R.A., Clifton L.A., Skoda M.W.A., Soltwedel O., Baglioni P., Nylander T. Molecular recognition of nucleic acids by nucleolipid/dendrimer surface complexes  
*Soft Matter* **10**, 8401-8405 (2014)
- Yanez Arteta M., Campbell R.A., Nylander T. Adsorption of mixtures of poly(amidoamine) dendrimers and sodium dodecyl sulfate at the air-water interface  
*Langmuir* **30**, 5817-5828 (2014)
- Yanez Arteta M., Campbell R.A., Watkins E.B., Obiols-Rabasa M., Schillén K., Nylander T. Interactions of small dendrimers with sodium dodecyl sulfate at the air-water interface  
*Journal of Physical Chemistry B* **118**, 11835-11848 (2014)
- Ye L., Chu X., Zhang Z., Kan Y., Xie Y., Grillo I., Zhao J., Dreiss C.A., Qiu D. Effect of particle polydispersity on the structure and dynamics of complex formation between small particles and large polymer  
*RSC Advances* **4**, 14896-14903 (2014)

# PUBLICATIONS

## Spectroscopy in Solid State Physics and Chemistry

Alekseev P.A., Nemkovski K.S., Mignot J.M., Clementyev E.S., Ivanov A.S., Rols S., Bewley R.I., Filipov V.B., Shitsevalova N.Y. Possible undercompensation effect in the Kondo insulator (Yb,Tm)B<sub>12</sub> *Physical Review B* **89**, 115121-1-115121-10 (2014)

Aramini M., Gaboardi M., Vlahopoulou G., Pontiroli D., Cavallari C., Milanese C., Riccò M. Muon spin relaxation reveals the hydrogen storage mechanism in light alkali metal fullerides *Carbon* **67**, 92-97 (2014)

Bahn E., Hedgeland H., Jardine A.P., Henry P.F., Hansen T.C., Fouquet P. The structure of deuterated benzene films adsorbed on the graphite (0001) basal plane: What happens below and above the monolayer coverage? *Physical Chemistry Chemical Physics* **16**, 22116-22121 (2014)

Bessas D., Simon R.E., Friese K., Koza M., Hermann R.P. Lattice dynamics in intermetallic Mg<sub>2</sub>Ge and Mg<sub>2</sub>Si *Journal of Physics: Condensed Matter* **26**, 485401-1-485401-7 (2014)

Calvo-Almazán I., Bahn E., Koza M.M., Zbiri M., Maccarini M., Telling M.T.F., Miret-Artés S., Fouquet P. Benzene diffusion on graphite described by a rough hard disk model *Carbon* **79**, 183-191 (2014)

Cavallari C., Pontiroli D., Jiménez-Ruiz M., Ivanov A., Mazzani M., Gaboardi M., Aramini M., Brunelli M., Riccò M., Rols S. Hydrogen on graphene investigated by inelastic neutron scattering *Journal of Physics: Conference Series* **554**, 012009-1-012009-7 (2014)

Chrissopoulou K., Fotiadou S., Frick B., Anastasiadis S.H. Structure and dynamics in hydrophilic polymer/layered silicate nanocomposites *Macromolecular Symposia* **331-332**, 50-57 (2013)

Claudio T., Stein N., Stroppa D.G., Klobes B., Koza M.M., Kudejova P., Petermann N., Wiggers H., Schierning G., Hermann R.P. Nanocrystalline silicon: Lattice dynamics and enhanced thermoelectric properties *Physical Chemistry Chemical Physics* **16**, 25701-25709 (2014)

Cousland G.P., Mole R.A., Elcombe M.M., Cui X.Y., Smith A.E., Stampfl C.M., Stampfl A.P.J. Investigation of the vibrational properties of cubic yttria-stabilised zirconia: A combined experimental and theoretical study *Journal of Physics and Chemistry of Solids* **75**, 351-357 (2014)

Euchner H., Pailhès S., Yamada T., Tamura R., Ishimasa T., Rols S., Schober H., Mihalkovic M., Trebin H.R., Schopf D., Paschen S., Haghighirad A., Ritter F., Assmus W., Grin Y., Nguyen L., de Boissieu M. Atomic dynamics in complex metallic alloys *MRS Proceedings* **1517**, 1-12 (2013)

Euchner H., Yamada T., Rols S., Ishimasa T., Ollivier J., Schober H., Mihalkovič M., de Boissieu M. Lattice dynamics of the icosahedral quasicrystals i-ZnMgSc and i-ZnAgSc and the cubic 1/1-approximant Zn<sub>5</sub>Sc *Journal of Physics: Condensed Matter* **26**, 055402-1-055402-7 (2014)

Frantsuzov I., Ford S.J., Evans I.R., Horsewill A.J., Trommsdorff H.P., Johnson M.R. Measurement of proton tunneling in short hydrogen bonds in single crystals of 3,5 pyridinedicarboxylic acid using nuclear magnetic resonance spectroscopy *Physical Review Letters* **113**, 018301-1-018301-5 (2014)

Frantsuzov I., Johnson M.R., Trommsdorff H.P., Horsewill A.J. Proton tunnelling in the hydrogen bonds of the benzoic acid dimer: <sup>18</sup>O substitution and isotope effects of the heavy atom framework *Journal of Physical Chemistry B* **118**, 7777-7784 (2014)

Gallo E., Piovano A., Marini C., Mathon O., Pascarelli S., Glatzel P., Lamberti C., Berlier G. Architecture of the Ti(IV) sites in TiAlPO-5 determined using Ti K-edge X-ray absorption and X-ray emission spectroscopies *Journal of Physical Chemistry C* **118**, 11745-11751 (2014)

Goel P., Gupta M.K., Mittal R., Rols S., Patwe S.J., Achary S.N., Tyagi A.K., Chaplot S.L. Phonons, lithium diffusion and thermodynamics of LiMPO<sub>4</sub> (M = Mn, Fe) *Journal of Materials Chemistry A* **2**, 14729-14738 (2014)

Goh K.S.K., Jiménez-Ruiz M., Johnson M.R., Rols S., Ollivier J., Denning M.S., Mamone S., Levitt M.H., Lei X., Li Y., Turro N.J., Murata Y., Horsewill A.J. Symmetry-breaking in the endofullerene H<sub>2</sub>O@C<sub>60</sub> revealed in the quantum dynamics of *ortho*- and *para*-water: A neutron-scattering investigation *Physical Chemistry Chemical Physics* **16**, 21330-21339 (2014)

Gupta M.K., Mittal R., Chaplot S.L., Rols S. Phonons, nature of bonding, and their relation to anomalous thermal expansion behaviour of M<sub>2</sub>O (M = Au, Ag, Cu) *Journal of Applied Physics* **115**, 093507-1-093507-9 (2014)

Gupta M.K., Mittal R., Zbiri M., Singh R., Rols S., Schober H., Chaplot S.L. Spin-phonon coupling, high-pressure phase transitions, and thermal expansion of multiferroic GaFeO<sub>3</sub>: A combined first principles and inelastic neutron scattering study *Physical Review B* **90**, 134304-1-134304-11 (2014)

- Haverkate L.A., Zbiri M., Johnson M.R., Carter E., Kotlewski A., Picken S., Mulder F.M., Kearley G.J. Electronic and vibronic properties of a discotic liquid-crystal and its charge transfer complex  
Journal of Chemical Physics **140**, 014903-1-014903-9 (2014)
- Huclier-Markai S., Kerdjoudj R., Alliot C., Bonraisin A.C., Michel N., Haddad F., Barbet J. Optimization of reaction conditions for the radiolabeling of DOTA and DOTA-peptide with  $^{44m/44}\text{Sc}$  and experimental evidence of the feasibility of an *in vivo* PET generator  
Nuclear Medicine and Biology **41**, e36-e43 (2014)
- Hureau M., Smirnov K.S., Moissette A., Jobic H. Vibrational dynamics of the salicylideneaniline molecule in the solid phase and the confined state  
Physical Chemistry Chemical Physics **16**, 7562-7570 (2014)
- Johnson M.R., Kearley G.J. Dynamics of atoms and molecules  
In « Experimental Methods in the Physical Sciences » Migdall A. et al. Eds. (2013, Elsevier) pp. 415-469
- Koskelo O., Köster U., Tuomisto F., Helariutta K., Sopanen M., Suihkonen S., Svensk O., Räisänen J. Migration kinetics of ion-implanted beryllium in ZnO and GaN  
Physica Scripta **88**, 035603-1-035603-5 (2013)
- Koza M.M., Leithe-Jasper A., Rosner H., Schnelle W., Mutka H., Johnson M.R., Grin Y. Vibrational dynamics of the filled skutterudite  $\text{Yb}_{1-x}\text{Fe}_4\text{Sb}_{12}$ : Debye-Waller factor, generalised density of states, and elastic structure factor  
Physical Review B **89**, 014302-1-014302-14 (2014)
- Koza M.M., Leithe-Jasper A., Sischka E., Schnelle W., Borrmann H., Mutka H., Grin Y. Effect of the electropositive elements  $A = \text{Sc}, \text{La},$  and  $\text{Ce}$  on the microscopic dynamics of  $\text{AV}_2\text{Al}_{20}$   
Physical Chemistry Chemical Physics **16**, 27119-27133 (2014)
- Krause C., Zorn R., Emmerling F., Falkenhagen J., Frick B., Huber P., Schönhals A. Vibrational density of states of triphenylene based discotic liquid crystals: Dependence on the length of the alkyl chain  
Physical Chemistry Chemical Physics **16**, 7324-7333 (2014)
- Krause C., Zorn R., Frick B., Schönhals A. Thermal properties and vibrational density of states of a nanoconfined discotic liquid crystal  
Colloid and Polymer Science **292**, 1949-1960 (2014)
- Kulszewicz-Bajer I., Louarn G., Djurado D., Skorka L., Szymanski M., Mevellec J.Y., Rols S., Pron A. Vibrational dynamics in dendritic oligoarylamines by raman spectroscopy and incoherent inelastic neutron scattering  
Journal of Physical Chemistry B **118**, 5278-5288 (2014)
- Kunkel N., Meijerink A., Kohlmann H. Bright yellow and green Eu(II) luminescence and vibronic fine structures in  $\text{LiSrH}_3$ ,  $\text{LiBaH}_3$  and their corresponding deuterides  
Physical Chemistry Chemical Physics **16**, 4807-4813 (2014)
- Micoulaut M., Coulet M.V., Piarristeguy A., Johnson M.R., Cuello G.J., Bichara C., Raty J.Y., Flores-Ruiz H., Pradel A. Effect of concentration in Ge-Te liquids: A combined density functional and neutron scattering study  
Physical Review B **89**, 174205-1-174205-13 (2014)
- Mishra S.K., Gupta M.K., Mittal R., Zbiri M., Rols S., Schober H., Chaplot S.L. Phonon dynamics and inelastic neutron-scattering of sodium niobate  
Physical Review B **89**, 184303-1-184303-9 (2014)
- Ondrejčović P., Kempa M., Kulda J., Frick B., Appel M., Combet J., Dec J., Lukaszewicz T., Hlinka J. Dynamics of nanoscale polarisation fluctuations in a uniaxial relaxor  
Physical Review Letters **113**, 167601-1-167601-5 (2014)
- Pajzderska A., Druźbicki K., González M.A., Jenczyk J., Peplińska B., Jarek M., Mielcarek J., Wasicki J. Experimental and solid-state computational study of structural and dynamic properties in the equilibrium form of temazepam  
Journal of Physical Chemistry B **118**, 6670-6679 (2014)
- Pontiroli D., Aramini M., Gaboardi M., Mazzani M., Sanna S., Caracciolo F., Carretta P., Cavallari C., Rols S., Tatti R., Aversa L., Verucchi R., Riccò M. Tracking the hydrogen motion in defective graphene  
Journal of Physical Chemistry C **118**, 7110-7116 (2014)
- Ramsahye N.A., Gao J., Jobic H., Llewellyn P.L., Yang Q., Wiersum A.D., Koza M.M., Guillerm V., Serre C., Zhong C.L., Maurin G. Adsorption and diffusion of light hydrocarbons in  $\text{UiO-66}(\text{Zr})$ : A combination of experimental and modeling tools  
Journal of Physical Chemistry C **118**, 27470-27482 (2014)
- Rao M.N., Lamago D., Ivanov A., Postnikov A.V., Hussein R.H., Basak T., Chaplot S.L., Firszt F., Paszkowicz W., Deb S.K., Pagès O. Lattice dynamics of the model percolation-type  $(\text{Zn},\text{Be})\text{Se}$  alloy: Inelastic neutron-scattering, *ab initio* study, and shell-model calculations  
Physical Review B **89**, 155201-1-155201-13 (2014)

## PUBLICATIONS

## Theory

Rosenbach N., Jobic H., Ghoufi A., Devic T., Koza M.M., Ramsahye N., Mota C.J., Serre C., Maurin G. Diffusion of light hydrocarbons in the flexible MIL-53(Cr) metal-organic framework: A combination of quasi-elastic neutron scattering experiments and molecular dynamics simulations  
*Journal of Physical Chemistry C* **118**, 14471-14477 (2014)

Sanz A., Nogales A., Puente-Orench I., García-Gutiérrez M.C., Campo J., Häussler W., Soccio M., Lotti N., Munari A., Ezquerro T.A. Confined dynamics in poly(ethylene terephthalate): A coherent and incoherent neutron-scattering study  
*Journal of Physics: Conference Series* **549**, 012011-1-012011-5 (2014)

Shoko E., Kearley G.J., Peterson V.K., Mutka H., Koza M.M., Yamaura J.I., Hiroi Z., Thorogood G.J. Novel rattling of K atoms in aluminium-doped defect pyrochlore tungstate  
*Journal of Physics: Condensed Matter* **26**, 305401-1-305401-9 (2014)

Wehinger B., Bosak A., Piccolboni G., Refson K., Chernyshov D., Ivanov A., Rumiantsev A., Krisch M. Diffuse scattering in metallic tin polymorphs  
*Journal of Physics: Condensed Matter* **26**, 115401-1-115401-9 (2014)

Xu M., Jiménez-Ruiz M., Johnson M.R., Rols S., Ye S., Carravetta M., Denning M.S., Lei X., Bačić Z., Horsewill A.J. Confirming a predicted selection rule in inelastic neutron scattering spectroscopy: The quantum translator-rotator H<sub>2</sub> entrapped inside C<sub>60</sub>  
*Physical Review Letters* **113**, 123001-1-123001-5 (2014)

Chakrabarti B., Pezzoli M.E., Sordi G., Haule K., Kotliar G.  $\alpha$ - $\gamma$  transition in cerium: Magnetic form factor and dynamic magnetic susceptibility in dynamical mean-field theory  
*Physical Review B* **89**, 125113-1-125113-4 (2014)

Denkmayr T., Geppert H., Sponar S., Lemmel H., Matzkin A., Tollaksen J., Hasegawa Y. Observation of a quantum Cheshire Cat in a matter-wave interferometer experiment  
*Nature Communications* **5**, 4492-1-4492-7 (2014)

Kawabata S., Asano Y., Tanaka Y., Golubov A.A. Robustness of spin-triplet pairing and singlet-triplet pairing crossover in superconductor/ferromagnet hybrids  
*Journal of the Physical Society of Japan* **82**, 124702-1-124702-9 (2013)

Kawai H., Yamashita K., Cannuccia E., Marini A. Electron-electron and electron-phonon correlation effects on the finite-temperature electronic and optical properties of zinc-blende GaN  
*Physical Review B* **89**, 085202-1-085202-6 (2014)

Kolokathis P.D., Pantatosaki E., Gatsiou C.A., Jobic H., Papadopoulos G.K., Theodorou D.N. Dimensionality reduction of free energy profiles of benzene in silicalite-1: Calculation of diffusion coefficients using transition state theory  
*Molecular Simulation* **40**, 80-100 (2014)

Lemmel H. Das Quantengrinsen der Cheshire-Katze  
*Physik in Unserer Zeit* **45**, 266-267 (2014)

Markovits A., Lepetit M.B. Approches pour le traitement des solides et des surfaces  
*L'Actualité Chimique* **382-383**, 29-36 (2014)

Mizuno H., Mossa S., Barrat J.L. Acoustic excitations and elastic heterogeneities in disordered solids  
*Proceedings of the National Academy of Sciences* **111**, 11949-11954 (2014)

Mizuno H., Mossa S., Barrat J.L. Elastic heterogeneity, vibrational states, and thermal conductivity across an amorphisation transition  
*EPL (Europhysics Letters)* **104**, 56001-p1-56001-p7 (2013)

Nicolas A., Martens K., Barrat J.L. Rheology of athermal amorphous solids: Revisiting simplified scenarios and the concept of mechanical noise temperature  
*Europhysics Letters* **107**, 44003-p1-44003-p6 (2014)

---

## Other

---

Nicolas A., Martens K., Bocquet L., Barrat J.L. Universal and non-universal features in coarse-grained models of flow in disordered solids

Soft Matter **10**, 4648-4661 (2014)

Nicolas A., Rottler J., Barrat J.L. Spatiotemporal correlations between plastic events in the shear flow of athermal amorphous solids

European Physical Journal E **37**, 50-1-50-11 (2014)

Puosi F., Rottler J., Barrat J.L. Time-dependent elastic response to a local shear transformation in amorphous solids

Physical Review E **89**, 042302-1-042302-7 (2014)

Singh K., Lepetit M.B., Simon C., Bellido N., Pailhès S., Varignon J., De Muer A. Analysis of the multiferroicity in the hexagonal manganite  $\text{YMnO}_3$

Journal of Physics: Condensed Matter **25**, 416002-1-416002-10 (2013)

Singh K., Simon C., Cannuccia E., Lepetit M.B., Corraze B., Janod E., Cario L. Orbital-ordering-driven multiferroicity and magnetoelectric coupling in  $\text{GeV}_4\text{S}_8$

Physical Review Letters **113**, 137602-1-137602-5 (2014)

Varignon J., Petit S., Gellé A., Lepetit M.B. An *ab initio* study of magneto-electric coupling of  $\text{YMnO}_3$

Journal of Physics: Condensed Matter **25**, 496004-1-496004-7 (2013)

Yoshida H., Mizuno H., Kinjo T., Washizu H., Barrat J.L.

Molecular dynamics simulation of electrokinetic flow of an aqueous electrolyte solution in nanochannels

Journal of Chemical Physics **140**, 214701-1-214701-12 (2014)

Aurelio G., Gardner J.S., Granado E., Kenzelmann M., Cuello G.

School on the fundamentals of neutron scattering held in Natal, Brazil

Neutron News **25**, 6-7 (2014)

Massa E., Mana G., Krempel J., Jentschel M. Polarisation delivery in heterodyne interferometry

Optics Express **21**, 27119-27126 (2013)

Mutka H. Go for the future, do not forget the past

Neutron News **25**, 2-3 (2014)

Xia F., Zhao J., Etschmann B.E., Brugger J., Garvey C.J., Rehm C., Lemmel H., Ilavsky J., Han Y.S., Pring A. Characterisation of porosity in sulfide ore minerals: A USANS/SANS study

American Mineralogist **99**, 2398-2404 (2014)





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