

Publications in 2012

In 2012, the ILL received notice of 552 publications by ILL staff and users. They are listed in the CD-ROM of this year's Annual Report.

The distribution by subject is as follows:

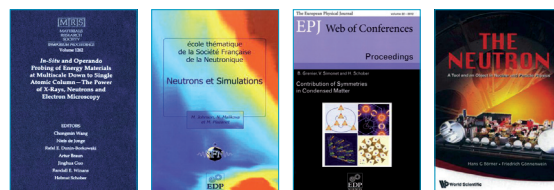
Applied Physics, Instrumentation and Techniques	28
Biology	49
Crystallography	92
Liquids and Glasses	34
Magnetic Excitations	64
Magnetic Structures	86
Materials Science and Engineering	53
Nuclear and Particle Physics	37
Theory	13
Soft Matter	72
Spectroscopy in Solid State Physics and Chemistry	24

ILL PhD studentships

PhD students at ILL in 2012*	32
PhD theses completed in 2012	7

* Receiving a grant from ILL

Books published in 2012





Sulyok G. - *Photon exchange and decoherence in neutron interferometry.*
From: Technische Universität Wien, Fakultät für Physik, Atominstitut, Germany, 2011.

Rivard C. - *Contribution à l'étude de la stabilité des minéraux constitutifs de l'argilite du Callovo-Oxfordien en présence de fer à 90°C.*
From: INP de Lorraine, Vandoeuvre-lès-Nancy, France, 2011.

Ouladdiaf S. - *Intérêt de la diffraction par les neutrons dans l'étude des biomatériaux dentaires. Caractérisation structurale de la dentine et d'un ciment silicate tricalcique, la Biodentine™.*
From: Université Claude Bernard de Lyon I, France, 2012.

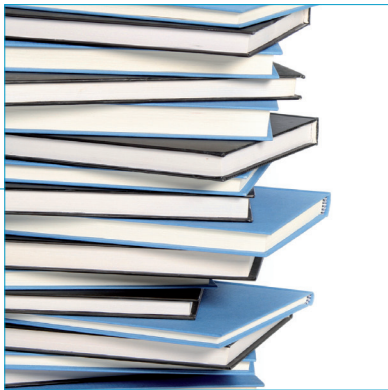
Jones A.O.F. - *Towards high throughput single crystal neutron diffraction of hydrogen bonded molecular complexes.*
From: University of Bath, UK, 2012.

Hennig M. - *Dynamics of globular proteins in crowded electrolyte solutions. Studied by neutron scattering.*
From: Eberhard Karls Universität Tübingen, Germany, 2011.

Gutfreund P. - *The microscopic origin of surface slip: A neutron and X-ray scattering study on the near surface structure of flowing liquids.*
From: Ruhr-Universität Bochum, Fakultät für Physik und Astronomie, Germany, 2011.

Groen D. - *Stratum corneum model membranes: molecular organisation in relation to skin barrier function.*
From: Universiteit Leiden, the Netherlands, 2011.



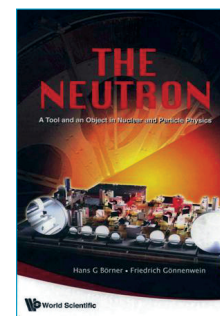
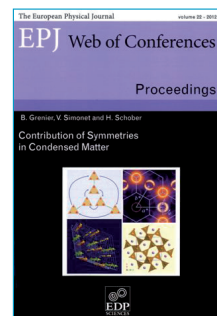
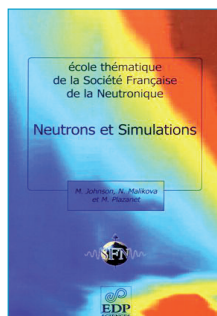
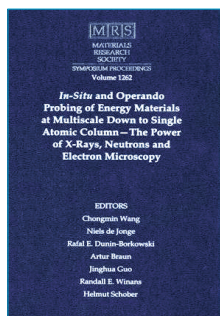


Wang C., de Jonge N., Dunin-Borkowski R.E., Braun A., Guo J., Winans R.E., Schober H.
- *In situ and Operando Probing of Energy Materials at Multiscale Down to Single Atomic Column*
- *The Power of X-Rays, Neutrons and Electron Microscopy*
Cambridge University Press (2010)

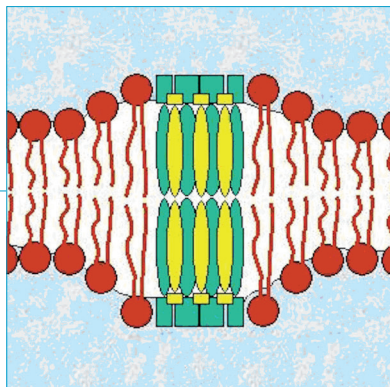
Johnson M.R., Malikova N., Plazanet M. - *Neutrons et Simulations*
EDP Sciences (2012)

Grenier B., Simonet V., Schober H.
- *Contribution of Symmetries in Condensed Matter*
EDP Sciences (2012)

Börner H.G., Gönnerwein F.
- *The Neutron: A Tool and an Object in Nuclear and Particle Physics*
World Scientific (2012)



Biology



Aurelio G., Sommadossi S.A., Cuello G.J. Crystal structure of Cu-Sn-In alloys around the η -phase field studied by neutron diffraction

Journal of Electronic Materials **41**, 3223-3231 (2012)

Chinchalikar A.J., Kumar S., Aswal V.K., Callow P., Wagh A.G. Co-existence of monomers and clusters in concentrated protein solutions

AIP Conference Proceedings **1447**, 161-162 (2012)

Christie M.P., Whitten A.E., King G.J., Hu S.H., Jarrott R.J., Chen K.E., Duff A.P., Callow P., Collins B.M., James D.E., Martin J.L. Low-resolution solution structures of Munc18:

Syntaxin protein complexes indicate an open binding mode driven by the Syntaxin N-peptide
Proceedings of the National Academy of Sciences of the USA **109**, 9816-9821 (2012)

Clifton L.A., Johnson C.L., Solovyova A.S., Callow P., Weiss K.L., Ridley H., Le Brun A.P., Kinane C.J., Webster J.R., Holt S.A., Lakey J.H. Low resolution structure and dynamics of a colicin-receptor complex determined by neutron scattering

Journal of Biological Chemistry **287**, 337-346 (2012)

Combet S., Zanotti J.M. Further evidence that interfacial water is the main "driving force" of protein dynamics: A neutron scattering study on perdeuterated C-phycoerythrin

Physical Chemistry Chemical Physics **14**, 4927-4934 (2012)

Engelbrecht T.N., Demé B., Dobner B., Neubert R.H.H. Study of the influence of the penetration enhancer isopropyl myristate on the nanostructure of stratum corneum lipid model membranes using neutron diffraction and deuterium labelling

Skin Pharmacology and Physiology **25**, 200-207 (2012)

Engelbrecht T.N., Schroeter A., Hauß T., Demé B., Scheidt H.A., Huster D., Neubert R.H.H. The impact of ceramides NP and AP on the nanostructure of *stratum corneum* lipid bilayer. Part I: neutron diffraction and ^2H NMR studies on multilamellar models based on ceramides with symmetric alkyl chain length distribution

Soft Matter **8**, 2599-2607 (2012)

Fragneto G., Charitat T., Daillant J. Floating lipid bilayers: Models for physics and biology

European Biophysics Journal **41**, 863-874 (2012)

Gabel F. Small angle neutron scattering for the structural study of intrinsically disordered proteins in solution: A practical guide

Methods in Molecular Biology **896**, 123-135 (2012)

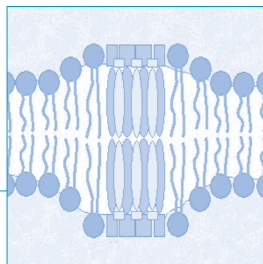
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Journal of the American Chemical Society **134**, 13168-13171 (2012)

Gallat F.X., Laganowsky A., Wood K., Gabel F., van Eijck L., Wuttke J., Moulin M., Härtlein M., Eisenberg D., Colletier J.P., Zaccai G., Weik M. Dynamical coupling of intrinsically disordered proteins and their hydration water: Comparison with folded soluble and membrane proteins

Biophysical Journal **103**, 129-136 (2012)

Biology



Garg S., Porcar L., Hamill A.C., Butler P.D., Perez-Salas U. Response to "How slow is the transbilayer diffusion (Flip-Flop) of cholesterol?"
Biophysical Journal **102**, 947-949 (2012)

Gerelli Y., Porcar L., Fragneto G. Lipid rearrangement in DSPC/DMPC bilayers:
A neutron reflectometry study
Langmuir **28**, 15922-15928 (2012)

Giménez V., James C., Armiñán A., Schweins R., Paul A., Vicent M.J. Demonstrating the importance of polymer-conjugate conformation in solution on its therapeutic output: Diethylstilbestrol (DES)-polyacetals as prostate cancer treatment
Journal of Controlled Release **159**, 290-301 (2012)

Heidebrecht T., Fish A., von Castelmur E., Johnson K.A., Zaccai G., Borst P., Perrakis A. Binding of the J-binding protein to DNA containing glucosylated hmU (base J) or 5-hmC: Evidence for a rapid conformational change upon DNA binding
Journal of the American Chemical Society **134**, 13357-13365 (2012)

Hughes R.C., Coates L., Blakeley M.P., Tomanicek S.J., Langan P., Kovalevsky A.Y., García-Ruiz J.M., Ng J.D. Inorganic pyrophosphatase crystals from *Thermococcus thio还原ens* for X-ray and neutron diffraction
Acta Crystallographica F **68**, 1482-1487 (2012)

Kennaway C.K., Taylor J.E., Song C.F., Potrzebowski W., Nicholson W., White J.H., Swiderska A., Obarska-Kosinska A., Callow P., Cooper L.P., Roberts G.A., Artero J.B., Bujnicki J.M., Trinick J., Kneale G.G., Dryden D.T.F. Structure and operation of the DNA-translocating type I DNA restriction enzymes
Genes & Development **26**, 92-104 (2012)

Kovalevsky A., Hanson B.L., Mason S.A., Forsyth V.T., Fisher Z., Mustyakimov M., Blakeley M.P., Keen D.A., Langan P. Inhibition of D-xylose isomerase by polyols: Atomic details by joint X-ray/neutron crystallography
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Neutron News **23**, 22-24 (2012)

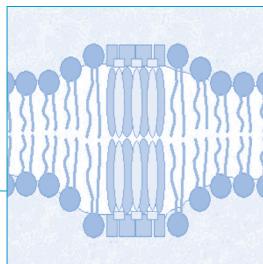
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European Biophysics Journal **41**, 361-367 (2012)

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Journal of Non-Crystalline Solids **358**, 2635-2640 (2012)

Merlino A., Vitiello G., Grimaldi M., Sica F., Busi E., Basosi R., D'Ursi A.M., Fragneto G., Paduano L., D'Errico G. Destabilisation of lipid membranes by a peptide derived from glycoprotein gp36 of feline immunodeficiency virus: A combined molecular dynamics/experimental study
Journal of Physical Chemistry B **116**, 401-412 (2012)

Biology



Myles D.A.A., Dauvergne F., Blakeley M.P., Meilleur F. Neutron protein crystallography at ultra-low (<15K) temperatures

Journal of Applied Crystallography **45**, 686-692 (2012)

Nagy G., Pieper J., Krumova S.B., Kovács L., Trapp M., Garab G., Peters J. Dynamic properties of photosystem II membranes at physiological temperatures characterised by elastic incoherent neutron scattering. Increased flexibility associated with the inactivation of the oxygen evolving complex
Photosynthesis Research **111**, 113-124 (2012)

Nagy G., Szabó M., Ünneper R., Káli G., Miloslavina Y., Lambrev P.H., Zsiros O., Porcar L., Timmins P., Rosta L., Garab G. Modulation of the multilamellar membrane organisation and of the chiral macrodomains in the diatom *Phaeodactylum tricornutum* revealed by small-angle neutron scattering and circular dichroism spectroscopy
Photosynthesis Research **111**, 71-79 (2012)

Ossowski S., Jackson A., Obiols-Rabasa M., Holt C., Lenton S., Porcar L., Paulsson M., Nylander T. Aggregation behavior of bovine κ - and β -casein studied with small angle neutron scattering, light scattering, and cryogenic transmission electron microscopy
Langmuir **28**, 13577-13589 (2012)

Paciaroni A., Orecchini A., Haertlein M., Moulin M., Conti Nibali V., De Francesco A., Petrillo C., Sacchetti F. Vibrational collective dynamics of dry proteins in the terahertz region
Journal of Physical Chemistry B **116**, 3861-3865 (2012)

Peters J., Trovaslet M., Trapp M., Nachon F., Hill F., Royer E., Gabel F., van Eijck L., Masson P., Tehei M. Activity and molecular dynamics relationship within the family of human cholinesterases
Physical Chemistry Chemical Physics **14**, 6764-6770 (2012)

Pieper J., Trapp M., Skomorokhov A., Natkaniec I., Peters J., Renger G. Temperature-dependent vibrational and conformational dynamics of photosystem II membrane fragments from spinach investigated by elastic and inelastic neutron scattering
Biochimica et Biophysica Acta **1817**, 1213-1219 (2012)

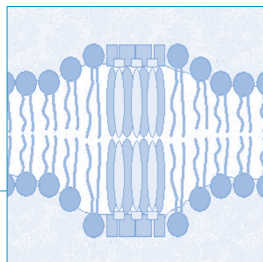
Posselt D., Nagy G., Kirkensgaard J.J.K., Holm J.K., Aagaard T.H., Timmins P., Rétfalvi E., Rosta L., Kovács L., Garab G. Small-angle neutron scattering study of the ultrastructure of chloroplast thylakoid membranes - Periodicity and structural flexibility of the stroma lamellae
Biochimica et Biophysica Acta **1817**, 1220-1228 (2012)

Prokeš K., Hiess A., Bao W., Wheeler E., Landsgesell S., Argyriou D.N. Anisotropy of the (π, π) dynamic susceptibility in magnetically ordered ($\chi=0.05$) and superconducting ($\chi=0.40$) $\text{Fe}_{1.02}\text{Te}_{1-\chi}\text{Se}_{\chi}$
Physical Review B **86**, 064503-1-064503-5 (2012)

Sawada D., Nishiyama Y., Langan P., Forsyth V.T., Kimura S., Wada M. Direct determination of the hydrogen bonding arrangement in anhydrous β -chitin by neutron fiber diffraction
Biomacromolecules **13**, 288-291 (2012)

Sawada D., Nishiyama Y., Langan P., Forsyth V.T., Kimura S., Wada M. Water in crystalline fibers of dihydrate β -chitin results in unexpected absence of intramolecular hydrogen bonding
PLoS One **7**, e39376-1-e39376-8 (2012)

Biology



Schiró G., Natali F., Cupane A. Physical origin of anharmonic dynamics in proteins: New insights from resolution-dependent neutron scattering on homomeric polypeptides
Physical Review Letters **109**, 128102-1-128102-5 (2012)

Schiró G., Vetri V., Frick B., Militello V., Leone M., Cupane A. Neutron scattering reveals enhanced protein dynamics in Concanavalin A amyloid fibrils
Journal of Physical Chemistry Letters **3**, 992-996 (2012)

Selvam P., Bharatwaj B., Porcar L., da Rocha S.R.P. Reverse aqueous microemulsions in hydrofluoroalkane propellants and their aerosol characteristics
International Journal of Pharmaceutics **422**, 428-435 (2012)

Sharma K.S., Durand G., Gabel F., Bazzacco P., Le Bon C., Billon-Denis E., Catoire L.J., Popot J.L., Ebel C., Pucci B. Non-ionic amphiphilic homopolymers: Synthesis, solution properties, and biochemical validation
Langmuir: the ACS journal of surfaces and colloids **28**, 4625-4639 (2012)

Stadler A.M., Fabiani E., Zaccai G. Changes in molecular dynamics of apomyoglobin during amyloid formation
Journal of Physics: Conference Series **340**, 012092-1-012092-9 (2012)

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Journal of the Royal Society Interface **9**, 2845-2855 (2012)

Stadler A.M., Pellegrini E., Johnson M., Fitter J., Zaccai G. Dynamics-stability relationships in apo- and holomyoglobin: A combined neutron scattering and molecular dynamics simulations study
Biophysical Journal **102**, 351-359 (2012)

Taylor J.E., Swiderska A., Artero J.B., Callow P., Kneale G. Structural and functional analysis of the symmetrical type I restriction endonuclease R.EcoR124_{NT}
PLoS One **7**, e35263-1-e35263-7 (2012)

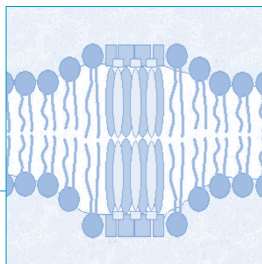
Teixeira S.C.M. Neutron protein crystallography at our table
Neutron News **23**, 19-21 (2012)

Trapp M., Trovaslet M., Nachon F., Koza M.M., van Eijck L., Hill F., Weik M., Masson P., Tehei M., Peters J. Energy landscapes of *human* acetylcholinesterase and its huperzine A-inhibited counterpart
Journal of Physical Chemistry B **116**, 14744-14753 (2012)

Wadsäter M., Laursen T., Singha A., Hatzakis N.S., Stamou D., Barker R., Mortensen K., Feidenhans'l R., Lindberg Møller B., Cárdenas M. Monitoring shifts in the conformation equilibrium of the membrane protein cytochrome P450 reductase (POR) in nanodiscs
Journal of Biological Chemistry **287**, 34596-34603 (2012)

Wood K., Gallat F.X., Otten R., van Heel A.J., Lethier M., van Eijck L., Moulin M., Haertlein M., Weik M., Mulder F.A.A. Protein surface and core dynamics show concerted hydration-dependent activation
Angewandte Chemie International Edition **51**, 1-5 (2012)

Biology



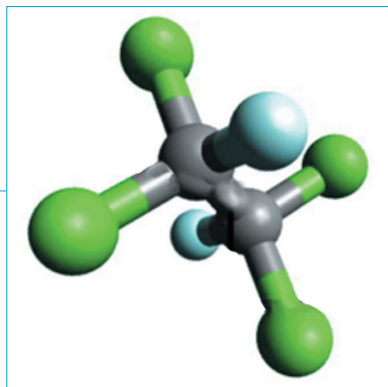
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Proceedings of the National Academy of Sciences of the USA **108**, 9839-9844 (2011)

Perkins S.J., Nan R., Li K., Khan S., Abe Y. Analytical ultracentrifugation combined with X-ray and neutron scattering: Experiment and modelling
Methods **54**, 181-199 (2011)



Liquids and Glasses



Amann-Winkel K., Löw F., Handle P.H., Knoll W., Peters J., Geil B., Fujara F., Loerting T. Limits of metastability in amorphous ices: The neutron scattering Debye-Waller factor
Physical Chemistry Chemical Physics **14**, 16386-16391 (2012)

Bafile U., Celli M., Colognesi D., Zoppi M., Guarini E., De Francesco A., Formisano F., Neumann M. Neutron study of non-Gaussian self dynamics in liquid parahydrogen
Journal of Physics: Conference Series **340**, 012076-1-012076-10 (2012)

Blochowicz T., Schramm S., Lusceac S., Vogel M., Stühn B., Gutfreund P., Frick B. Signature of a type-A glass transition and intrinsic confinement effects in a binary glass-forming system
Physical Review Letters **109**, 035702-1-035702-5 (2012)

Chathoth S.M., Koza M.M., Meyer A. Complex atomic dynamics in a deep-eutectic binary metallic melt
Materials Chemistry and Physics **136**, 296-299 (2012)

Chiapponi C., Di Bari M.T., Gerelli Y., Deriu A., Chiessi E., Finelli I., Paradossi G., Russina M., Izaola Z., Garcia Sakai V. Water dynamics in physical hydrogels based on partially hydrophobized hyaluronic acid
Journal of Physical Chemistry B **116**, 12915-12921 (2012)

Comez L., Corezzi S., Orecchini A., Paciaroni A., Petrillo C., Santucci S.C., Sacchetti F., Fioretto D. A comparison between acoustic compliance and self-particle susceptibility in associated liquids: The case of water and glycerol
Journal of Molecular Liquids **176**, 76-78 (2012)

Dawidowski J., Cuello G.J. Experimental corrections in neutron diffraction of ambient water using H/D isotopic substitution
Journal of Physics: Conference Series **340**, 012004-1-012004-11 (2012)

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Physics and Chemistry of Liquids **50**, 31-38 (2012)

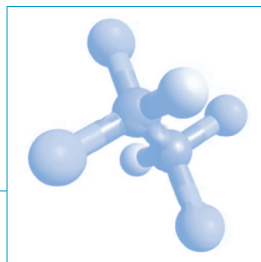
Drewitt J.W.E., Hennet L., Zeidler A., Jahn S., Salmon P.S., Neuville D.R., Fischer H.E. Structural transformations on vitrification in the fragile glass-forming system CaAl_2O_4
Physical Review Letters **109**, 235501-1-235501-5 (2012)

Fernandez-Martin C., Bruno G., Crochet A., Ovono Ovono D., Comte M., Hennet L. Nucleation and growth of nanocrystals in glass-ceramics: An *in situ* SANS perspective
Journal of the American Ceramic Society **95**, 1304-1312 (2012)

Hofmann T., Wallacher D., Mayorova M., Zorn R., Frick B., Huber P. Molecular dynamics of n-hexane: A quasi-elastic neutron scattering study on the bulk and spatially nanochannel-confined liquid
Journal of Chemical Physics **136**, 124505-1-124505-9 (2012)

Holland-Moritz D., Yang F., Kordel T., Klein S., Kargl F., Gegner J., Hansen T., Bednarcik J., Kaban I., Shuleshova O., Mattern N., Meyer A. Does an icosahedral short-range order prevail in glass-forming Zr-Cu melts?
Europhysics Letters **100**, 56002-p1-56002-p6 (2012)

Liquids and Glasses



Jakse N., Bouhadja M., Kozaily J., Drewitt J.W.E., Hennet L., Neuville D.R., Fischer H.E., Cristiglio V., Pasturel A. Interplay between non-bridging oxygen, triclusters, and fivefold Al coordination in low silica content calcium aluminosilicate melts

Applied Physics Letters **101**, 201903-1-201903-5 (2012)

Kofu M., Someya T., Tatsumi S., Ueno K., Ueki T., Watanabe M., Matsunaga T., Shibayama M., García Sakai V., Tyagi M., Yamamuro O. Microscopic insights into ion gel dynamics using neutron spectroscopy

Soft Matter **8**, 7888-7897 (2012)

Mamontov E., De Francesco A., Formisano F., Laloni A., Sani L., Leu B.M., Said A.H., Kolesnikov A.I. Water dynamics in a lithium chloride aqueous solution probed by Brillouin neutron and X-ray scattering

Journal of Physics Condensed Matter **24**, 064102-1-064102-9 (2012)

Martin R.A., Moss R.M., Lakhkar N.J., Knowles J.C., Cuello G.J., Smith M.E., Hanna J.V., Newport R.J. Structural characterisation of titanium-doped Bioglass using isotopic substitution neutron diffraction

Physical Chemistry Chemical Physics **14**, 15807-15815 (2012)

Mason P.E., Wernersson E., Jungwirth P. Accurate description of aqueous carbonate ions: An effective polarisation model verified by neutron scattering

Journal of Physical Chemistry B **116**, 8145-8153 (2012)

Meyer A., Kargl F., Horbach J. Channel diffusion in sodium silicate melts

Neutron News **23**, 35-37 (2012)

Orecchini A., Paciaroni A., Petrillo C., Sebastiani F., De Francesco A., Sacchetti F. Water dynamics as affected by interaction with biomolecules and change of thermodynamic state: A neutron scattering study

Journal of Physics Condensed Matter **24**, 064105-1-064105-8 (2012)

Orecchini A., Sebastiani F., Jasnin M., Paciaroni A., De Francesco A., Petrillo C., Moulin M., Haertlein M., Zaccai G., Sacchetti F. Collective dynamics of intracellular water in living cells

Journal of Physics: Conference Series **340**, 012091-1-012091-7 (2012)

Piarristeguy A.A., Cuello G.J., Fernández-Martínez A., Cristiglio V., Johnson M., Ribes M., Pradel A. Short range order and Ag diffusion threshold in $\text{Ag}_x(\text{Ge}_{0.25}\text{Se}_{0.75})_{100-x}$ glasses

Physica Status Solidi (b) **249**, 2028-2033 (2012)

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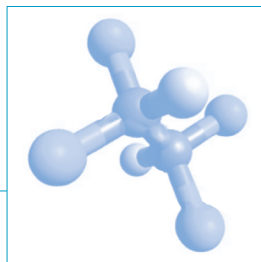
Russo D., Orecchini A., De Francesco A., Formisano F., Laloni A., Petrillo C., Sacchetti F. Brillouin neutron spectroscopy as a probe to investigate collective density fluctuations in biomolecules hydration water

Spectroscopy: An International Journal **27**, 293-305 (2012)

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Journal of Physics Condensed Matter **24**, 415102-1-415102-17 (2012)

Liquids and Glasses



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Structure and triclustering in Ba-Al-O glass
Physical Review B **85**, 064201-1-064201-12 (2012)

Violini N., Orecchini A., Paciaroni A., Petrillo C., Sacchetti F. Neutron scattering investigation of high-frequency dynamics in glassy glucose
Physical Review B **85**, 134204-1-134204-7 (2012)

Wezka K., Salmon P.S., Zeidler A., Whittaker D.A.J., Drewitt J.W.E., Klotz S., Fischer H.E., Marrocchelli D. Mechanisms of network collapse in GeO₂ glass: High-pressure neutron diffraction with isotope substitution as arbitrator of competing models
Journal of Physics Condensed Matter **24**, 502101-1-502101-9 (2012)

Wright A.C., Sinclair R.N., Stone C.E., Shaw J.L., Feller S.A., Kiczinski T.J., Williams R.B., Berger H.A., Fischer H.E., Vedishcheva N.M. A neutron diffraction study of 2M₂O.5B₂O₃ (M=Li, Na, K, Rb, Cs & Ag) and 2MO.5B₂O₃ (M=Ca & Ba) glasses
Physics and Chemistry of Glasses **53**, 191-204 (2012)

Wu B., Kerkeni B., Egami T., Do C., Liu Y., Wang Y., Porcar L., Hong K., Smith S.C., Liu E.L., Smith G.S., Chen W.R. Structured water in polyelectrolyte dendrimers: Understanding small angle neutron scattering results through atomistic simulation
Journal of Chemical Physics **136**, 144901-1-144901-9 (2012)

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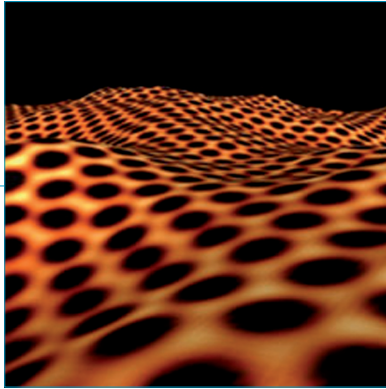
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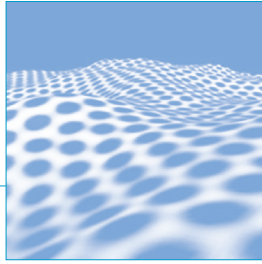
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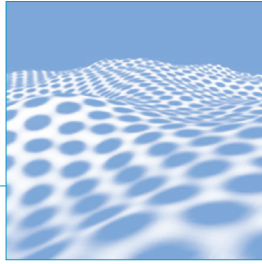
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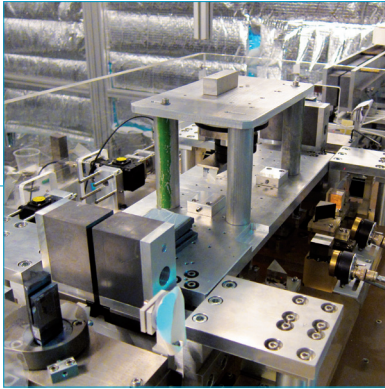
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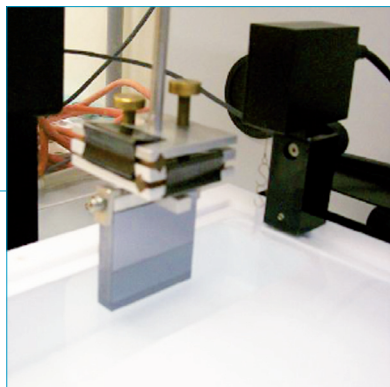


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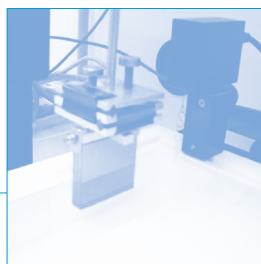
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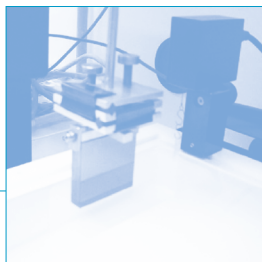
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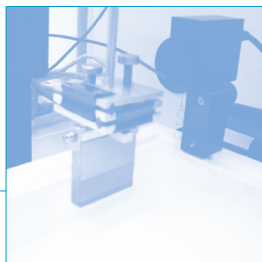
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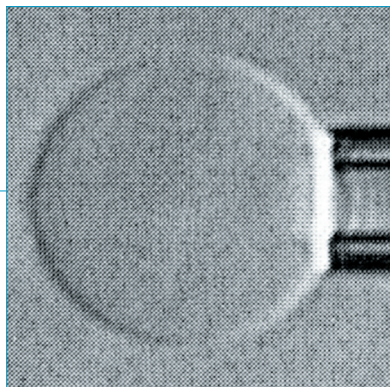
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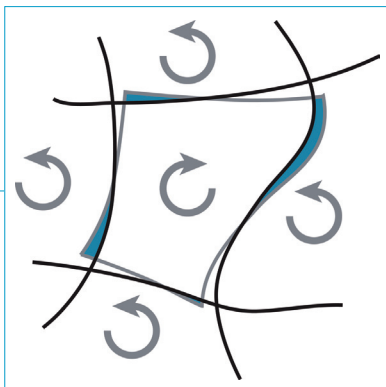
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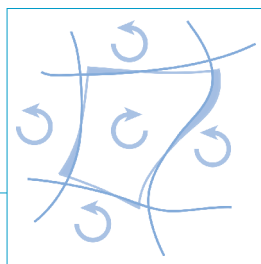
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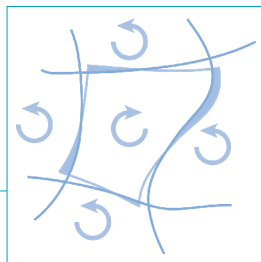
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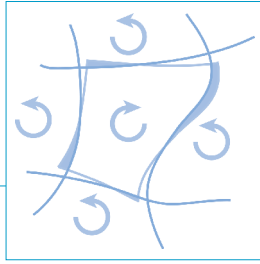
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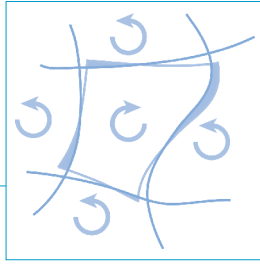
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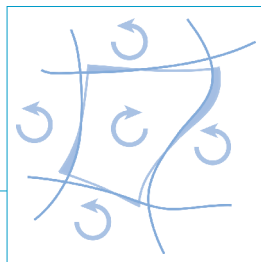
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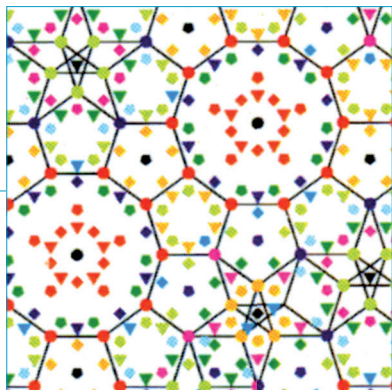
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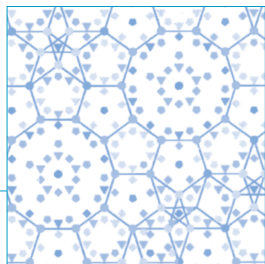
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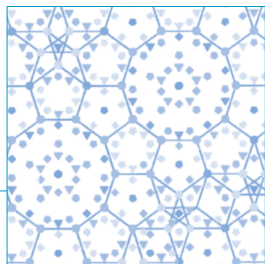
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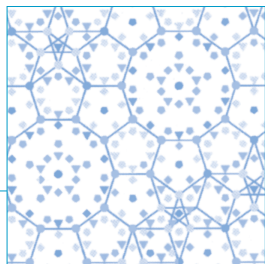
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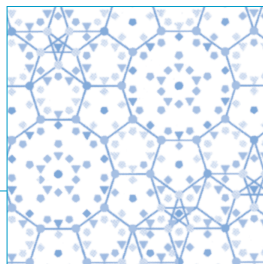
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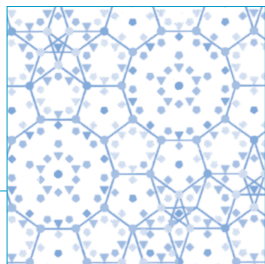
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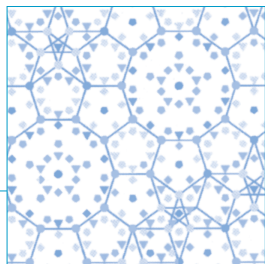
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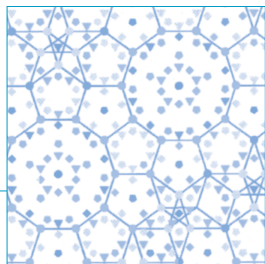
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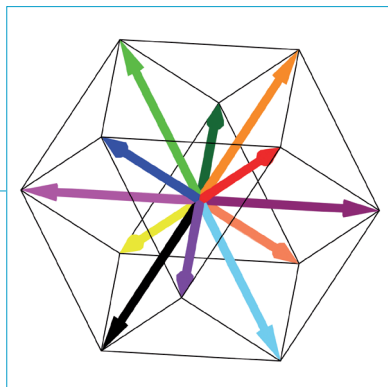
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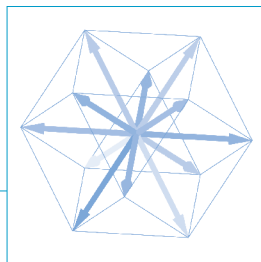
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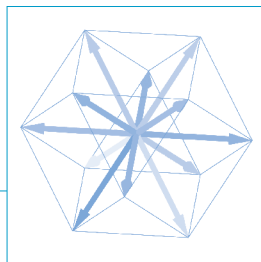
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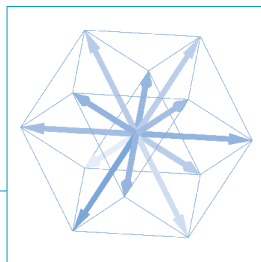
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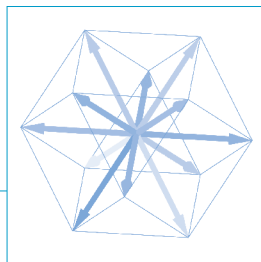
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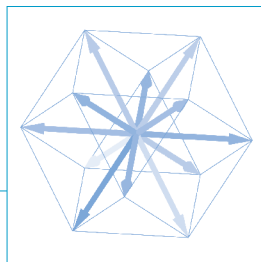
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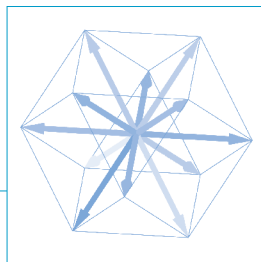
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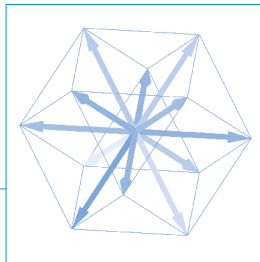
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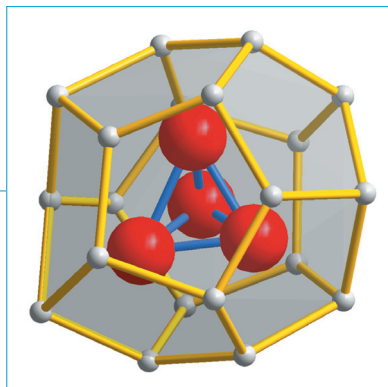
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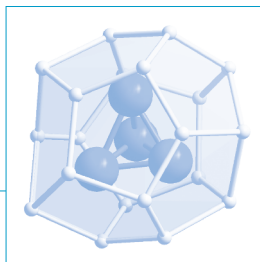
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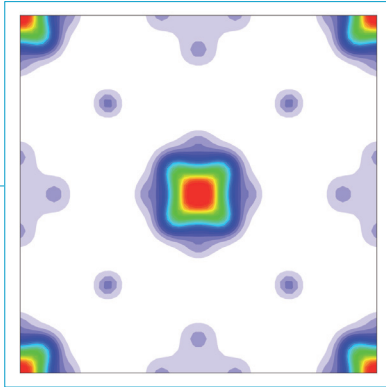
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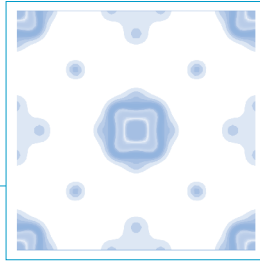
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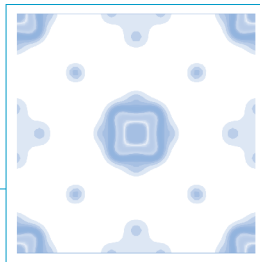
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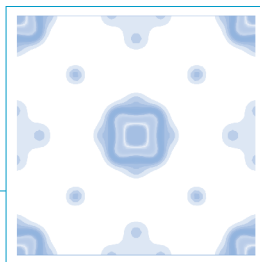
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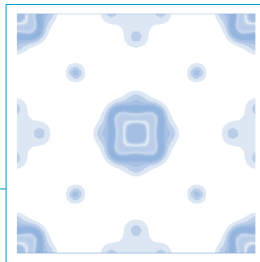
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