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Condensed Matter Science at Molecular Spectroscopy Group

Sanghamitra Mukhopadhyay

ISIS Facility, Rutherford Appleton Laboratory, Oxfordshire

Science & Technology Facilities Council
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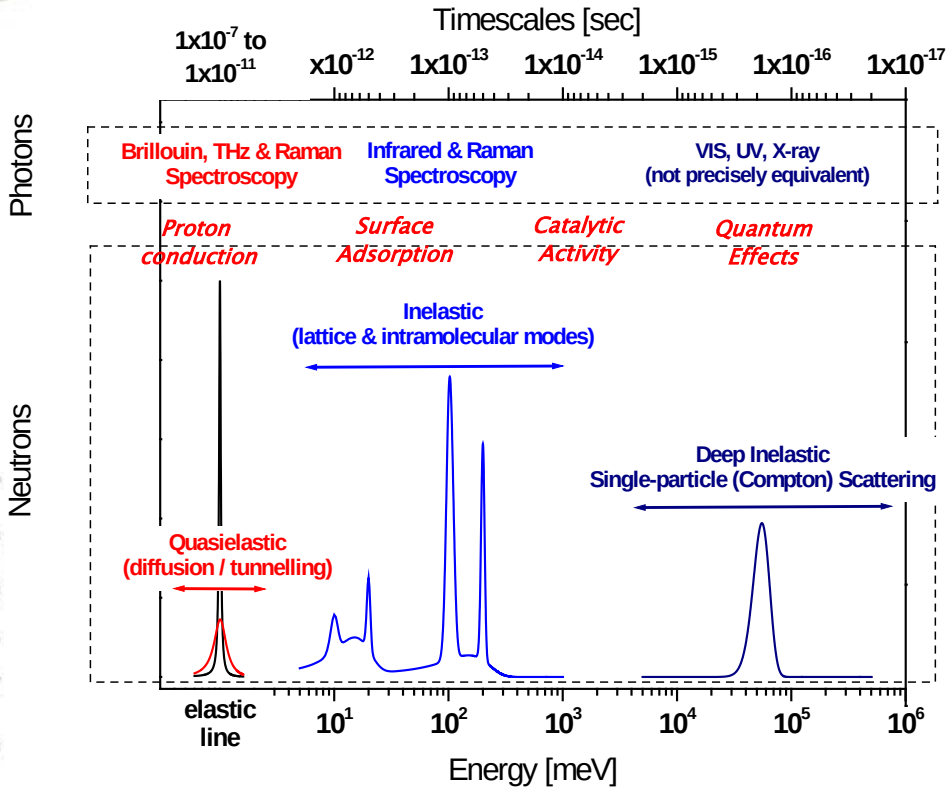
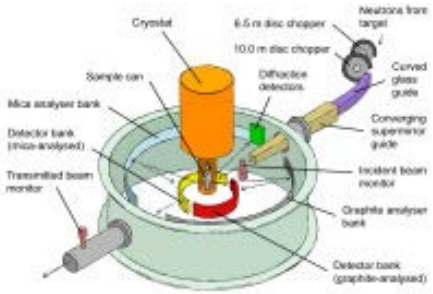
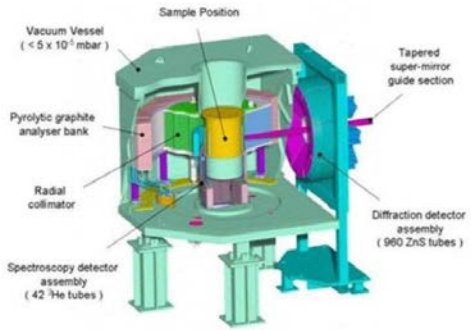
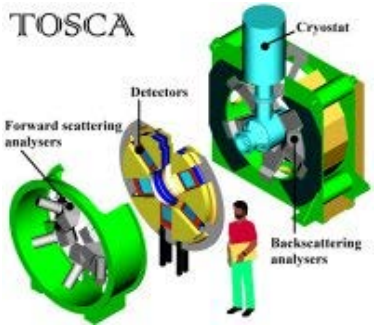
Chemical Spectroscopy









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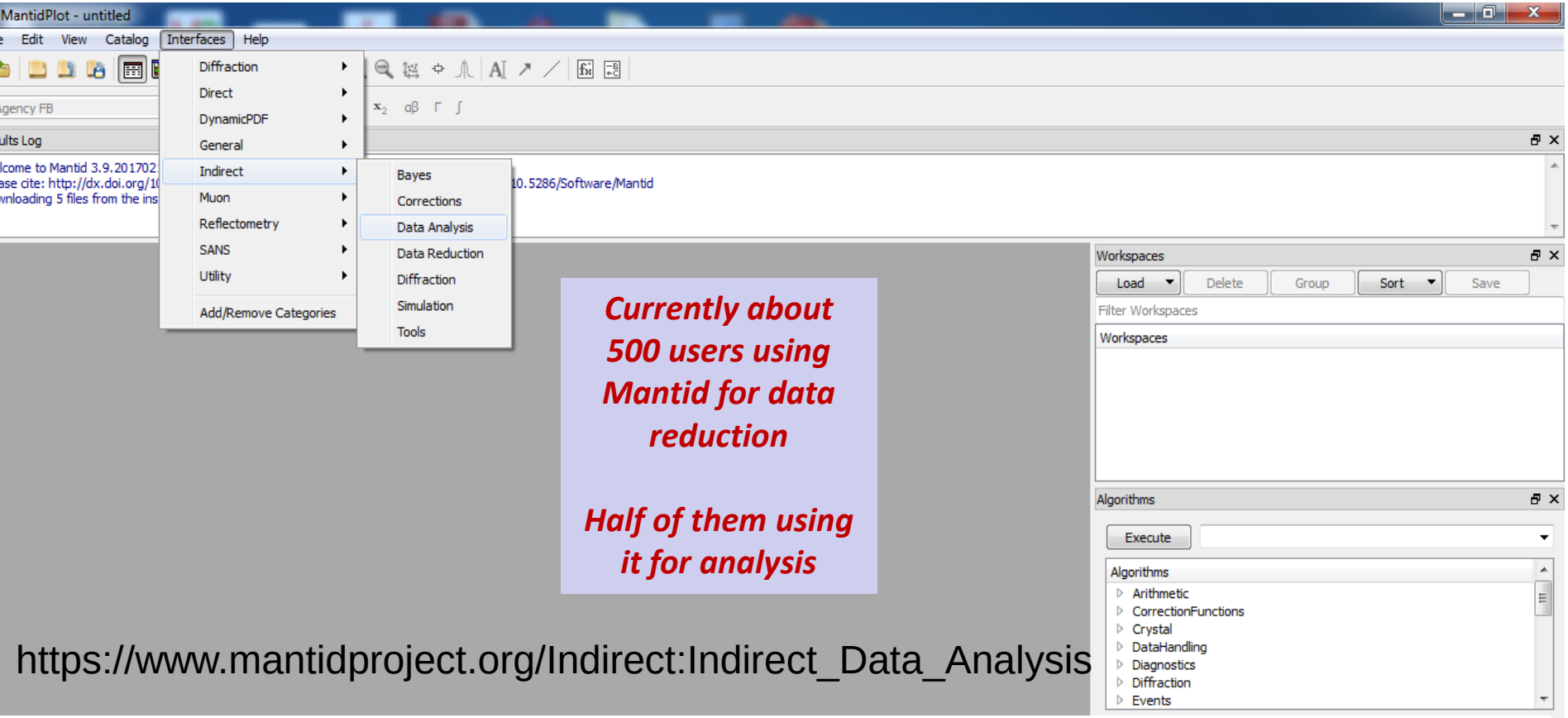
Indirect Interface in Mantid



Currently about 500 users using Mantid for data reduction

Half of them using it for analysis

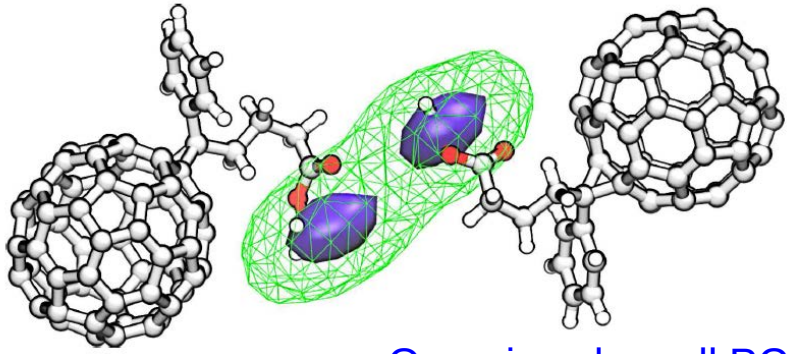
https://www.mantidproject.org/Indirect:Indirect_Data_Analysis

10 Reports/papers are on ePubs on the implementations.

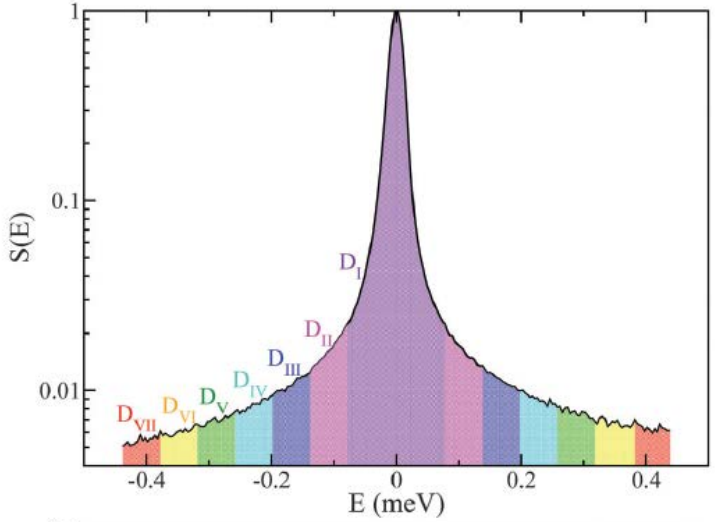
About 130 research papers/theses published in 2016-17 from the group have used Mantid in some form

iiref -> A brief reference about the graphical user interface.

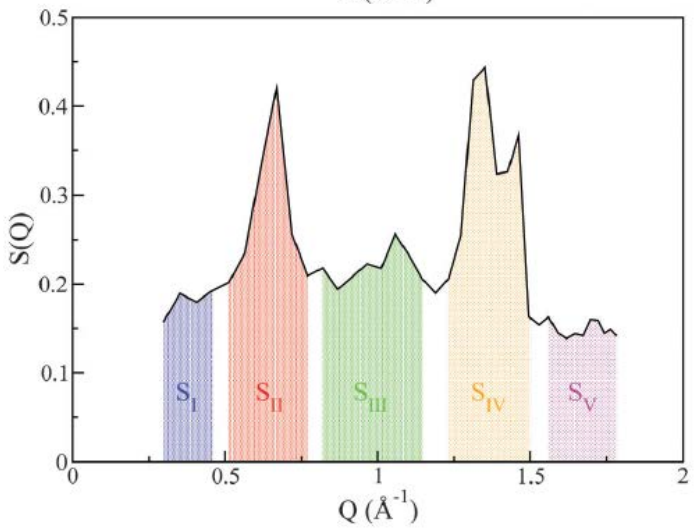
QENS on Organic Photovoltaic Materials



Organic solar cell PCBM



Analysis shows that the melting of this material is entirely driven by its tail motions



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PAPER

View Article Online
View Journal | View Issue

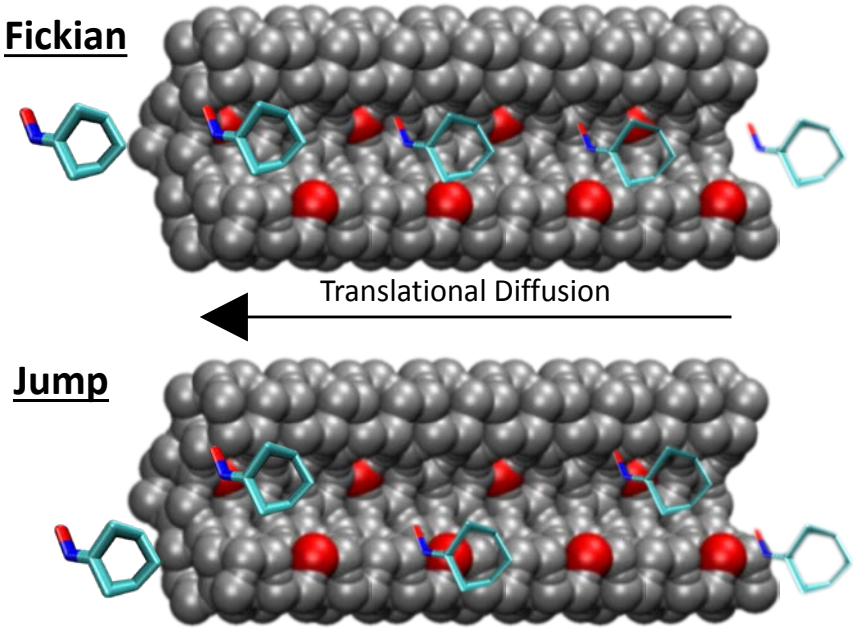
CrossMark

Cite this: *Phys. Chem. Chem. Phys.*, 2016, **18**, 17202

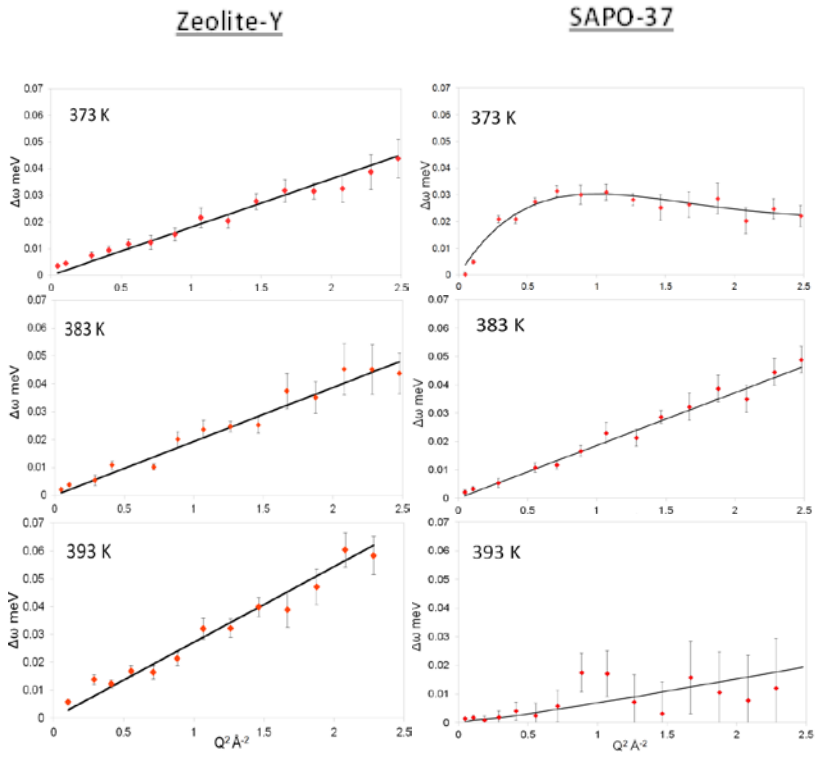
Heads or tails: how do chemically substituted fullerenes melt?

Jeff Armstrong,*[ab] Sanghamitra Mukhopadhyay,[ab] Fernando Bresme[ac] and Felix Fernandez-Alonso*[bd]

QENS Experiment to design solid acid catalyst



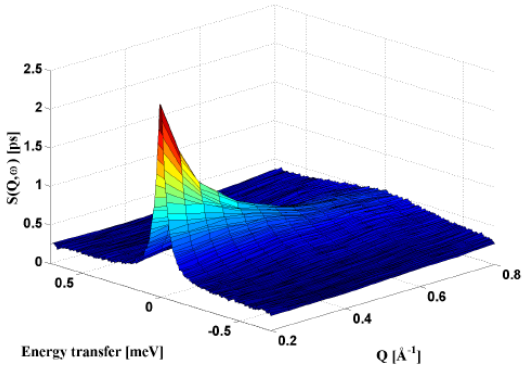
Diffusion modes of cyclohexanone oxime passing through a pore with active sites (red), Top: Smooth Fickian diffusion means the oxime diffuses straight down the pore. Bottom: Jump diffusion sees the oxime move between active sites with a specific residence time.



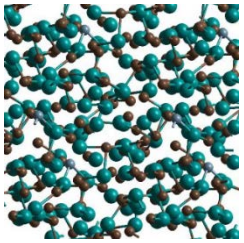
The *Q* dependence of the HWHM of the Lorentzian for Zeolite-Y (left) and SAPO-37 (right) obtained from QENS experiment on OSIRIS

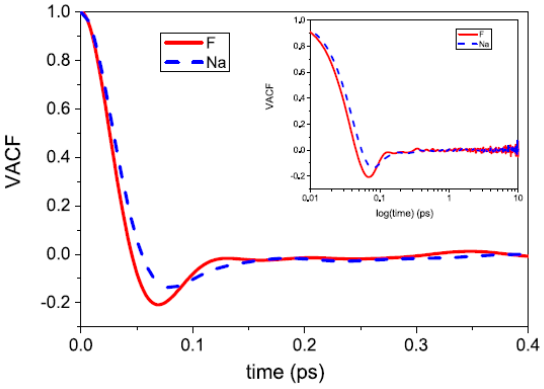
ME Potter, et al. ACS Catalysis **7** 2926-2934 (2017)

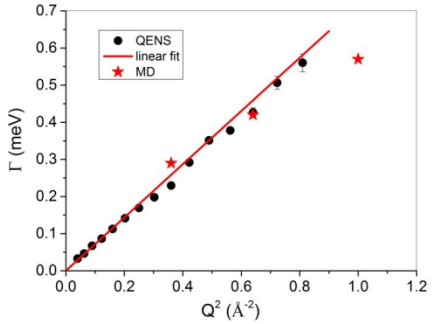
Single particle dynamics from molten salt

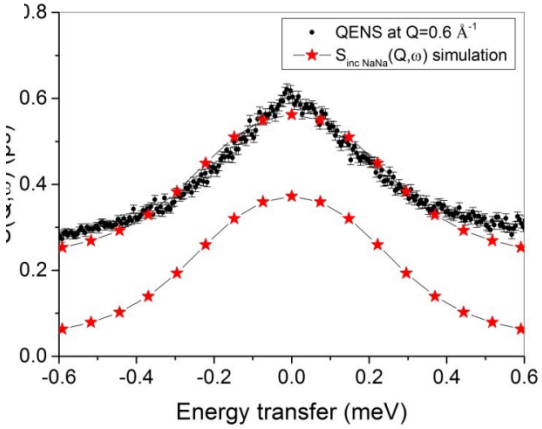


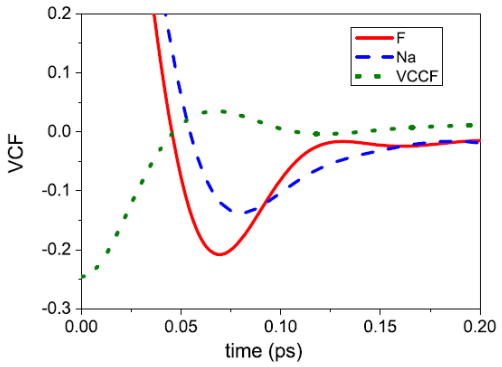
OSIRIS Experiment is compared with DFT-MD











THE JOURNAL OF CHEMICAL PHYSICS **144**, 014503 (2016)

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Quasielastic neutron scattering measurements and *ab initio* MD-simulations on single ion motions in molten NaF

F. Demmel[1] and S. Mukhopadhyay[1,2]
[1]*ISIS Facility, Rutherford Appleton Laboratory, Didcot OX11 0QX, United Kingdom*
[2]*Department of Materials, Imperial College London, Exhibition Road, London SW7 2AZ, United Kingdom*

(Received 17 September 2015; accepted 15 December 2015; published online 7 January 2016)

Soft Confinement Nanoparticles

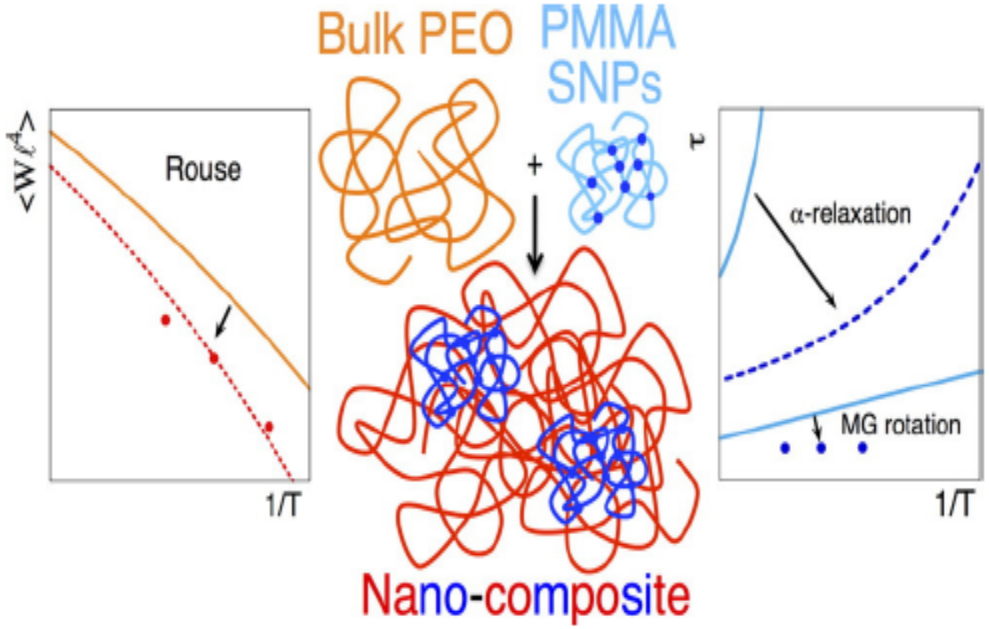
Macromolecules

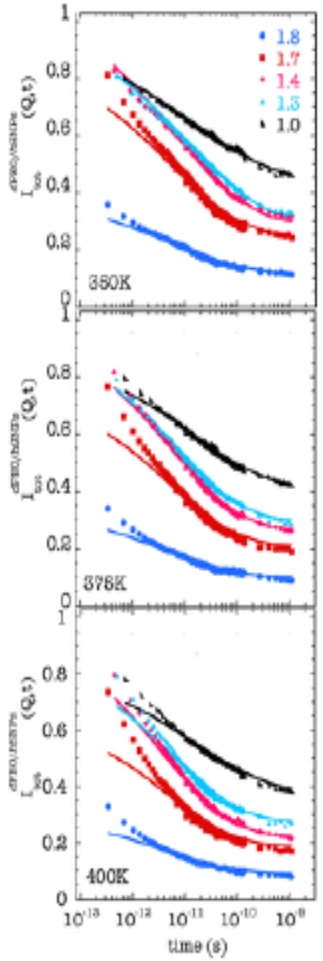
Article

pubs.acs.org/Macromolecules

Microscopic Dynamics in Nanocomposites of Poly(ethylene oxide) and Poly(methyl methacrylate) Soft Nanoparticles: A Quasi-Elastic Neutron Scattering Study

D. Bhowmik,[†] J. A. Pomposo,[‡,¶,§] F. Juranyi,[∥] V. García-Sakai,[⊥] M. Zamponi,[#] Y. Su,[#] A. Arbe,[*,‡] and J. Colmenero[†,‡]





Design of Drug Delivery Vectors

Soft Matter

Cite this: *Soft Matter*, 2011, **7**, 3929

www.rsc.org/softmatter **PAPER**

Conformational and segmental dynamics in lipid-based vesicles†

Yuri Gerelli,‡*[a][b] Victoria Garcia Sakai,[c] Jacques Ollivier[d] and Antonio Deriu[a][b]

Received 11th November 2010, Accepted 14th January 2011
DOI: 10.1039/c0sm01301c

ELSEVIER

Available online at www.sciencedirect.com
ScienceDirect
Chemical Physics 345 (2008) 239–244

Chemical Physics
www.elsevier.com/locate/chemphys

Dynamics of lipid–saccharide nanoparticles by quasielastic neutron scattering

M.T. Di Bari [a], Y. Gerelli [a], F. Sonvico [b], A. Deriu [a,*], F. Cavatorta [a], G. Albanese [a], P. Colombo [b], F. Fernandez-Alonso [c]

[a] *Dipartimento di Fisica and Unità CNISM, Università degli Studi di Parma, Italy*
[b] *Dipartimento Farmaceutico, Università degli Studi di Parma, Italy*
[c] *ISIS Facility, Rutherford Appleton Laboratory, Chilton, Didcot, Oxfordshire OX11 0QX, UK*

Received 31 January 2007; accepted 3 August 2007
Available online 11 August 2007

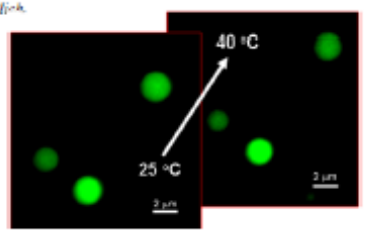
J. Phys. Chem. B **2010**, *114*, 10285–10293 **10285**

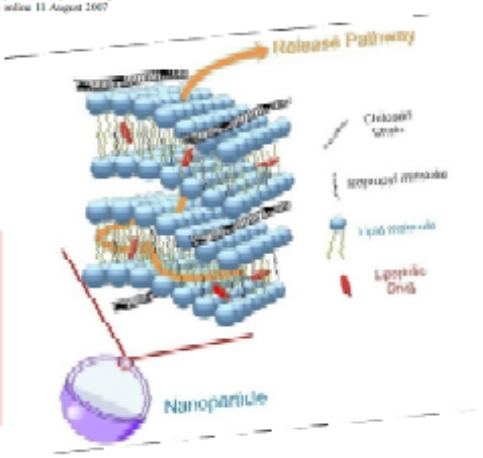
Structure and Dynamics of a Thermoresponsive Microgel around Its Volume Phase Transition Temperature

Shivkumar V. Ghugare,[†] Ester Chiessi,[†] Mark T. F. Telling,[‡] Antonio Deriu,[§] Yuri Gerelli,[§] Joachim Wuttke,[∥] and Gaio Paradossi*[,†]

Dipartimento di Scienze e Tecnologie Chimiche, Università di Roma Tor Vergata and SOFT, CNR-INFM, Rome, Italy; ISIS Facility, Rutherford Appleton Laboratory, Chilton Didcot, Oxfordshire OX11 0QX, U.K.; Dipartimento di Fisica, Università di Parma, Parma, Italy; and JCNS at FRM II, Forschungszentrum Jülich, 85747 Garching, Germany

Received: February 1, 2010; Revised Manuscript Received: June 18, 2010





Soft Matter

Cite this: *Soft Matter*, 2012, **8**, 2494

www.rsc.org/softmatter **PAPER**

Biodegradable dextran based microgels: a study on network associated water diffusion and enzymatic degradation†

Shivkumar V. Ghugare,[a] Ester Chiessi,[a] Barbara Cerroni,[a] Mark T. F. Telling,[b,c] Victoria Garcia Sakai[b] and Gaio Paradossi*[a]

Received 1st August 2011, Accepted 12th December 2011
DOI: 10.1039/c2sm06476f

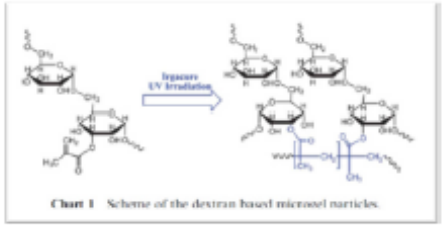


Chart 1 Scheme of the dextran based microsol particles.

Magnetism in Rare-Earths

PHYSICAL REVIEW B 86, 064203 (2012)

Coexistence of long- and short-range magnetic order in the frustrated magnet $SrYb_2O_4$

D. L. Quintero-Castro,[1,2,*] B. Lake,[1,2] M. Reehuis,[1] A. Niazi,[3] H. Ryll,[1,2] A. T. M. N. Islam,[1] T. Fennell,[4,5] S. A. J. Kimber,[1,6] B. Klemke,[1] J. Ollivier,[4] V. Garcia Sakai,[7] P. P. Deen,[4,8] and H. Mutka[4]

[1]*Helmholtz-Zentrum Berlin für Materialien und Energie, D-14109 Berlin, Germany*

[2]*Institut für Festkörperphysik, Technische Universität Berlin, D-10623 Berlin, Germany*

[3]*Department of Physics, Faculty of Natural Sciences, Jamia Millia Islamia University, New Delhi 110025, India*

[4]*Institut Laue Langevin, 6 rue Jules Horowitz, BP 156, F-38042, Grenoble Cedex 9, France*

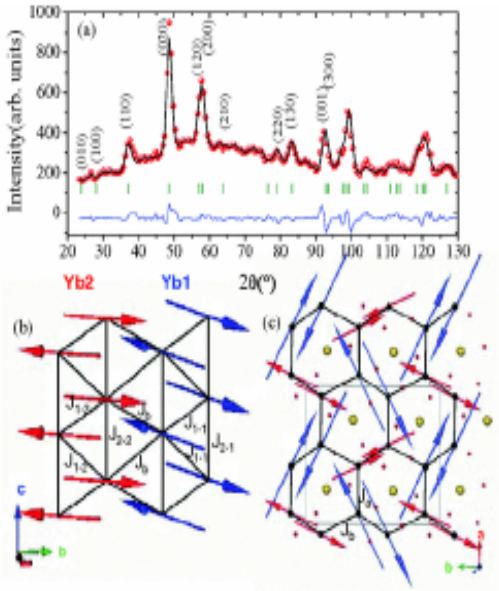
[5]*Laboratory for Neutron Scattering, PSI, CH-5232 Villigen, Switzerland*

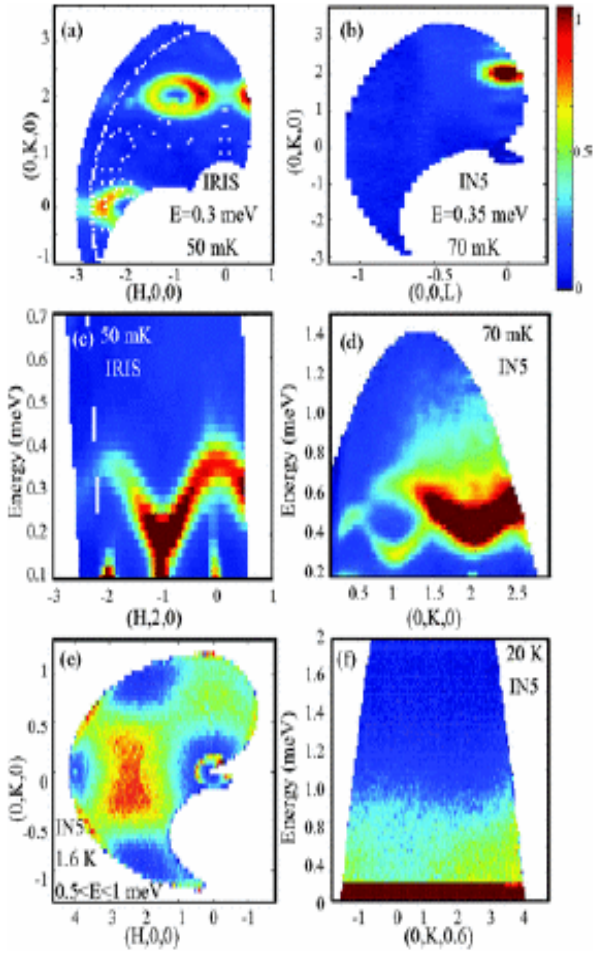
[6]*ESRF, 6 Rue Jules Horowitz BP 220, F-38043 Grenoble Cedex 9, France*

[7]*ISIS Pulsed Source, Rutherford Appleton Laboratory, Chilton, Didcot, United Kingdom*

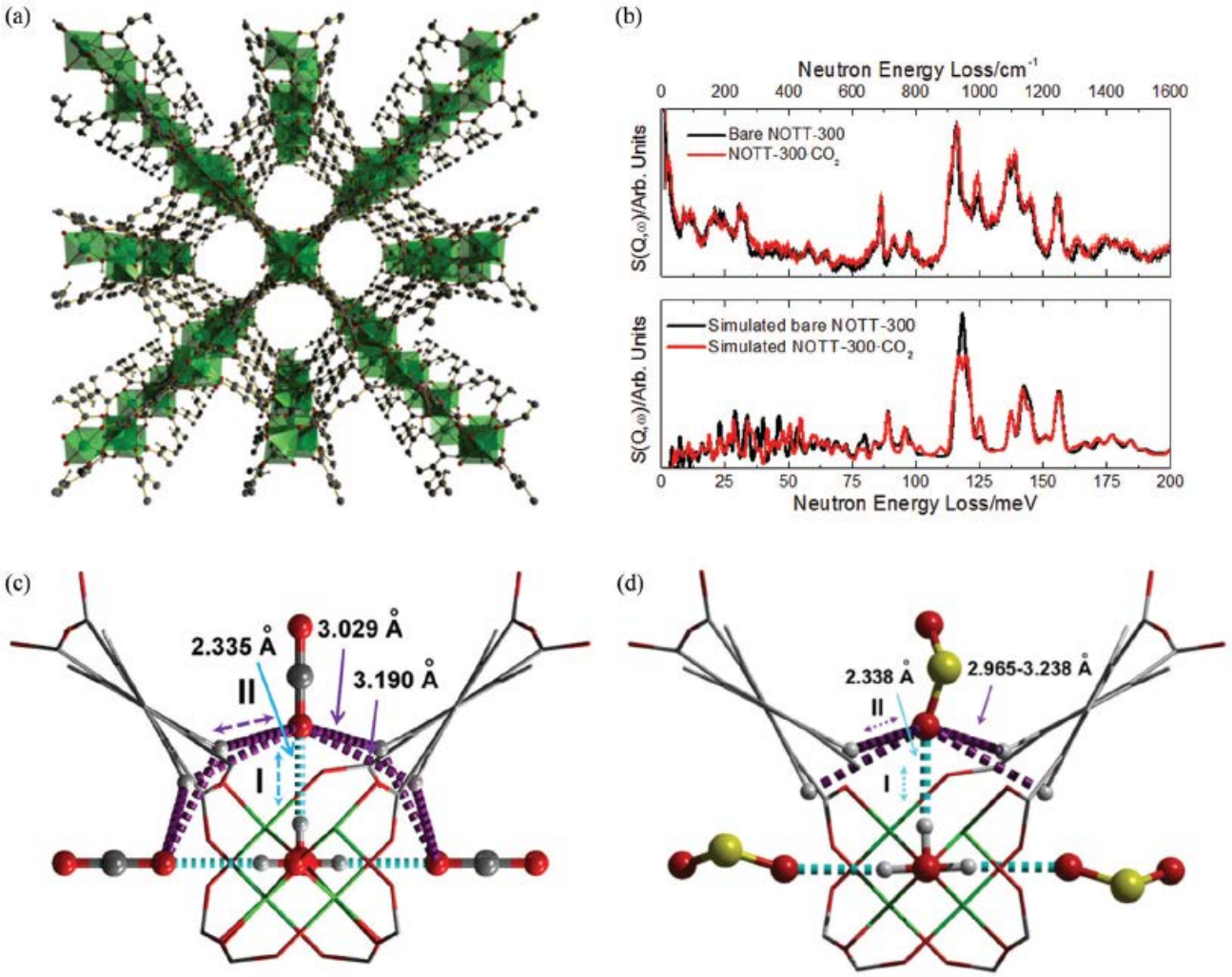
[8]*European Spallation Source ESS AB, P.O. Box 176, SE-22100 Lund, Sweden*

(Received 29 May 2012; published 13 August 2012)





Metal-Organic Frameworks – structural and dynamic studies of substrate binding



T.L. Easun, et al. Chem. Soc. Rev. 46, 239 (2017).

Anharmonic Effects in Organic Ferroelectric Croconic Acid

Diffraction from powdered sample compared with DFT

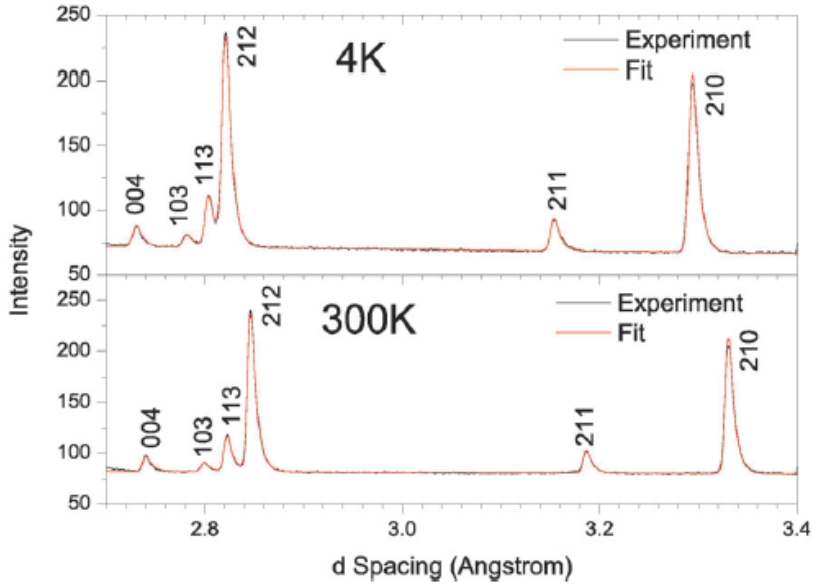
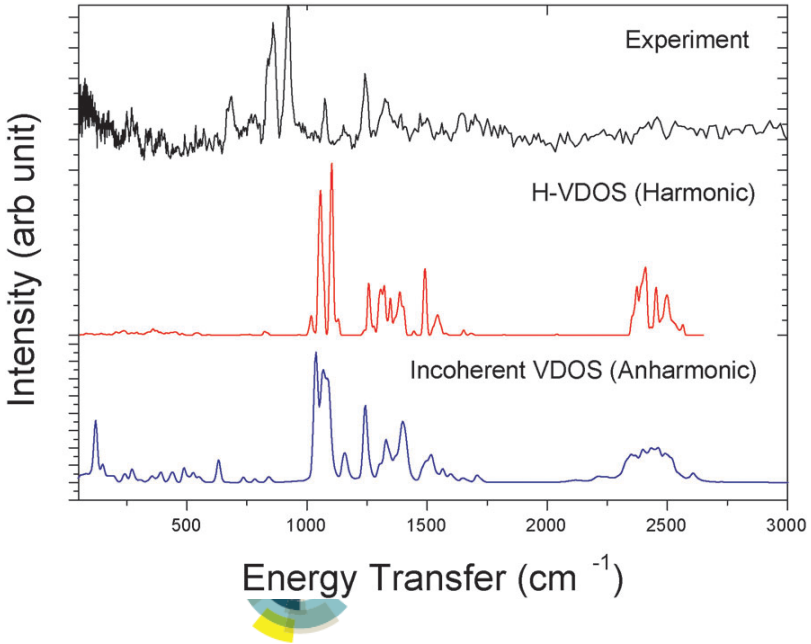


Fig. 2 ND patterns (black) and associated fits (red) obtained on IRIS at two selected temperatures. The numbers on the figure denote (*hkl*) reflections.

Anharmonic DOS is compared with INS experiments



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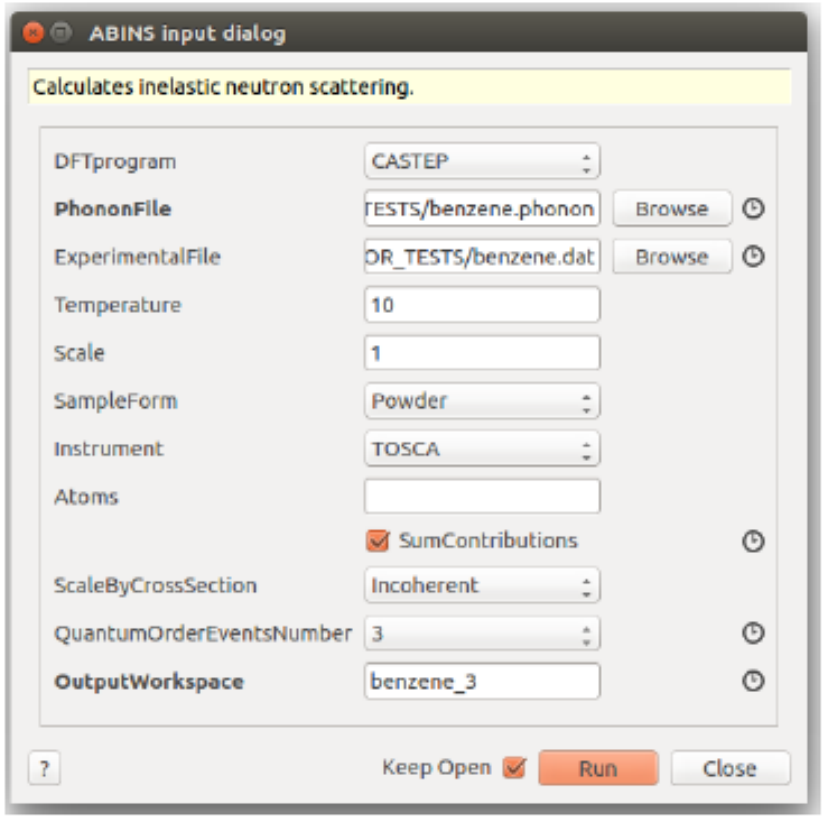
Cite this: *Phys. Chem. Chem. Phys.*, 2014, **16**, 26234

Hydrogen-bond structure and anharmonicity in croconic acid

Sanghamitra Mukhopadhyay,*[ab] Matthias Gutmann[a] and Felix Fernandez-Alonso[ac]

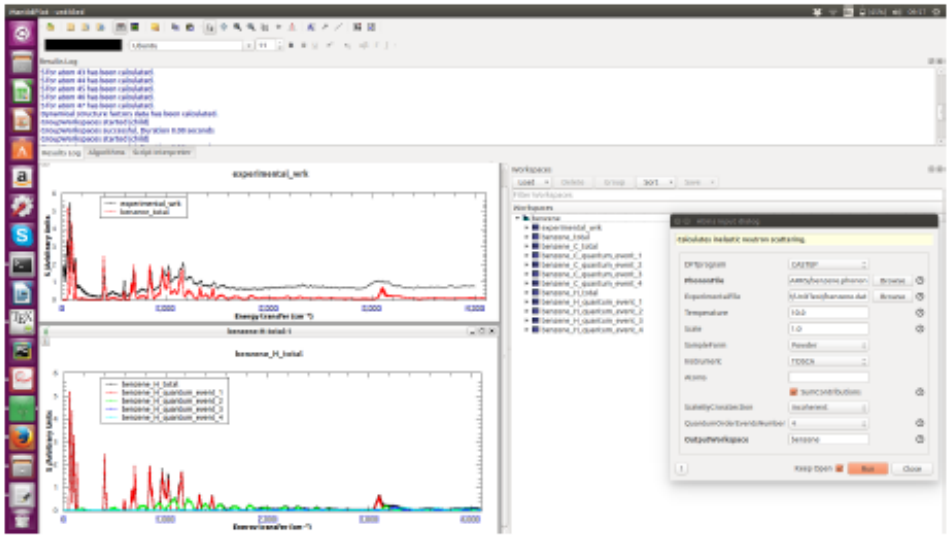
abINS : An open source algorithm for interpretation of INS data



- Allows direct comparison of simulated and measured inelastic neutron scattering spectra
- Implemented as a plugin to Mantid data reduction and visualization tool
- User friendly GUI based on Mantid
- User can plot data by means of Mantid plotting functions

- All data is saved to ASCII file so that user can later visualize it in the software of choice

abINS : An open source algorithm for interpretation of INS data



- Can be run from GUI (MantidPlot) or from command line
- AbINS is open source and runs on Linux, Windows and MacOS

- Works for powder samples and both low and high temperatures
- Allows calculations of fundamentals together with higher order quantum events (up to 4-th order)
- Allows for calculation of INS for other atoms than H
- Supports Tosca and Tosca-like instruments
- Supports CASTEP and CRYSTAL DFT programs

http://docs.mantidproject.org/nightly/algorithms/Abins-v1.html

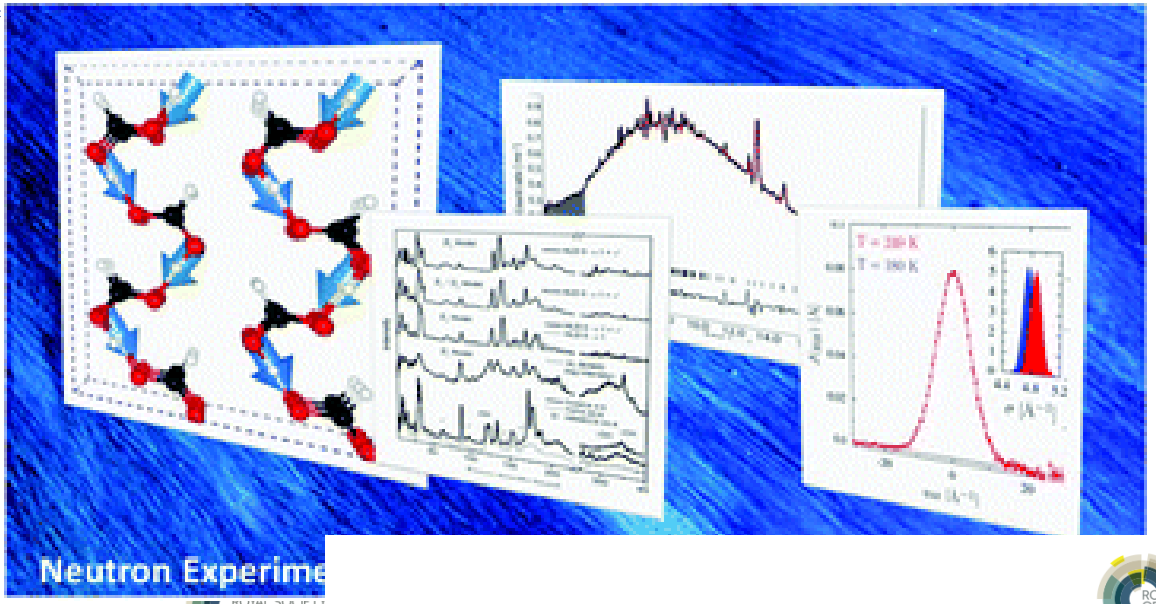
Hydrogen Dynamics in Water Adsorbed on Graphite Oxide Surface

THE JOURNAL OF PHYSICAL CHEMISTRY Letters
Letter
pubs.acs.org/JPCL

Direct Measurements of Quantum Kinetic Energy Tensor in Stable and Metastable Water near the Triple Point: An Experimental Benchmark

Carla Andreani,[†,‡] Giovanni Romanelli,[¶] and Roberto Senesi*[,†,‡]

The proton dynamics is probed beyond classical limit



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Probing the effects of 2D confinement on hydrogen dynamics in water and ice adsorbed in graphene oxide sponges†

Giovanni Romanelli,‡*[a] Roberto Senesi,[ab] Xuan Zhang,[c] Kian Ping Loh[c] and Carla Andreani[a]

Cite this: *Phys. Chem. Chem. Phys.*, 2015, **17**, 31680

PCCP
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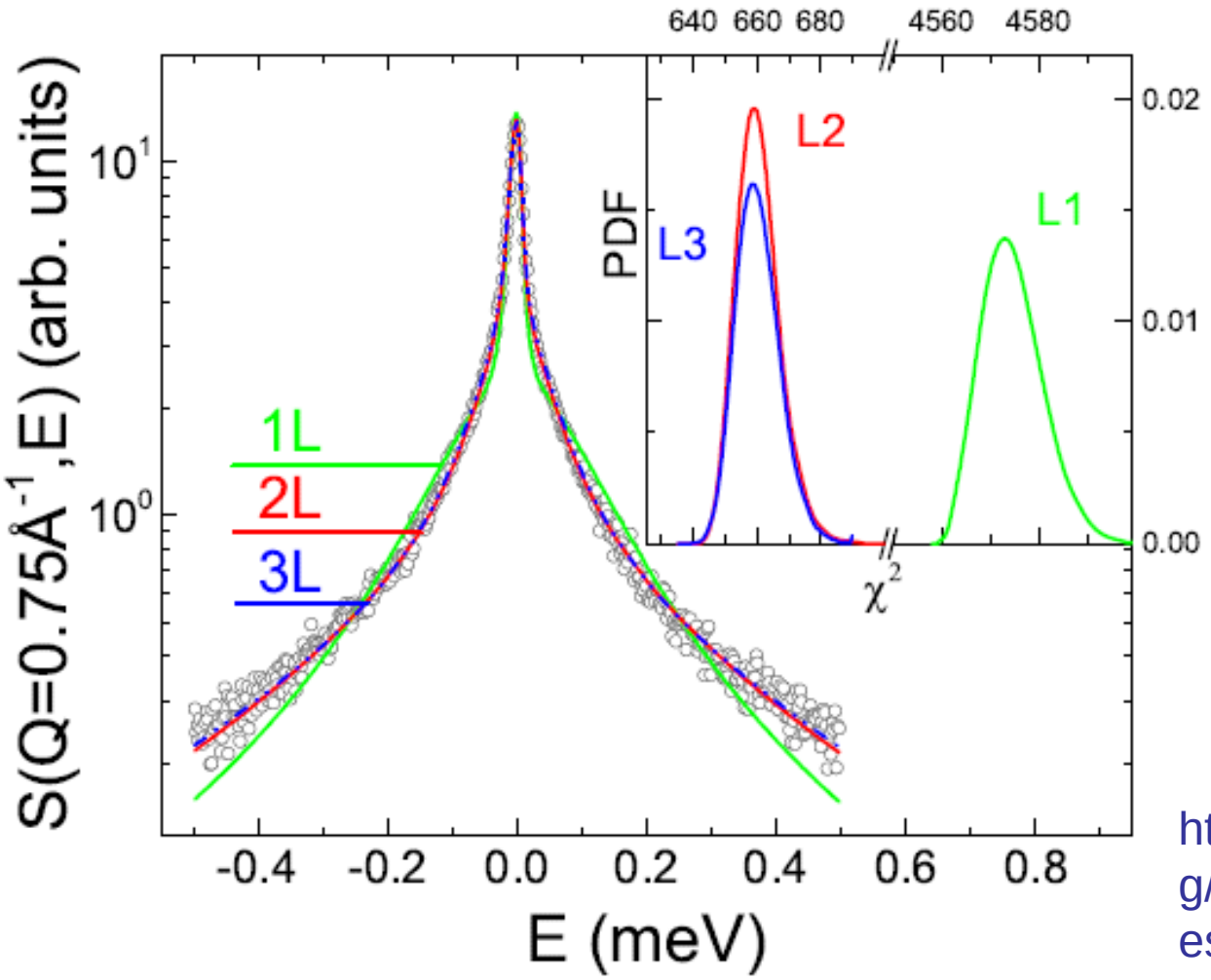
Nuclear dynamics and phase polymorphism in solid formic acid

Maciej Krzystyniak,*[ab] Kacper Drużbicki,[c] Giovanni Romanelli,[a] Matthias J. Gutmann,[a] Svemir Rudić,[a] Silvia Imberti[a] and Felix Fernandez-Alonso[ad]

Cite this: *Phys. Chem. Chem. Phys.*, 2017, **19**, 9064

Understanding dynamics during liquid-liquid phase transition using Bayesian analysis



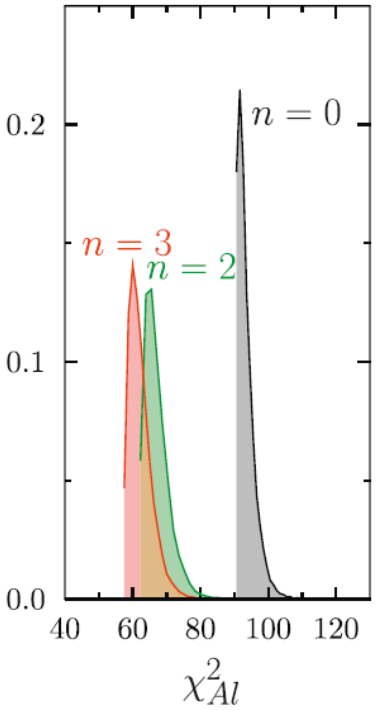
FABADA is used to fit QENS data obtained from IRIS instrument at ISIS.

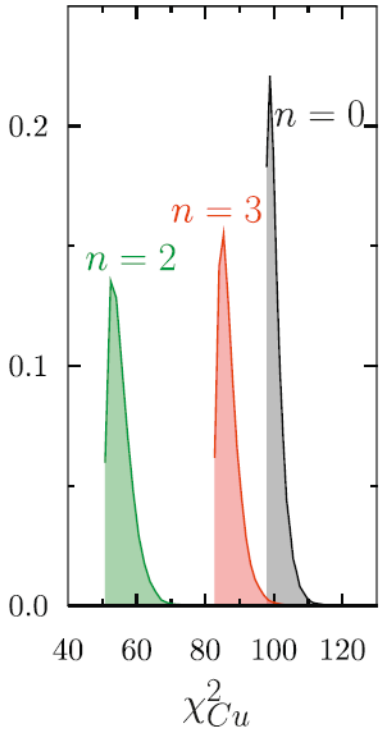
There is no gain by using L=3 over L=2 for this QENS fitting

http://www.mantidproject.org/Fitting_QENS_using_Bayesian_Routine_FABADA

A. Vispa, D. Monserrat, G. J. Cuello, F. Fernandez-Alonso,S. Mukhopadhyay, F. Demmel, J.Ll. Tamarit, and L. C. Pardo, submitted PCCP (2017).

Fitting Neutron Compton Profile





Gaussian peaks are fitted using FIM for analysing data obtained from VESUVIO instrument at ISIS

N=3 is the better fitting for Al but not for Cu

Physics Research A 819 (2016) 84–88

Contents lists available at ScienceDirect

Nuclear Instruments and Methods in Physics Research A

journal homepage: www.elsevier.com/locate/nima

Technical notes

On the line-shape analysis of Compton profiles and its application to neutron scattering

G. Romanelli [a,*], M. Krzystyniak [a,b]

[a] ISIS Facility, Rutherford Appleton Laboratory, Chilton, Didcot, Oxfordshire OX11 0QX, United Kingdom
[b] School of Science and Technology, Nottingham Trent University, Clifton Campus, Nottingham, NG11 8NS, United Kingdom

Science & Technology Facilities Council
ISIS

Future Work: High throughput QENS

Data reduction and preliminary analysis

Genetic algorithm in FABADA to be used in future