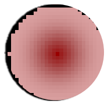
Inelastic Neutron Scattering and Material Dynamics

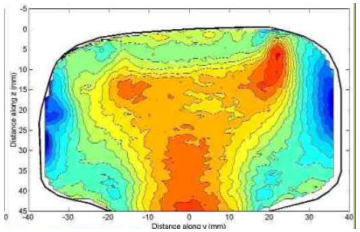
Dehong Yu, ACNS, ANSTO

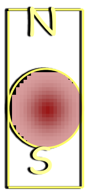
Inelastic Neutron Scattering
Instrumentation
What can be done
Examples

Properties of Neutrons - close to ideal

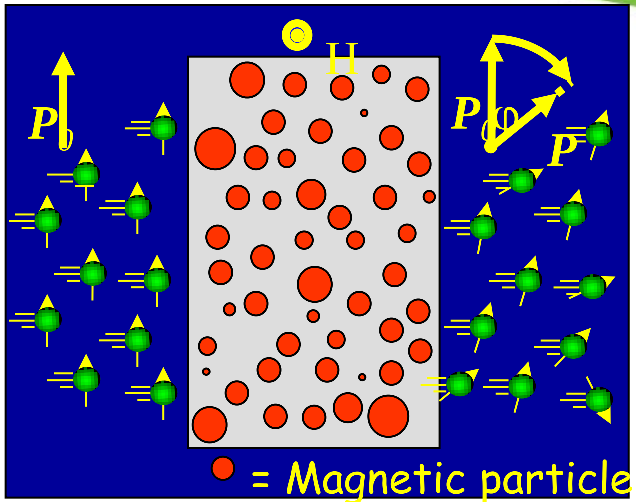


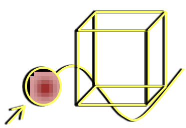
•no electric charge - can penetrate deep into a specimen



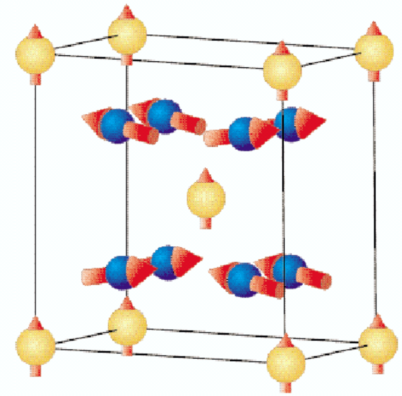


•has a magnetic moment - can see magnetic effects;

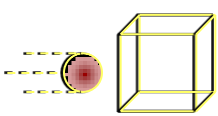




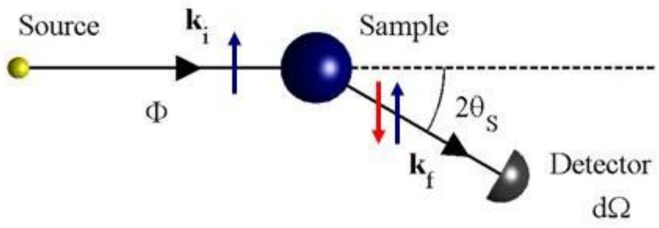
•Thermal neutrons have wavelength similar to atomic spacing -can be used to determine the positions of atoms.



•Thermal neutrons move at a speed similar to that of atoms at room temperature - can investigate motion of atoms.



The Scattering Function - S(Q,ω)

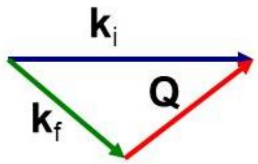


$$\frac{d^2\sigma}{d\Omega d\omega} \propto \frac{k_f}{k_i}\frac{\sigma}{4\pi} S(\boldsymbol{Q},\omega)$$

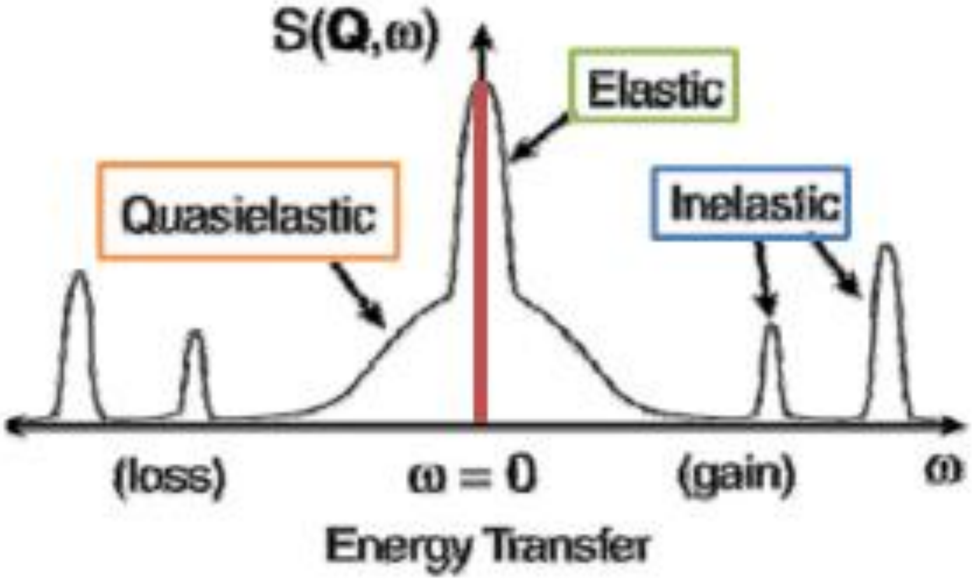
The scattering function, S(Q,ω) contains all the physics of the system (in space and time) and depends only on the system. This is what we measure in a scattering experiment.

Momentum	$\vec{Q} = \vec{k}_i - \vec{k}_f$
Energy	$\hbar\omega = E_i - E_f$

Scattering triangle



Inelastic Neutron Spectrum



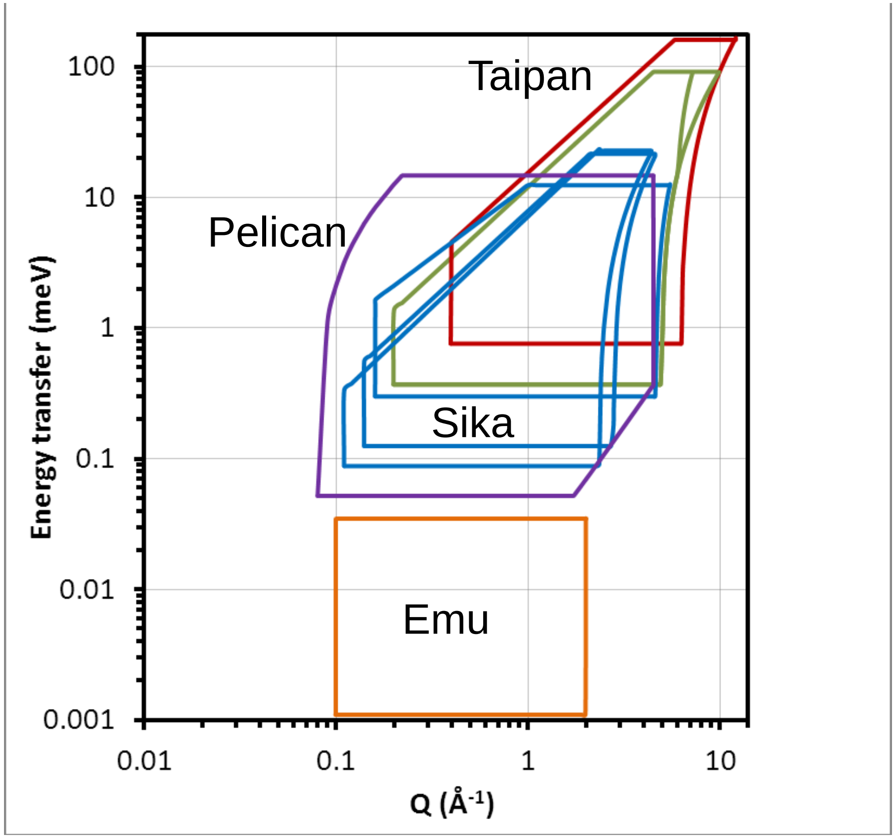
Elastic scattering – no energy exchange ħω=0. Diffraction process - Structure information.

Inelastic scattering – energy exchange ħω≠0. Dynamic processes such as phonons, vibrational modes, stretching modes, magnons, tunnelling, etc.

Quasi-elastic scattering (QENS)– small energy exchange ħω≠0≈neV or μeV . Dynamic processes with a distribution of energies, such as diffusion, rotations, translations….

Instrumentation

Time of Flight Spectrometer – Pelican
Triple Axis Spectrometers – Taipan & Sika
Backscattering Spectrometer – Emu
Be-filter Spectrometer – Option of Taipan



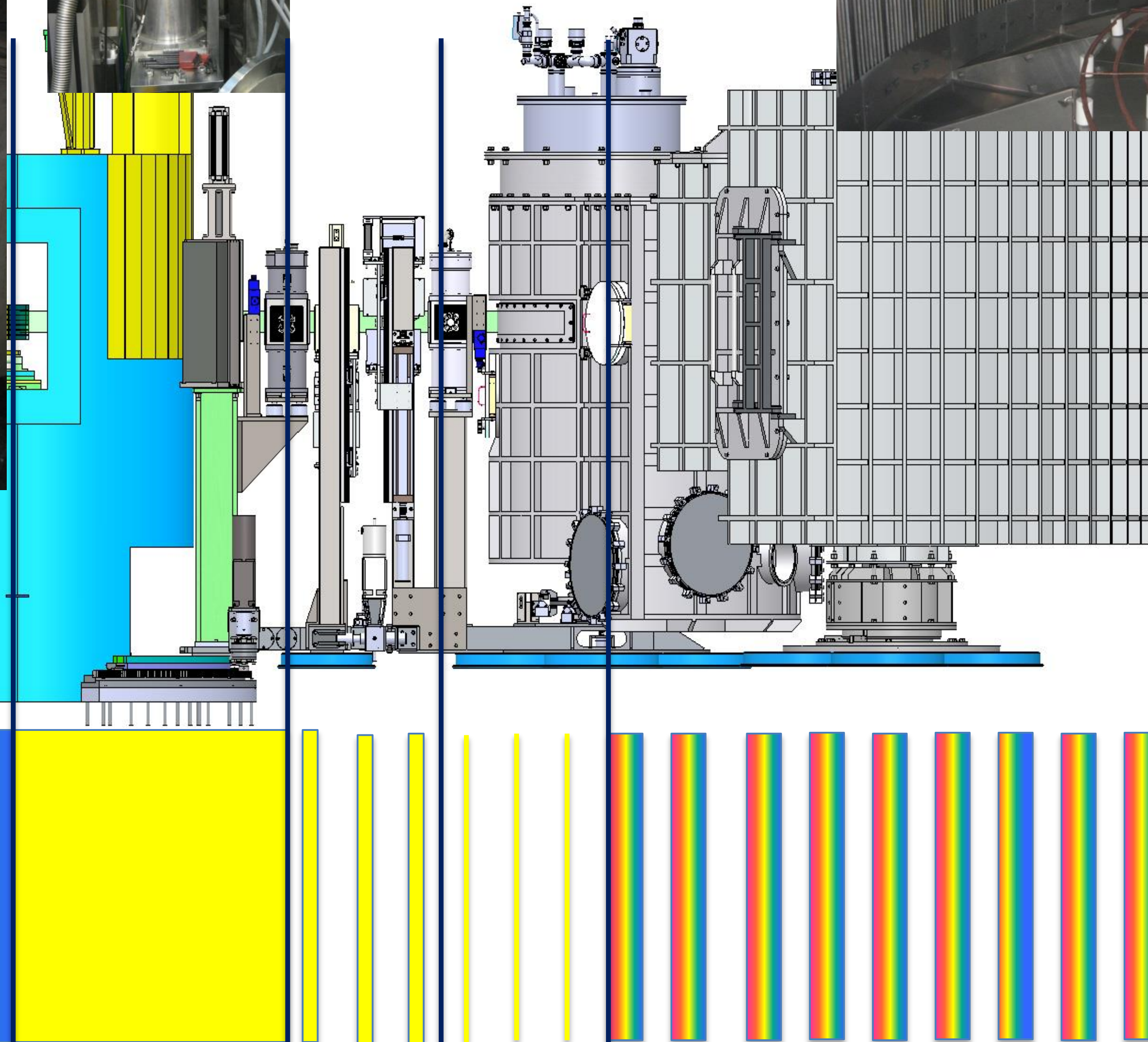
Fields: Physics, Chemistry, Biology, Materials
Topics: Lattice dynamics, Spin dynamics,
Materials: magnetic, thermoelectric, etc.
Sample: single crystals, powder, liquid, etc

Sample Environment

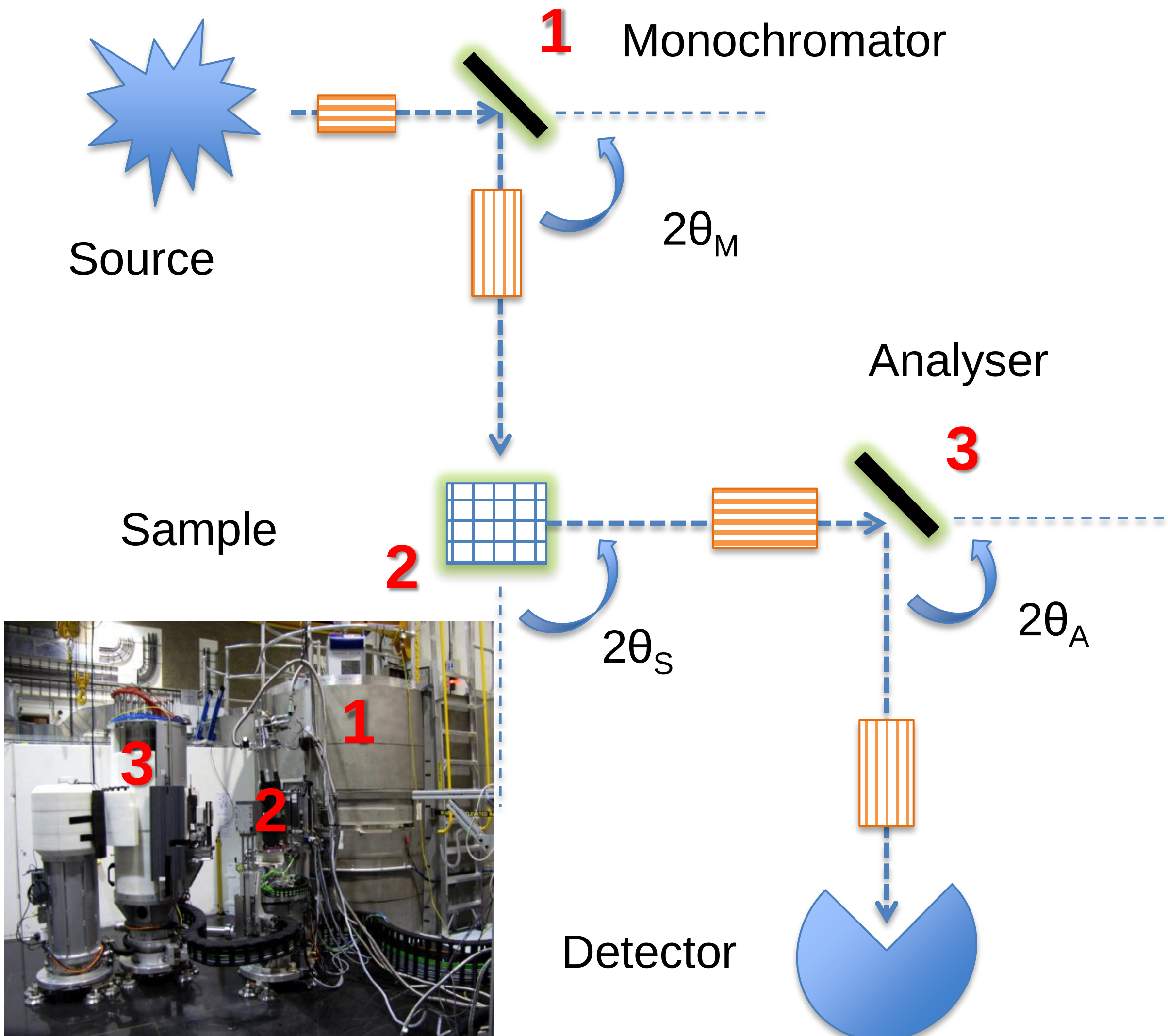
- 1.5 K to 700 K, up to 1600 ^{o}C and down to 50 mK.
- High magnetic field – 12 T.
- Electrical field.
- In situ gas or vapour delivery.

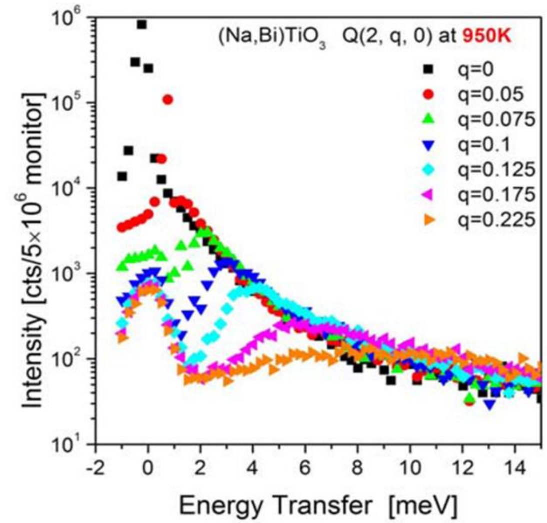
Australian Government

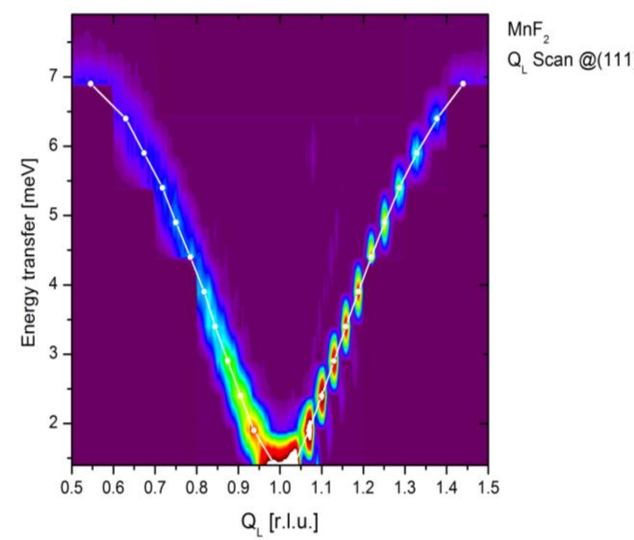
PELICAN



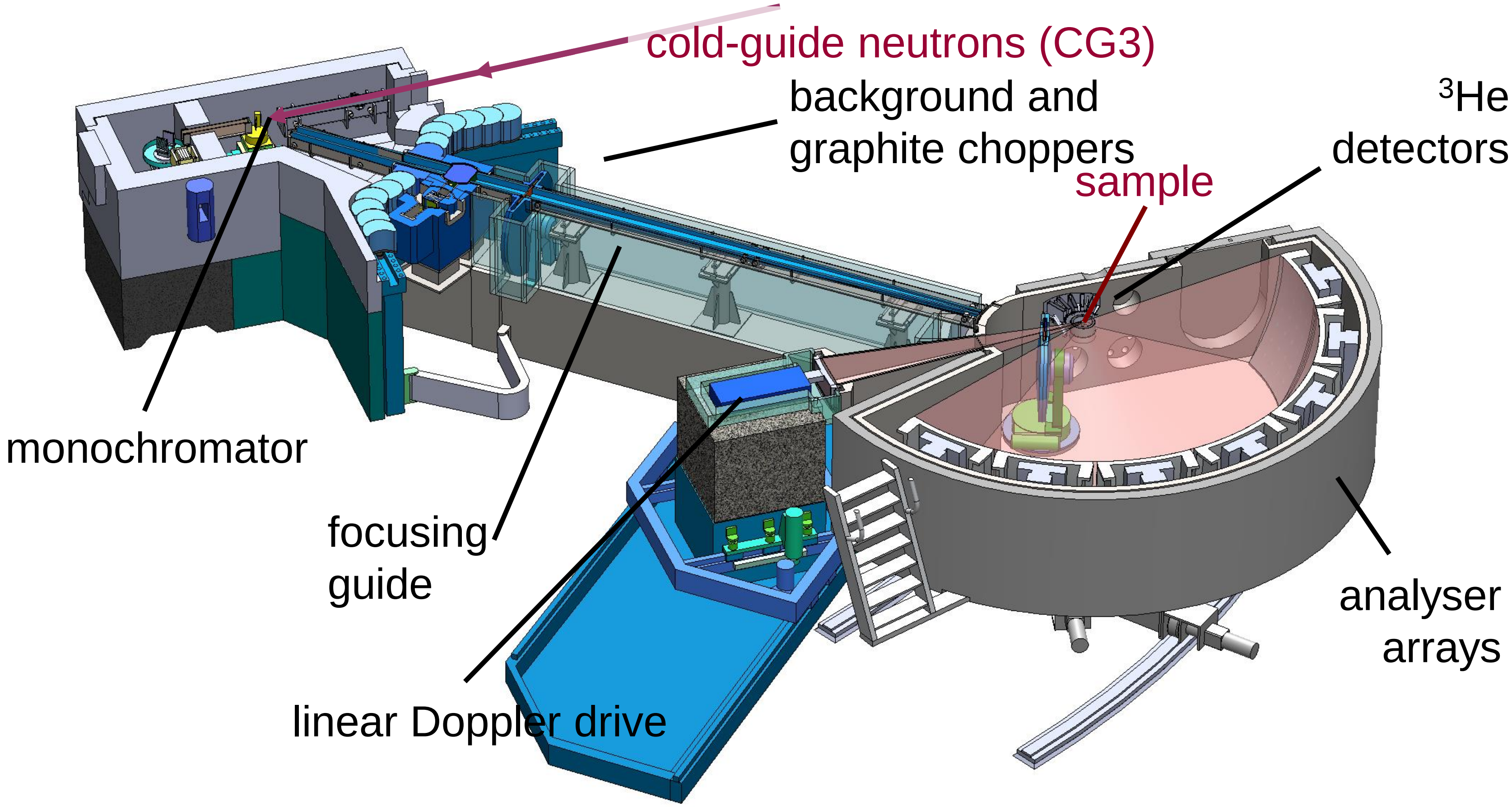
Triple Axis Spectrometers – TAIPAN & SIKA



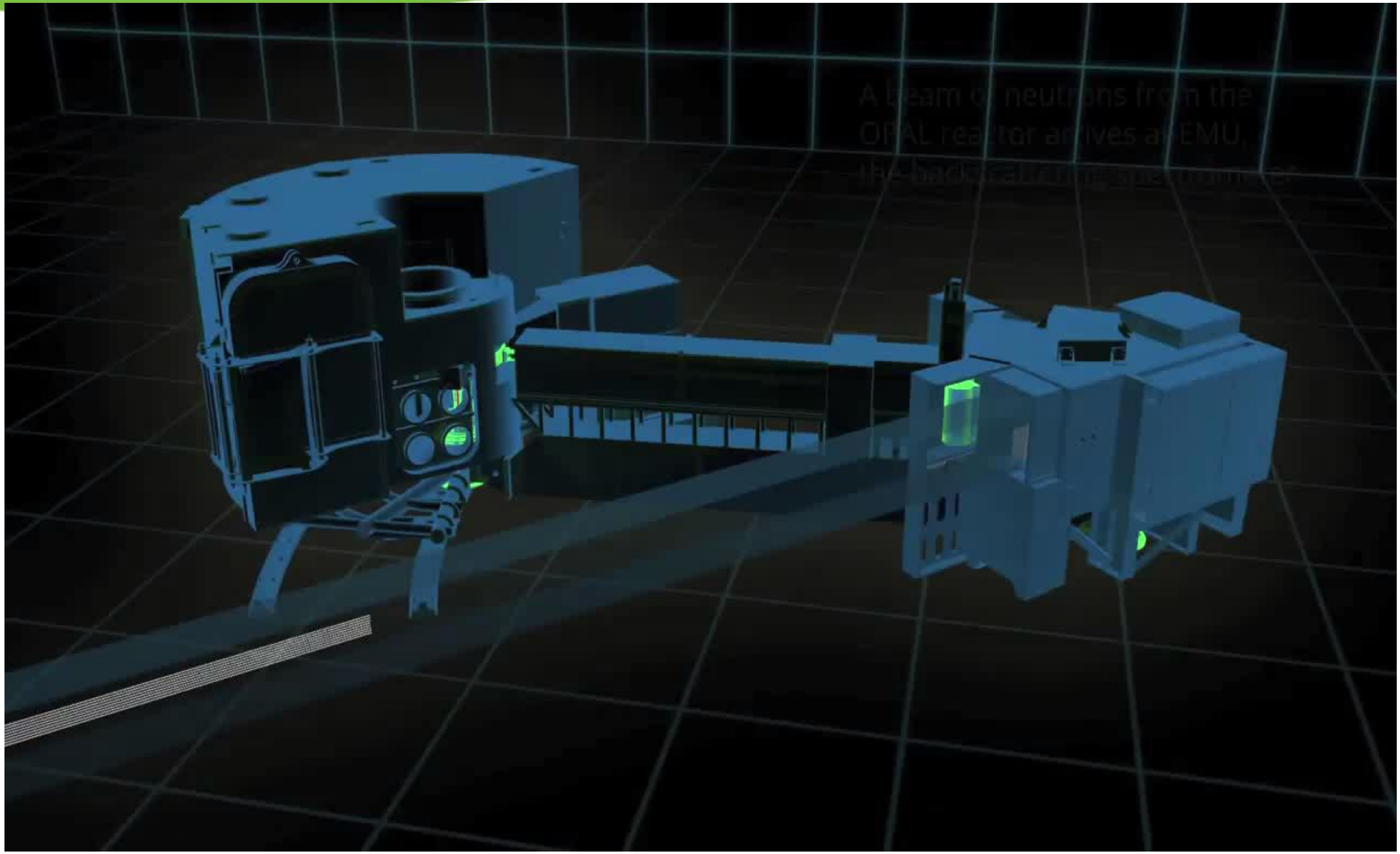




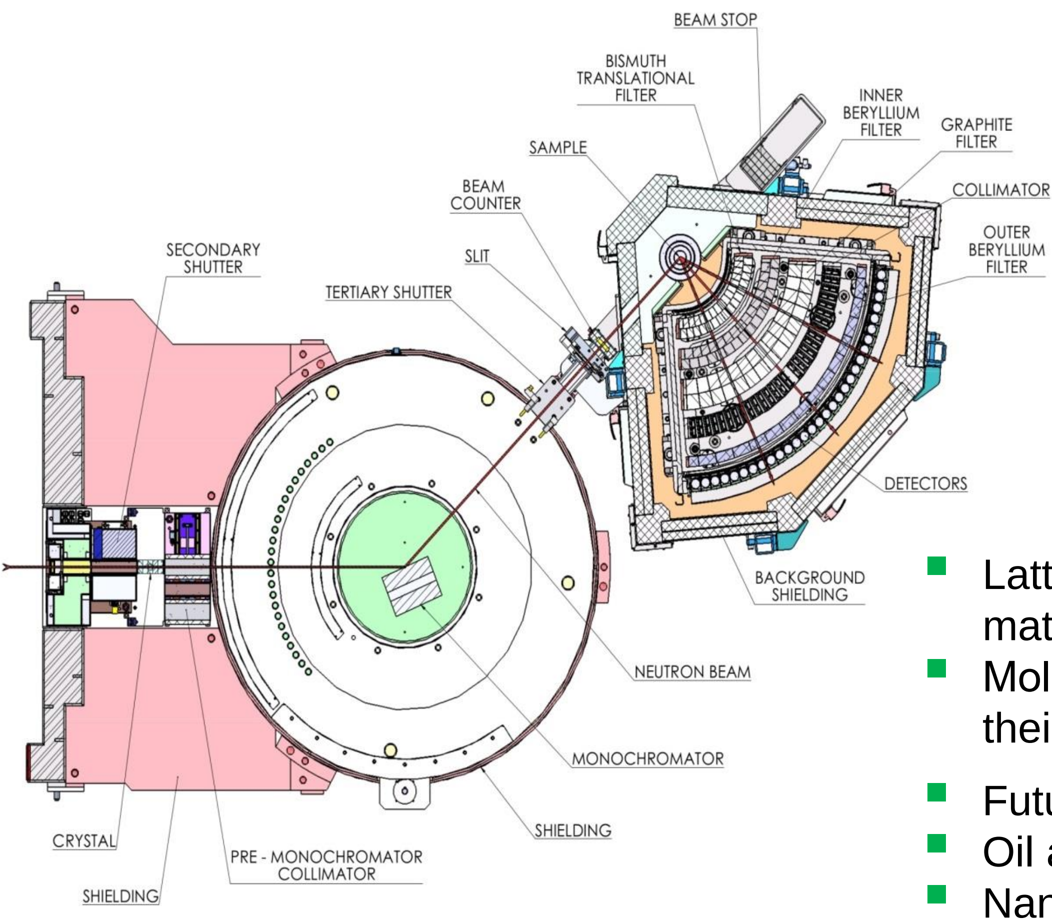
EMU – Back-scattering spectrometer



EMU – Back-scattering spectrometer



Be-Filter



TAIPAN BERYLLIUM FILTER INSTRUMENT LAYOUT

- Lattice and molecular excitations in complex materials in the form of phonon density of states
- Molecular vibrations acting as “fingerprints” of their surroundings
- Future energy storage (hydrides)
- Oil and chemical industry catalysts (zeolites)
- Nano-crystalline materials for industry and applications
- Coal studies
- Nuclear Fuels

CrystEngComm

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Driving forces for the phase transition of CuQ_2-TCNQ molecular crystals†

Dehong Yu,*[a] Gordon J. Kearley,[a] Guangfeng Liu,[b] Richard A. Mole,[a] Garry J. McIntyre[a] and Xutang Tao*[b]

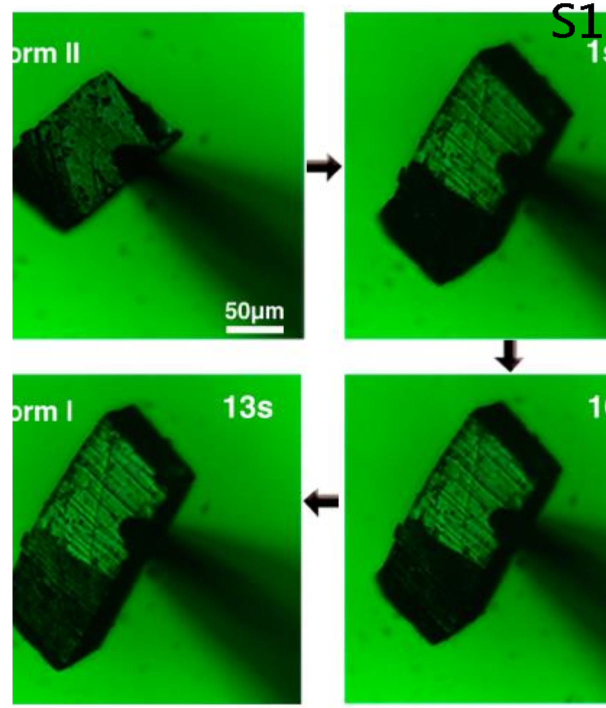
S1.mov

CuQ2-TCNQ:
7, 7, 8, 8 - tetracyanoquinodimethane-p-bis (8-hydroxyquinolinato) copper(II)

Under mechanical stimulation: Phase transition with about 100% increase in length and 50% reduction in thickness, maintaining the crystal form.

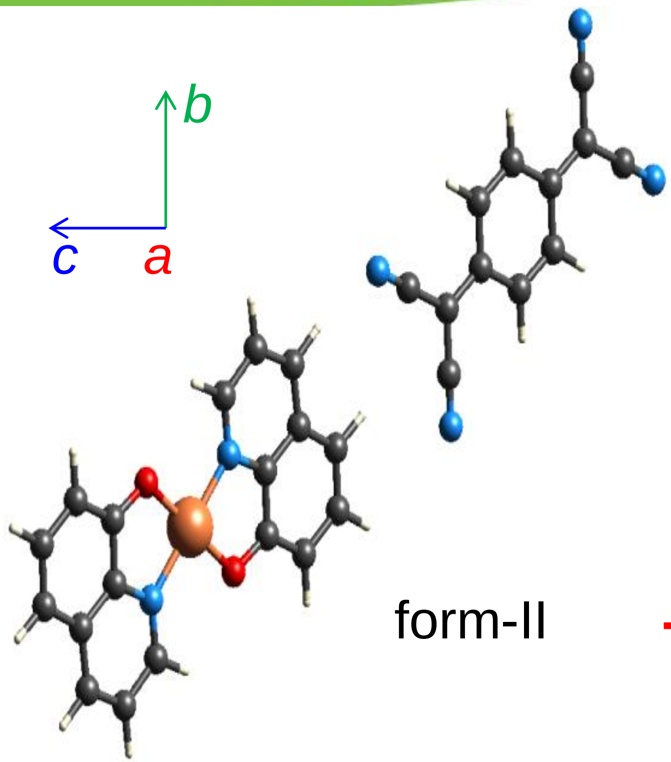
Potential applications in molecular mechanical actuators and artificial muscles

How does the phase transition occur at atomic level? What are the driving forces?

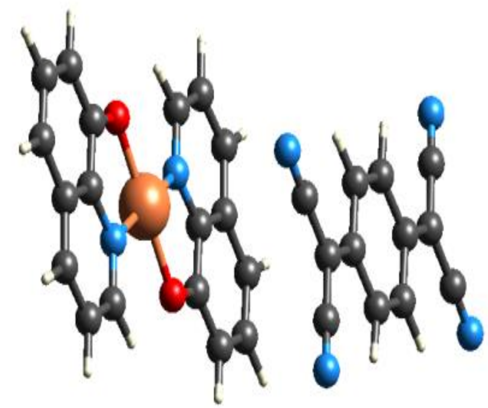


re 1. SCSC phase transition process with the (001) plane of
pressure-bearing surface.

Form II to Form I



form-II

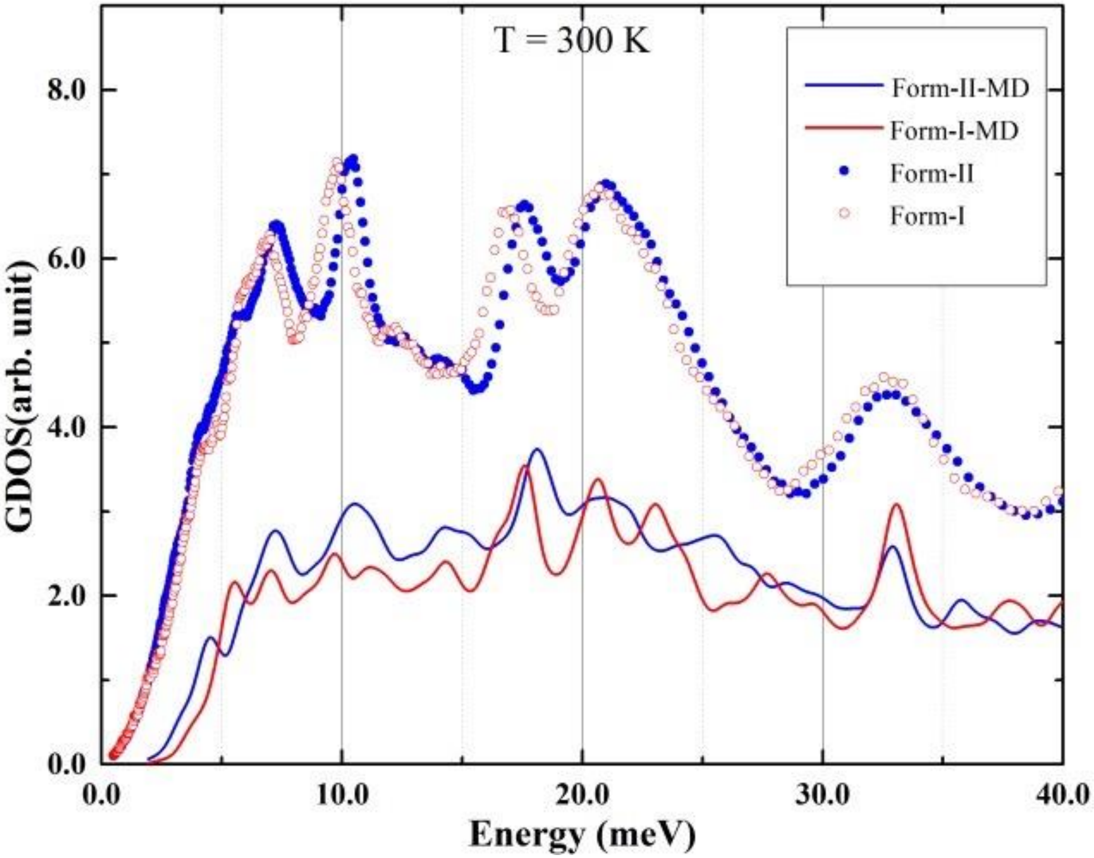


form-I

0 K, E(I)-E(II) = +33 meV
300 K, E(I)-E(II) = -63 meV

Low T, Form II metastable state

GDOS – Form II to Form I



Phonon softening effect

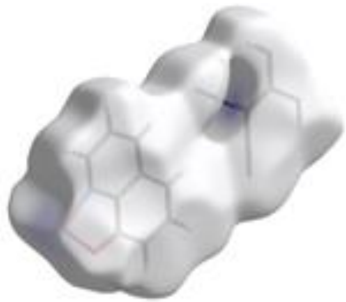
Spectra difference is still “surprising” small. Why?

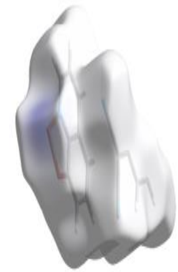
MD-simulation agrees with experimental observation.

Reflect the small change of the in plan H-bond interaction.

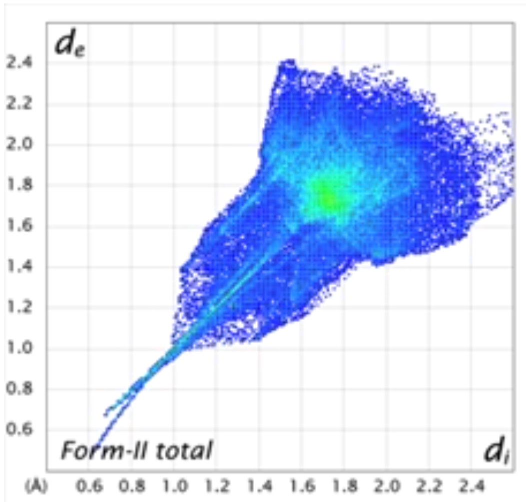
Hirshfeld Electron Density Surfaces
interlayer π - π interaction

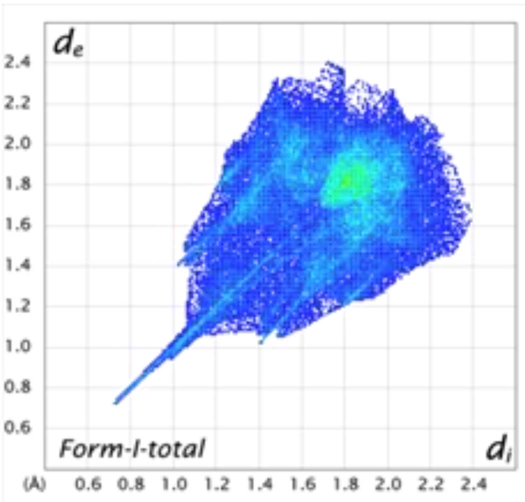
Form II





Form I





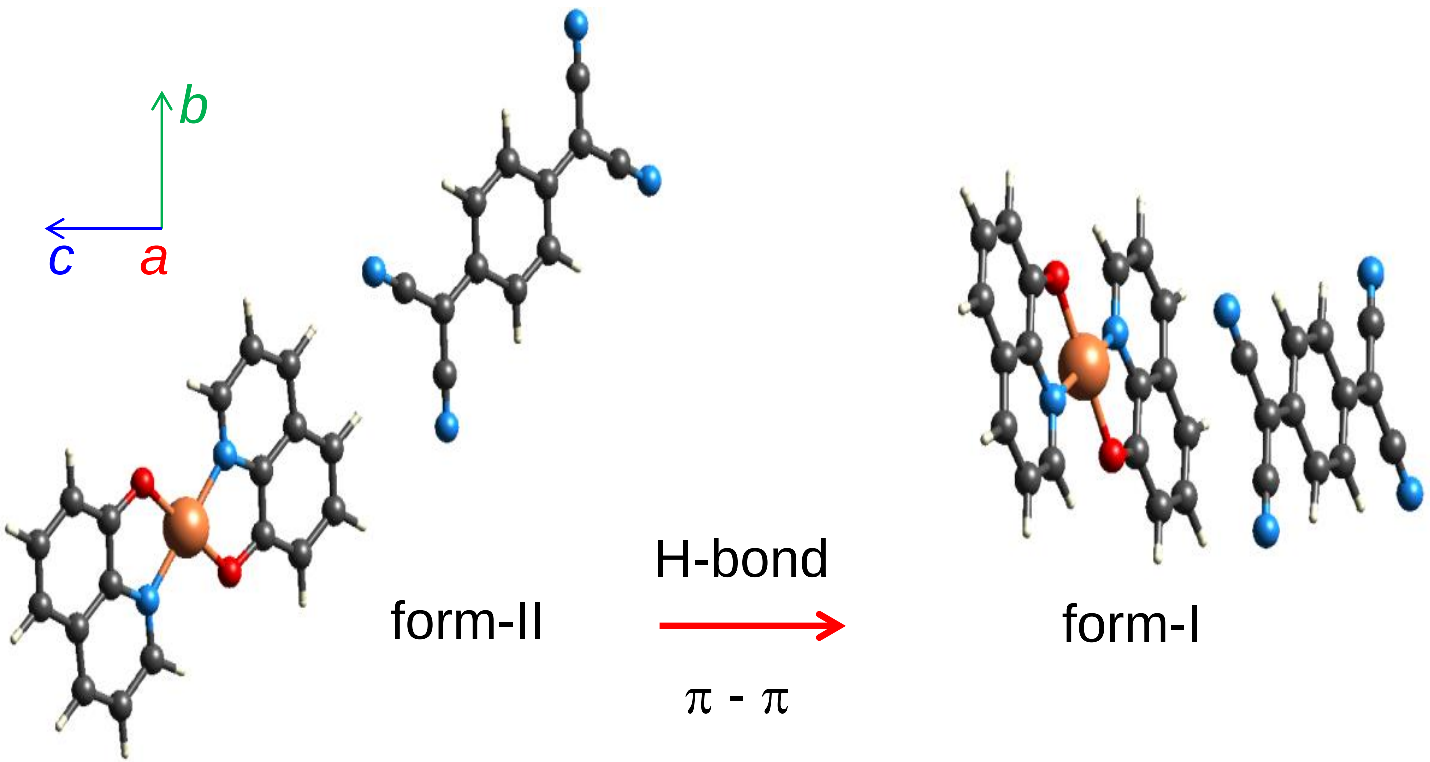
de = *di* = 1.7 Å

π-π stacking contacts

de = *di* = 1.8 Å

di and *de* are the distances from the hirshfeld surface to the nearest atoms, interior and exterior to the surface, respectively.

Interplay between strong H-bond and weak π - π interactions

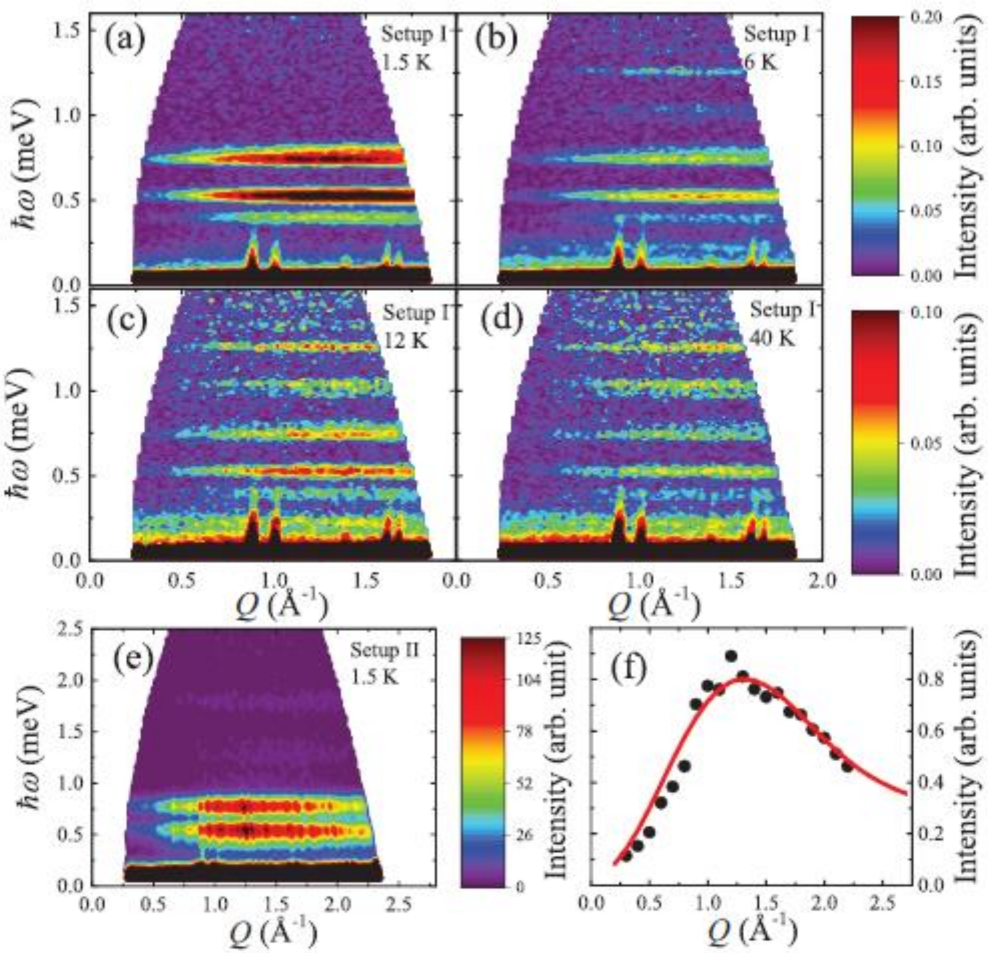


RAPID COMMUNICA

PHYSICAL REVIEW B **93**, 220407(R) (2016)

Low-energy excitations and ground-state selection in the quantum breathing pyrochlore antiferromagnet $Ba_3Yb_2Zn_5O_{11}$

T. Haku,[1] K. Kimura,[2] Y. Matsumoto,[1] M. Soda,[1] M. Sera,[2] D. Yu,[3] R. A. Mole,[3] T. Takeuchi,[4] S. Nakatsuji,[1] Y. Kono,[1] T. Sakakibara,[1] L.-J. Chang,[5] and T. Masuda[1]



General Hamiltonian was established:

$$\mathcal{H} = -\sum_{i<j}\sum_{\nu\mu} J_{ij}^{\nu\mu} S_i^{\nu} S_j^{\mu}.$$

Exchange interactions were determined:

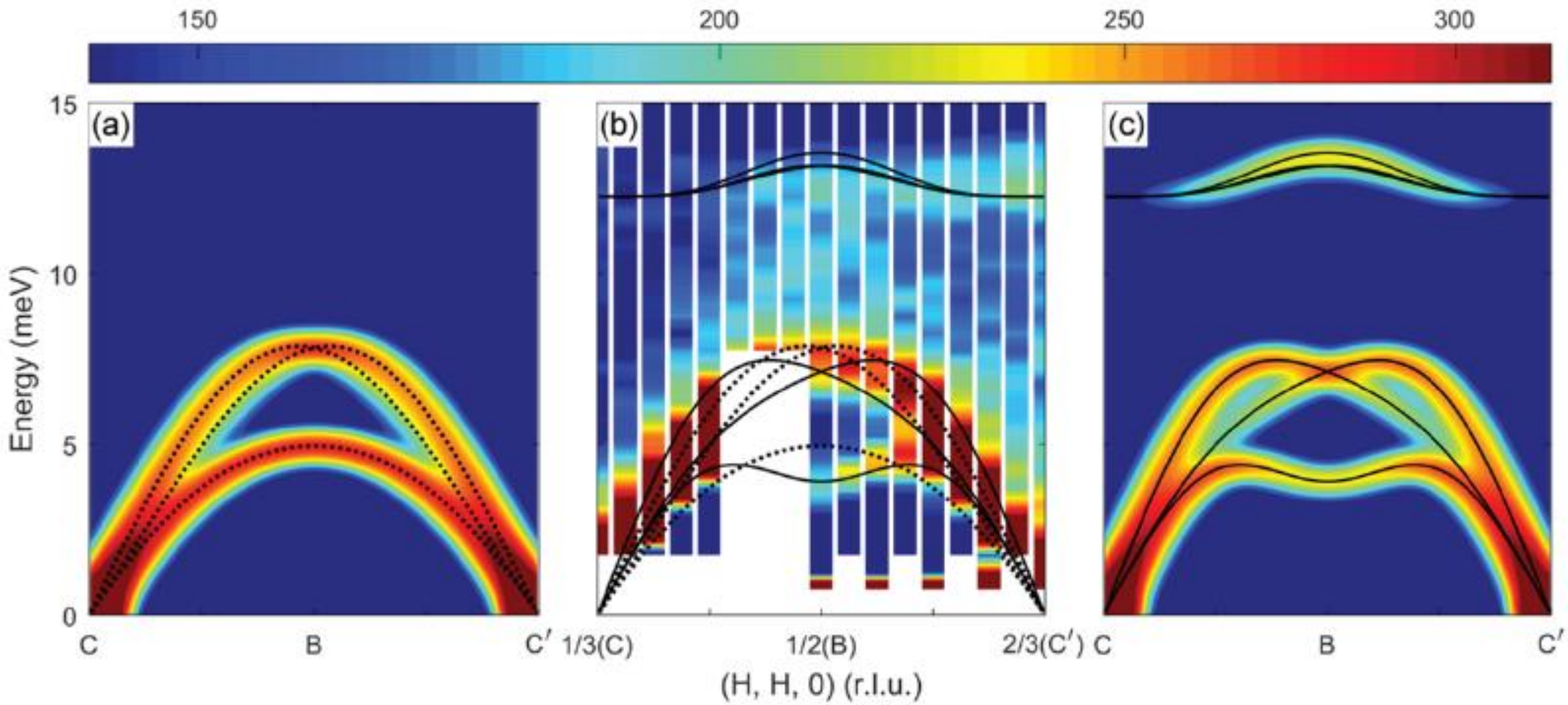
$$J_1 = -0.570 \pm 0.033 \text{ meV},$$
$$J_2 = -0.558 \pm 0.028 \text{ meV},$$
$$J_3 = 0.000 \pm 0.023 \text{ meV},$$
$$J_4 = 0.113 \pm 0.014 \text{ meV}.$$

More complex spin state was suggested:

Possible spin-liquid state

Magnon-phonon coupling and two-magnon continuum in two-dimensional triangular antiferromagnet $CuCrO_2$

Kisoo Park,[1,2] Joosung Oh,[1,2] Jonathan C. Leiner,[1,2] Jaehong Jeong,[1,2,3] Kirrily C. Rule,[4] Manh Duc Le,[1,2,5] and Je-Geun Park[1,2,*]



Experiment from Taipan measured the strong magnon-phonon coupling (spin-lattice coupling). To be published in PRB. T = 5 K

ChemComm

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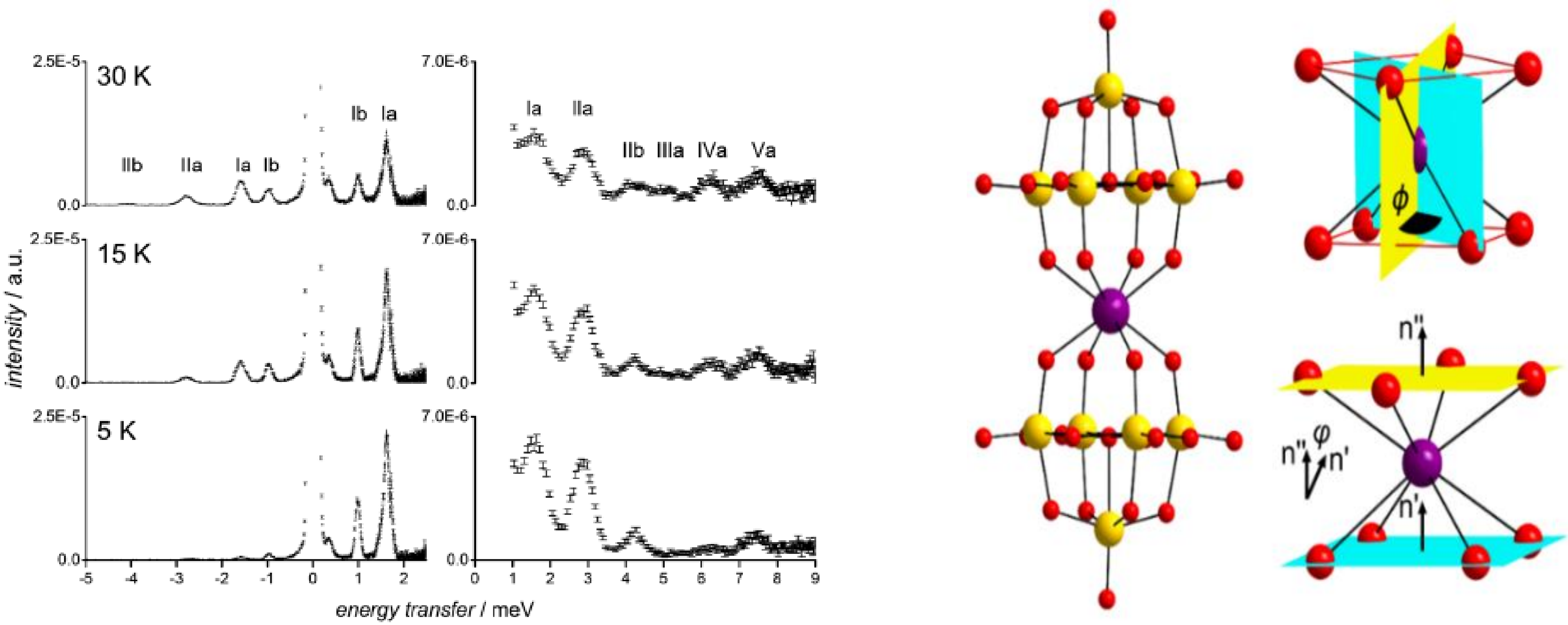
DOI: 10.1039/c5cc07541f

Ab initio calculations as a quantitative tool in the inelastic neutron scattering study of a single-molecule magnet analogue†

Michele Vonci,[a] Marcus J. Giansiracusa,[a] Robert W. Gable,[a] Willem Van den Heuvel,[a] Kay Latham,[b] Boujemaa Moubaraki,[c] Keith S. Murray,[c] Dehong Yu,[d] Richard A. Mole,*[d] Alessandro Soncini*[a] and Colette Boskovic*[a]



Nanoscale

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Received 19th February 2016,
Accepted 16th March 2016

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Enhanced ionic liquid mobility induced by confinement in 1D CNT membranes†

Q. Berrod,[a] F. Ferdeghini,[a] P. Judeinstein,[a] N. Genevaz,[a] R. Ramos,[b] A. Fournier,[b] J. Dijon,[b] J. Ollivier,[c] S. Rols,[c] D. Yu,[d] R. A. Mole[d] and J.-M. Zanotti*[a]

Scientific Reports (in press)

The logarithmic relaxation process and freezing of liquids in nano-confined states

Changjiu Chen[1, 2], Kaikin Wong[1,2], Richard A. Mole[3], Dehong Yu[3] and Suresh M. Chathoth[1,2,*]

More Scientific Examples

ARTICLES
PUBLISHED ONLINE: 5 JUNE 2011 | DOI: 10.1038/NMAT3035
nature materials

Giant anharmonic phonon scattering in PbTe

O. Delaire[1*], J. Ma[1], K. Marty[1], A. F. May[2], M. A. McGuire[2], M-H. Du[2], D. J. Singh[2], A. Podlesnyak[1], G. Ehlers[1], M. D. Lumsden[1] and B. C. Sales[2]

Understanding the microscopic processes affecting the bulk thermal conductivity is crucial to develop more efficient thermoelectric materials. PbTe is currently one of the leading thermoelectric materials, largely thanks to its low thermal conductivity. However, the origin of this low thermal conductivity in a simple rocksalt structure has so far been elusive. Using a combination of inelastic neutron scattering measurements and first-principles computations of the phonons, we identify a strong anharmonic coupling between the ferroelectric transverse optic mode and the longitudinal acoustic modes in PbTe. This interaction extends over a large portion of reciprocal space, and directly affects the heat-carrying longitudinal acoustic phonons. The longitudinal acoustic–transverse optic anharmonic coupling is likely to play a central role in explaining the low thermal conductivity of PbTe. The present results provide a microscopic picture of why many good thermoelectric materials are found near a lattice instability of the ferroelectric type.

More Scientific Examples

LETTERS

PUBLISHED ONLINE: 17 JANUARY 2010 | DOI: 10.1038/NPHYS1512

nature physics

Evolution of spin excitations into the superconducting state in $FeTe_{1-x}Se_x$

M. D. Lumsden[1]*, A. D. Christianson[1]*, E. A. Goremychkin[2,3], S. E. Nagler[1], H. A. Mook[1], M. B. Stone[1], D. L. Abernathy[1], T. Guidi[3], G. J. MacDougall[1], C. de la Cruz[4], A. S. Sefat[1], M. A. McGuire[1], B. C. Sales[1] and D. Mandrus[1]

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