Quantum Materials & ESS

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KTH Royal Institute of Technology

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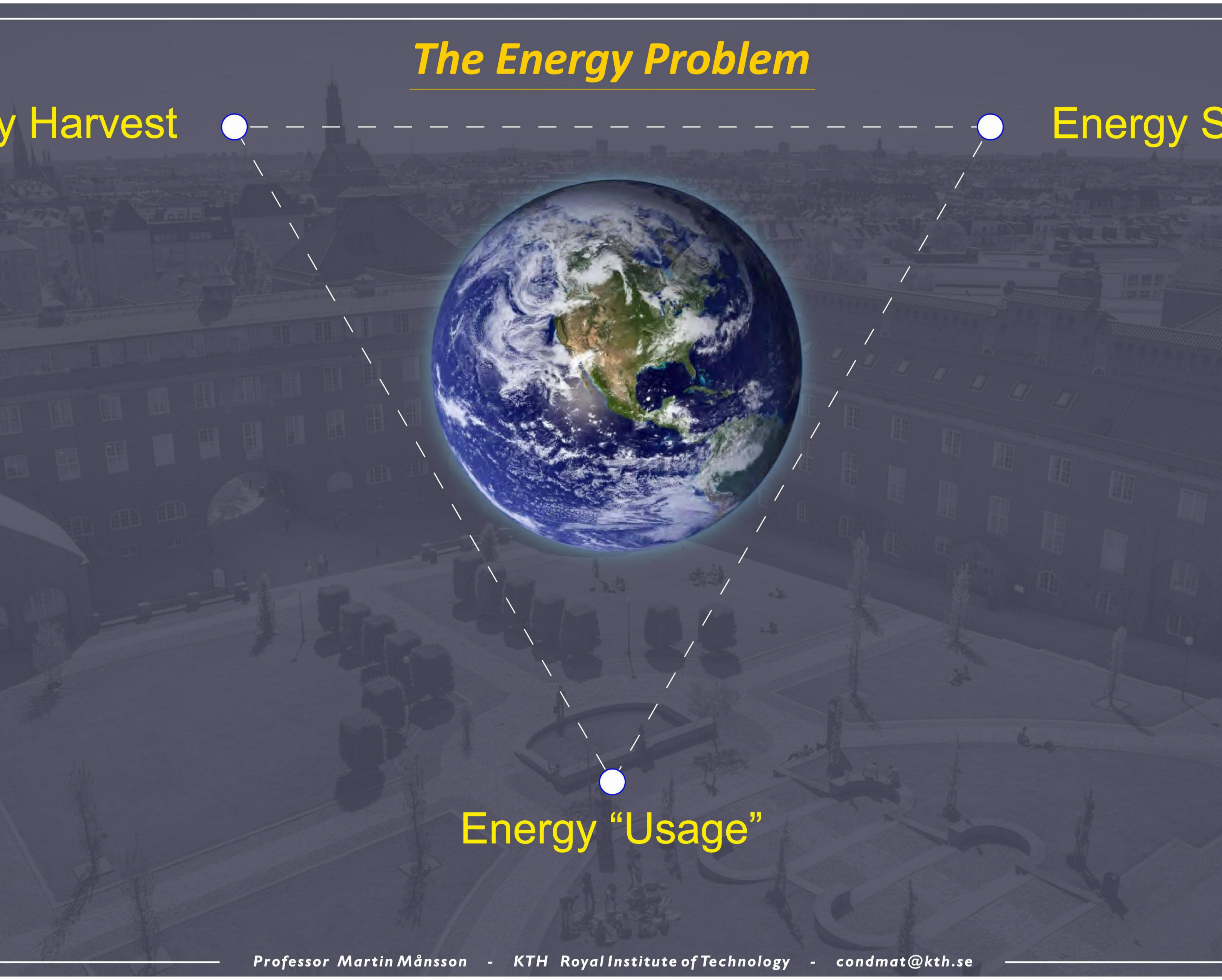
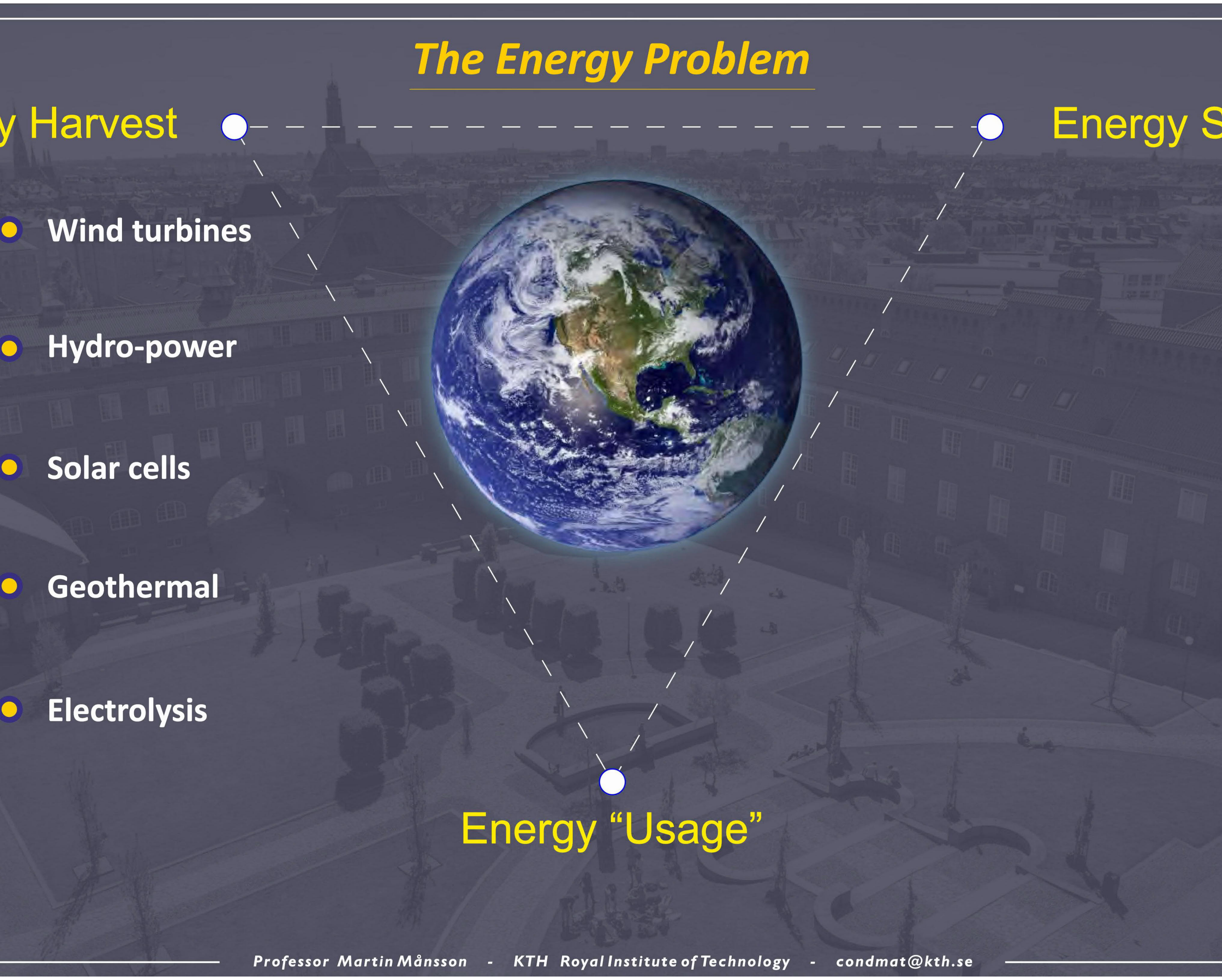

The Energy Problem
y Harvest
Energy S
Energy "Usage"
Professor Martin Månsson - KTH Royal Institute of Technology - condmat@kth.se


The Energy Problem
y Harvest
Energy S
Wind turbines
Hydro-power
Solar cells
Geothermal
Electrolysis
Energy "Usage"
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The Energy Problem

y Harvest

Energy S

- **Wind turbines**
- **Hydro-power**
- **Solar cells**
- **Geothermal**
- **Electrolysis**

Energy “Usage”

The Energy Problem

y Harvest

- Wind turbines
- Hydro-power
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- Geothermal
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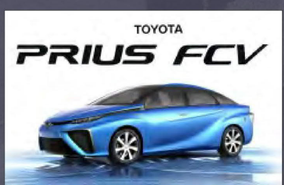
Energy S

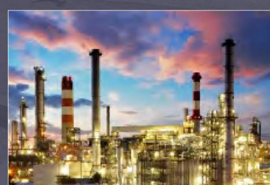
(Metal, paper

Energy “Usage”



- Transport

- Heat/Cool

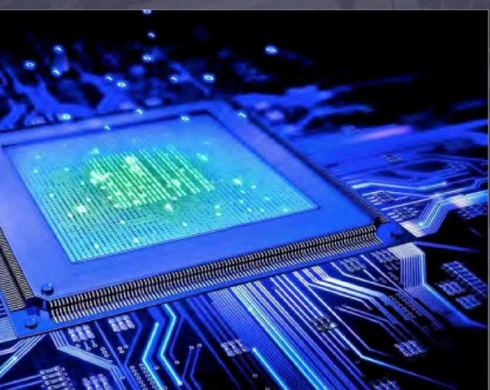


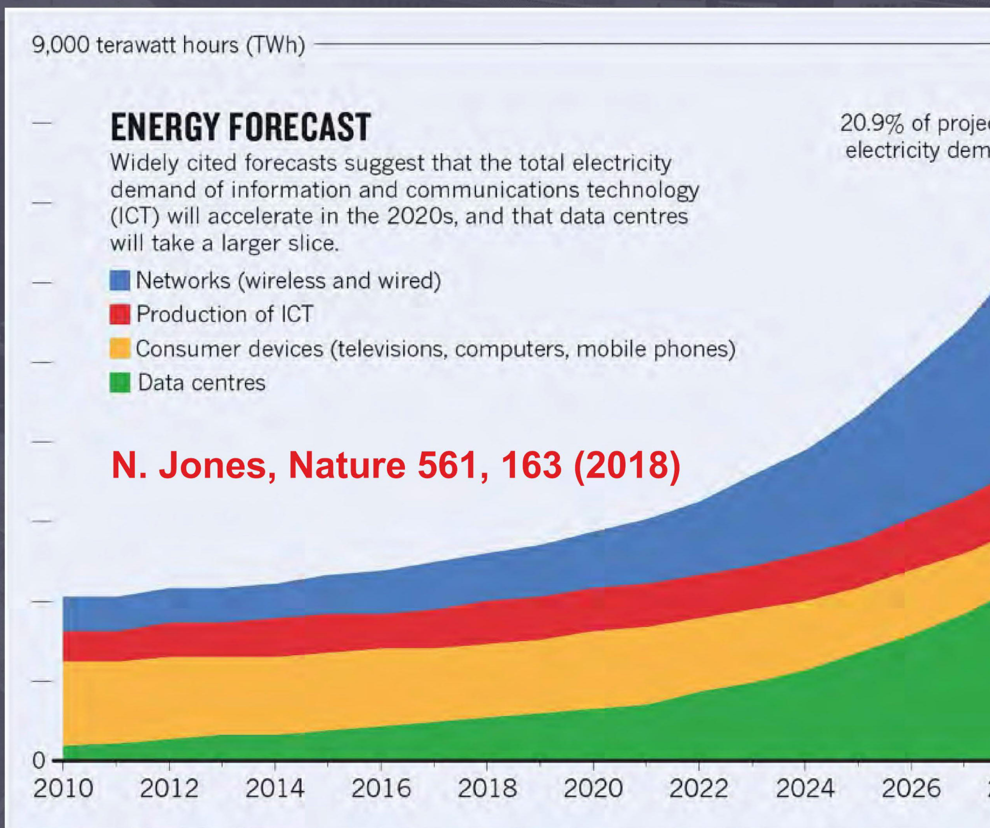
- Industry

Information & Communications Technology (ICT)

stimated to constitute 21% (or more) of the global electricity demand by 20

erver halls and networks are the areas that will increase the most.





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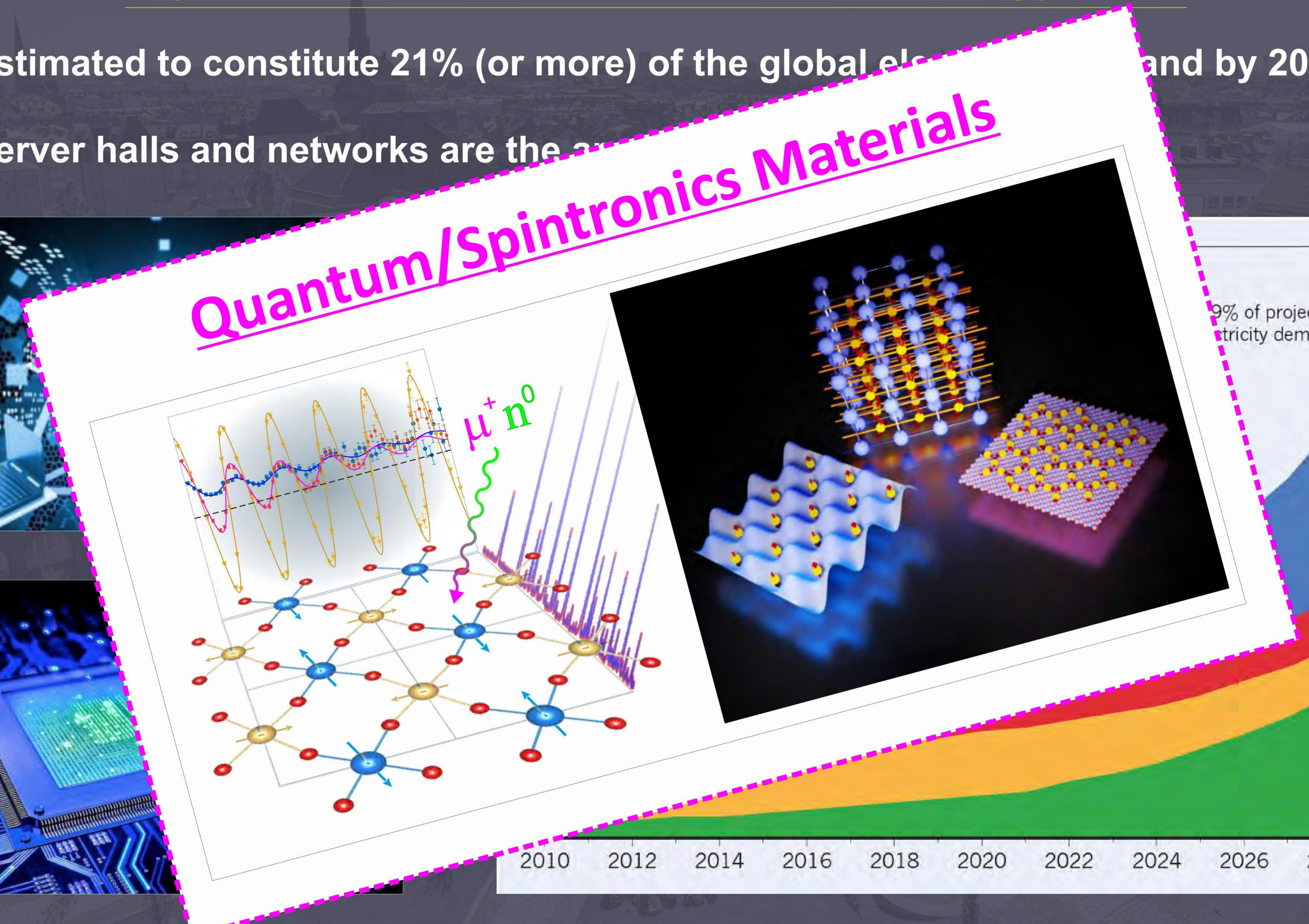
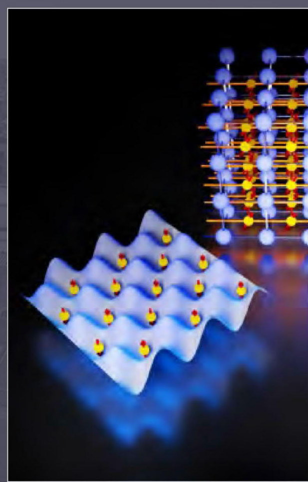


Why Quantum Materials ?

Spintro

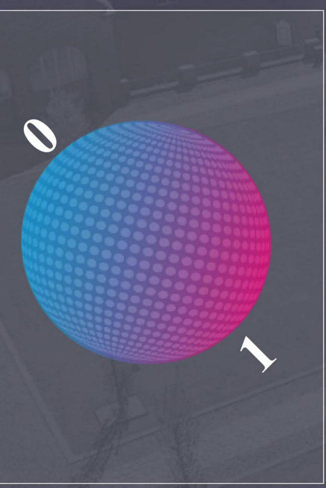


driving forces for looking at magnetic materials is clearly the
s evolution.

mmunication society to move forward, replacement of the
harge-based" electronics is essential.

the flow of charge through transistors with flipping of spins is
faster and energy efficient.

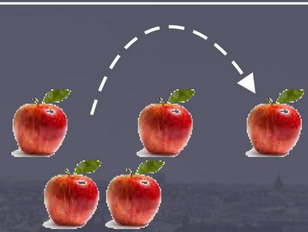
omputing/Qubits



- To increase computing power and improve security, using
  entanglement (bits $\rightarrow$ Qubits) in quantum computers is o
- If realized we could solve certain computing problems exp
  faster than with today's traditional algorithms.

To obtain a paradigm shift in this important area we
need to develop & understand new **QUANTUM MATER**

What is a Quantum Material



ıme for correlated electron physics"

es cannot be explained by the simple sum of the individual parts (atoms, electr

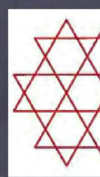
operties are instead governed by how the individual LEGO pieces are interactin

antum effects (= strenght of exchange interaction) are usually (but not always)

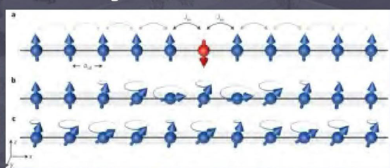
nhanced and/or protected for certain cases:

aterials that contains magnetic ions with small spin values (*S* = 1/2...)

e interactions are restricted = reduced dimensionality and/or frustrated



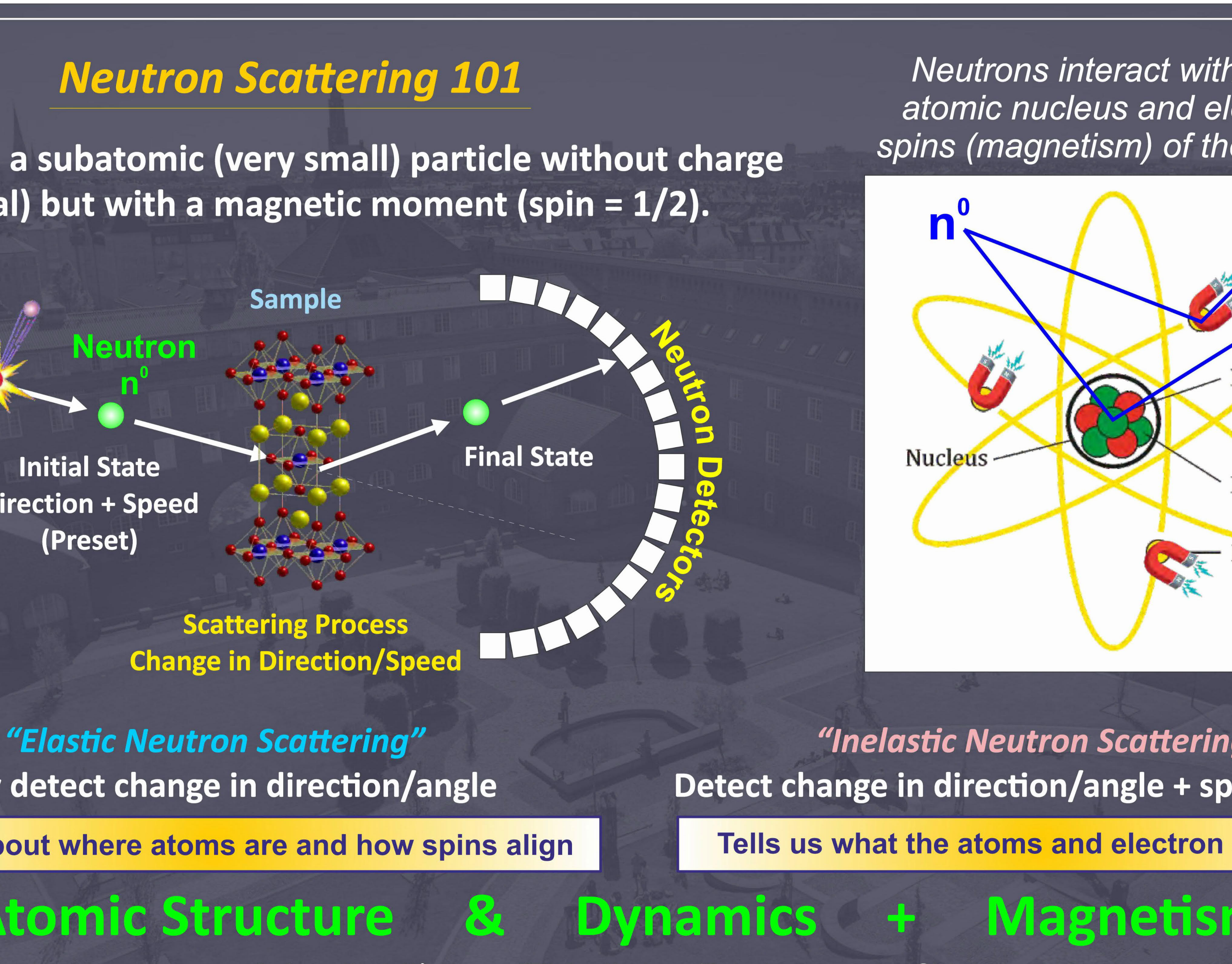
pologically proteced



s governed not only by thermal fluctuations but also quantum fluctuations (ev

c materials without magnetic order but a strong spin response to external pert

: "The Rise of Quantum Materials", Nature Physics 12, 105 (2016): https://doi.org/10.1038%2Fnp



Neutron Scattering 101
a subatomic (very small) particle without charge
al) but with a magnetic moment (spin = 1/2).
Sample
Neutron
n0
Initial State
irection + Speed
(Preset)
Final State
Neutron Detectors
Scattering Process
Change in Direction/Speed
Neutrons interact with
atomic nucleus and el
spins (magnetism) of th
n0
Nucleus
"Elastic Neutron Scattering"
detect change in direction/angle
bout where atoms are and how spins align
"Inelastic Neutron Scatterin
Detect change in direction/angle + sp
Tells us what the atoms and electron
tomic Structure & Dynamics + Magnetis
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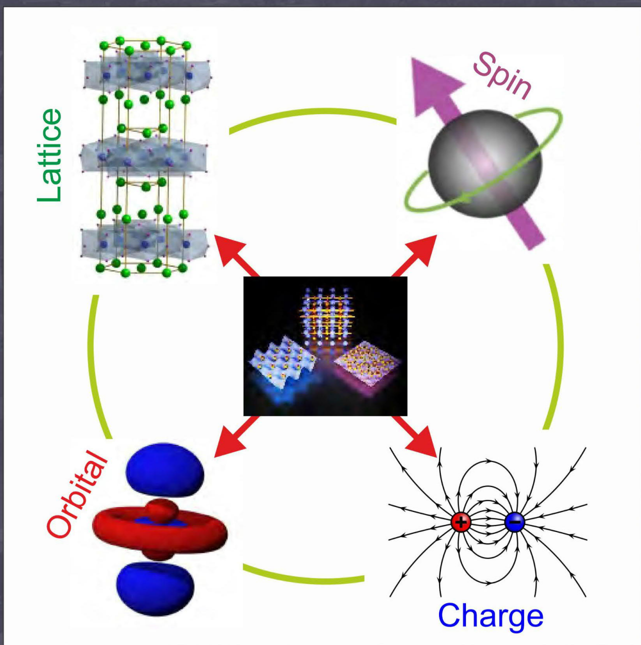
y Neutrons for Quantum Materials

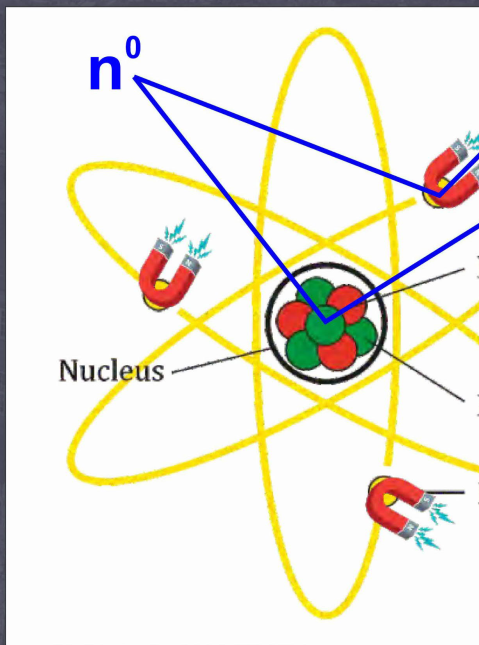
give direct access
ucture + low-
n excitations
 with X-rays)

d correlated
f freedom can
ed.

a wide range of
erturbations:
T, 100 GPa...
hemical "doping"

Neutrons interact with
atomic nucleus and el
spins (magnetism) of th





"Elastic Neutron Scattering"

"Inelastic Neutron Scatterin

bout where atoms are and how spins align

Tells us what the atoms and electron

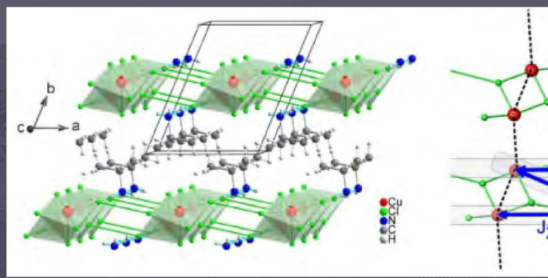
tomic Structure & Dynamics + Magnetis

Organometallics

pounds can create magnetic model systems

al ions (magnetic) into a tunable organic (non-
framework = endless combinations

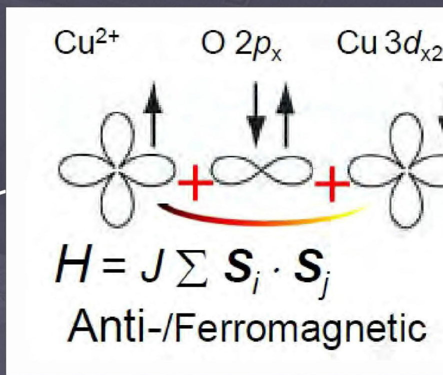
thesize (also for applications), accessible phase
H), "mechanically soft" (pressure).



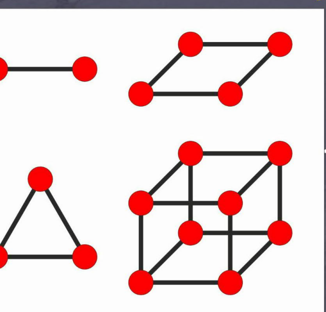
Spins

$S = ½, 1, ...$

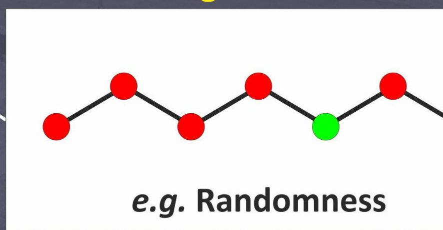
Interactions



Architecture
ension & connectivity)



Tuning Possibilities

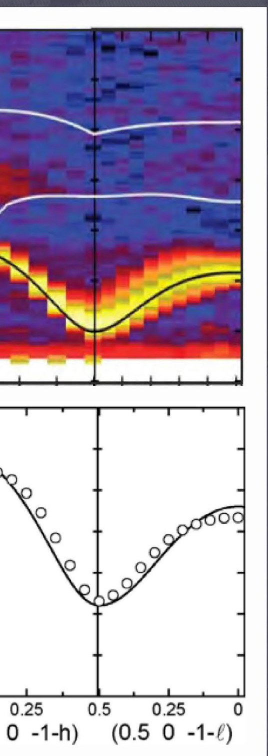


Example: PHCC

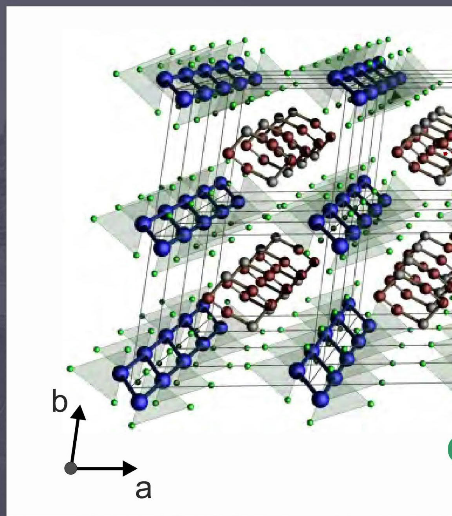
...um hexachloro-dicuprate or PHCC = $[C_4H_{12}N_2][Cu_2Cl_6]$

...=1/2) form slightly skewed spin-ladders along the c-axis.

...s not order even at lowest T (no magnetic Bragg peaks)



Ground state of PHCC is a quantum spin liquid



- The magnetic excitation spectrum (INS) is a single mode with ... singlet/triplet gap Δ = 1 meV and magnon band-width of 1.8 ... (h 0 l) plane, while flat along b* = ac-planes magnetically deco...
- Such data was originally acquired using traditional triple-axis s... that measure "point-by-point" in a limited range of the Brillou...

...ture 440, 187 (2006)

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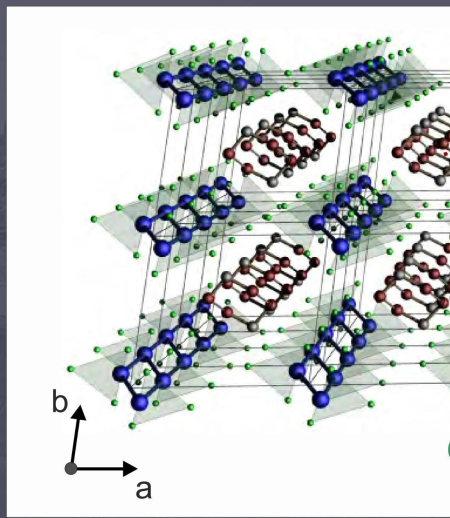

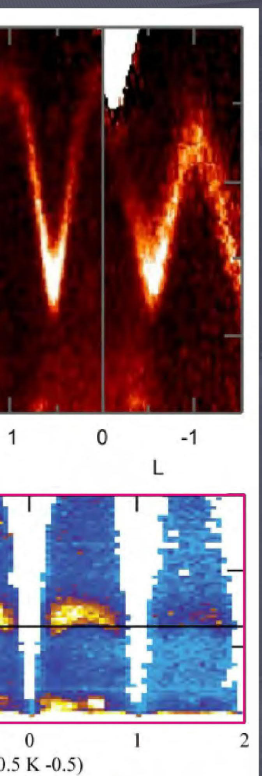

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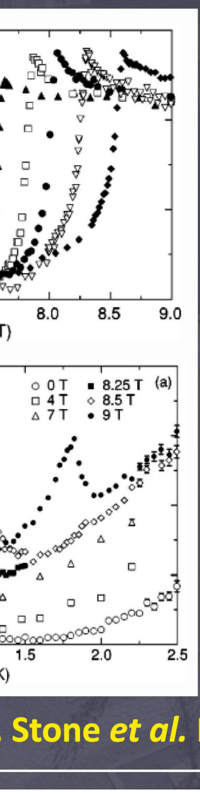
- Such data was originally acquired using traditional triple-axis ... that measure "point-by-point" in a limited range of the Brillou...
- If same material is measured using modern time-of-flight INS ... it is clear that a dispersion is present along $(0\ k\ 0)$ = interplane...

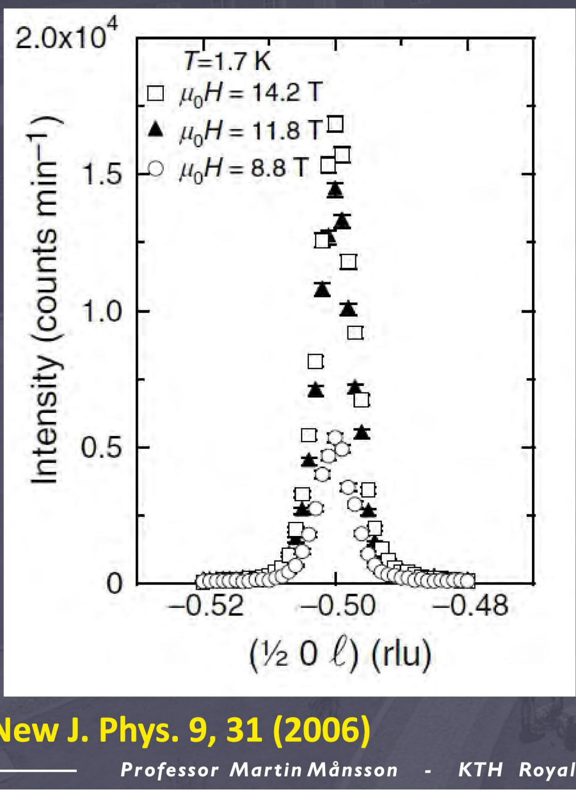
Inducing Magnetic Order in PHCC - Bose Einstein Condensation

xternal perturbations, we can close the spin gap and induce magnetic order (BEC)

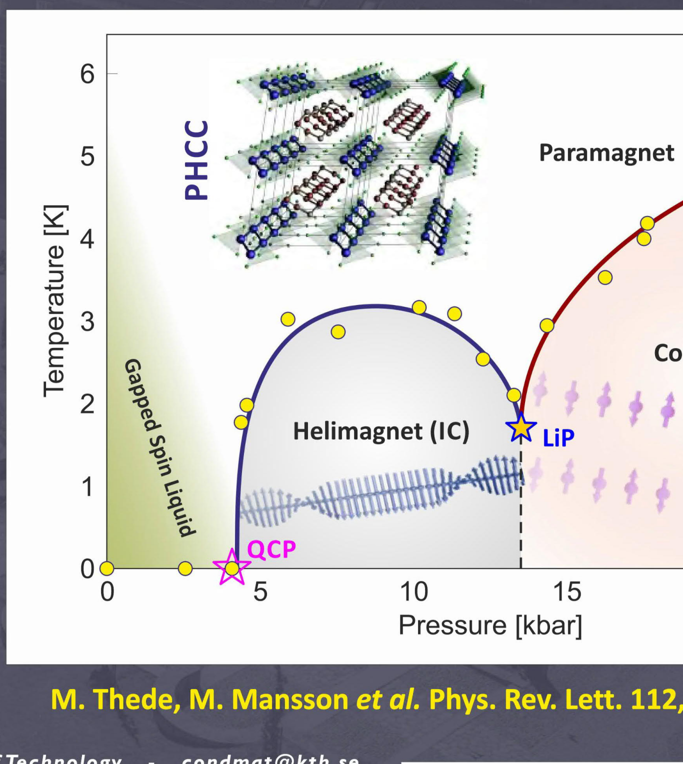
surements and neutron diffraction
l-induced AF magnetic order in
≈ 7.5 T

- High-pressure INS + muon spin ro
show that BEC is achieved at p_c ≈
where incommensurate AFM orde





. Stone *et al.* New J. Phys. 9, 31 (2006)



M. Thede, M. Mansson *et al.* Phys. Rev. Lett. 112,

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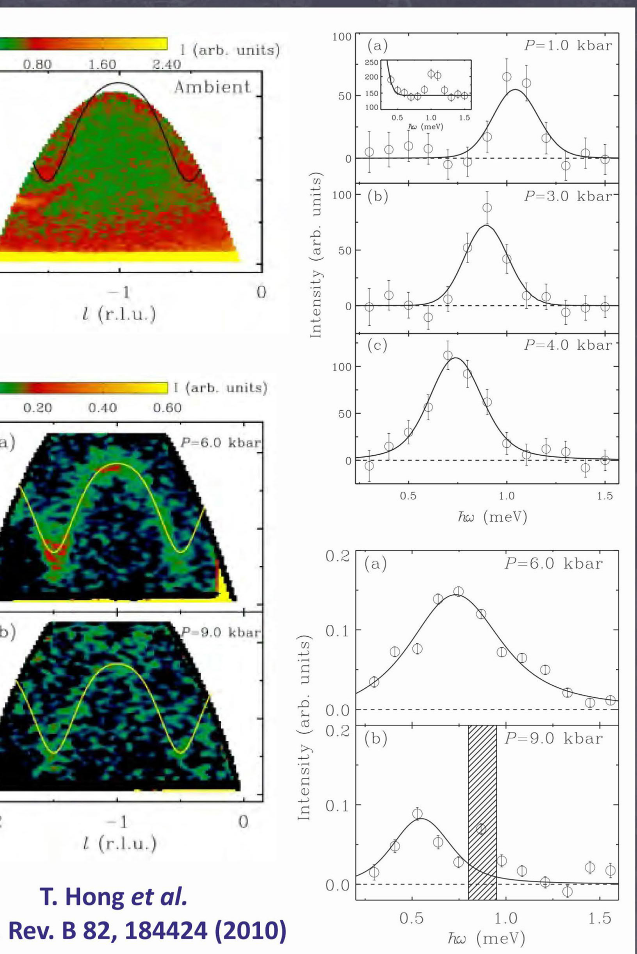

T. Hong *et al.*
Rev. B 82, 184424 (2010)

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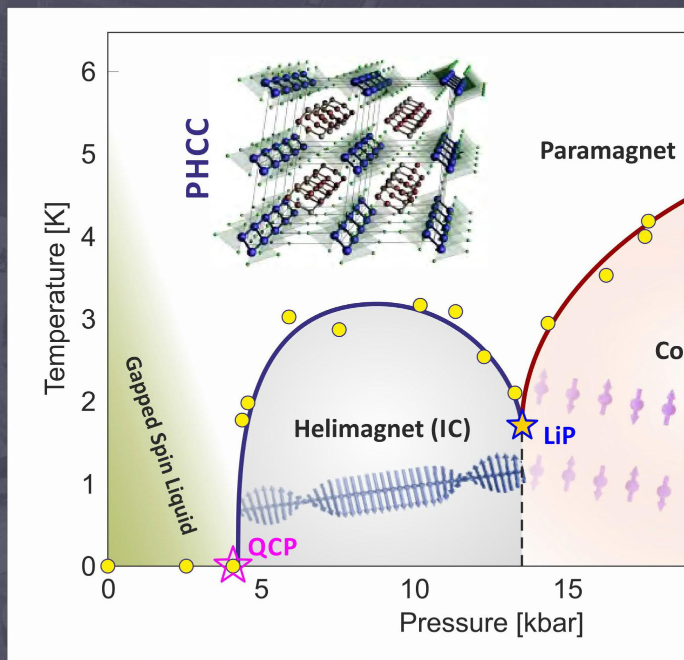


M. Thede, M. Mansson *et al.* Phys. Rev. Lett. 112,

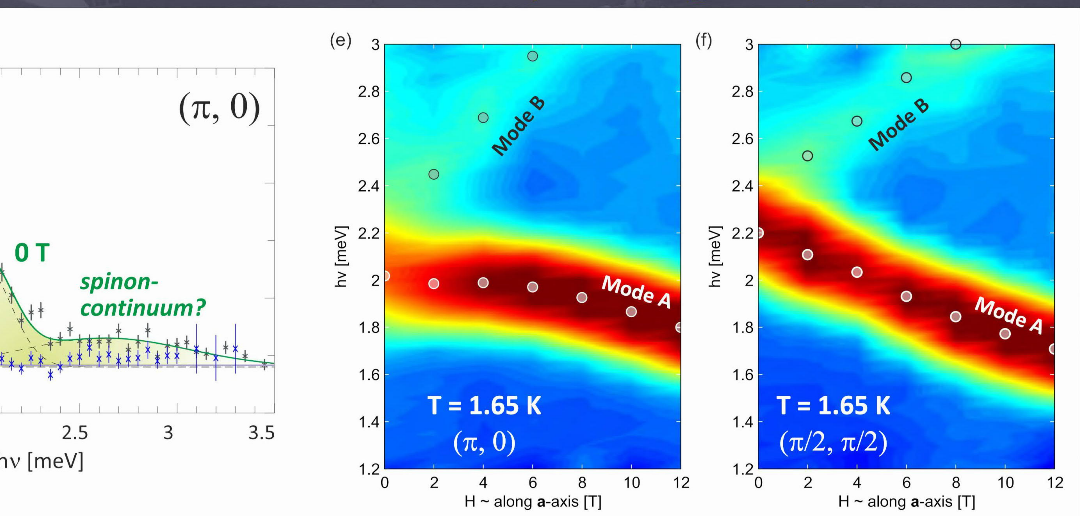
Next Generation Neutron Scattering

instrument for Quantum Materials and INS under
nditions (T, P, H) is BIFROST (c.f. CAMEA @ PSI).

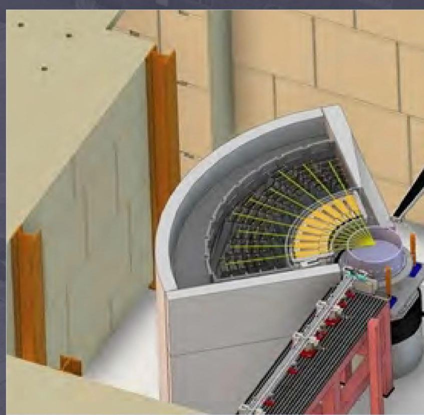
neutron flux in + efficient detection of scattered
will be 30 times better than any existing instrument!

samples AND/OR higher magnetic fields A/O higher energy
A/O lower background using high pressure environment.

~2 Weeks of beamtime (TASP @ PSI)



BIF



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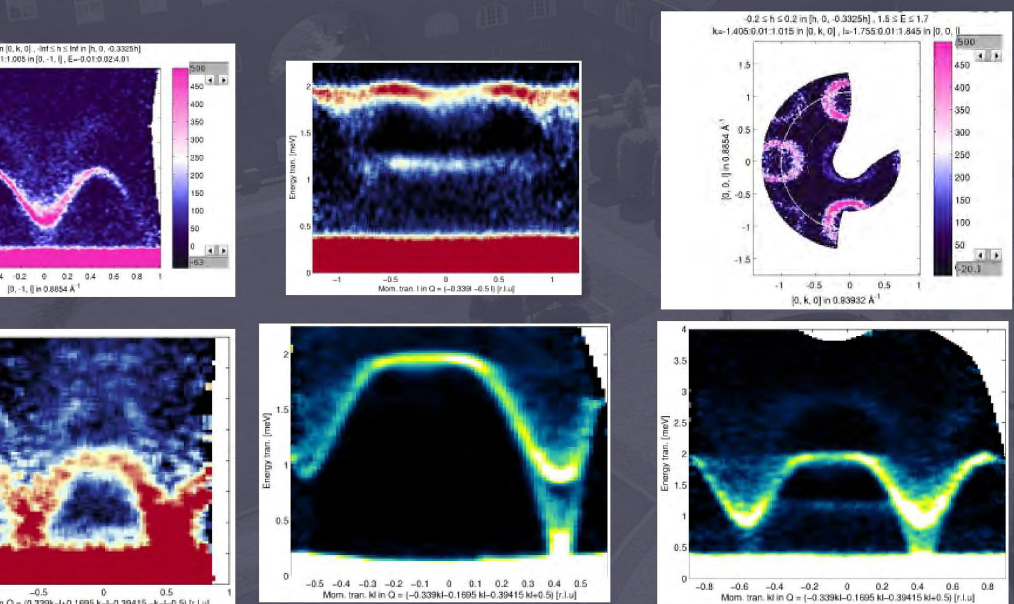
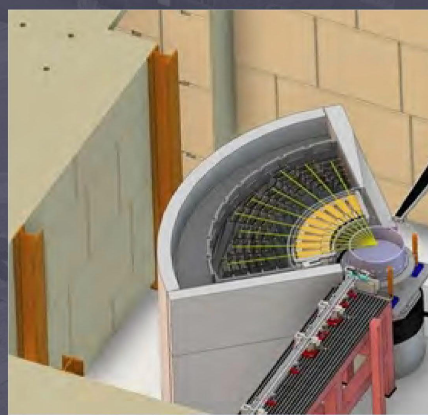
BIFI





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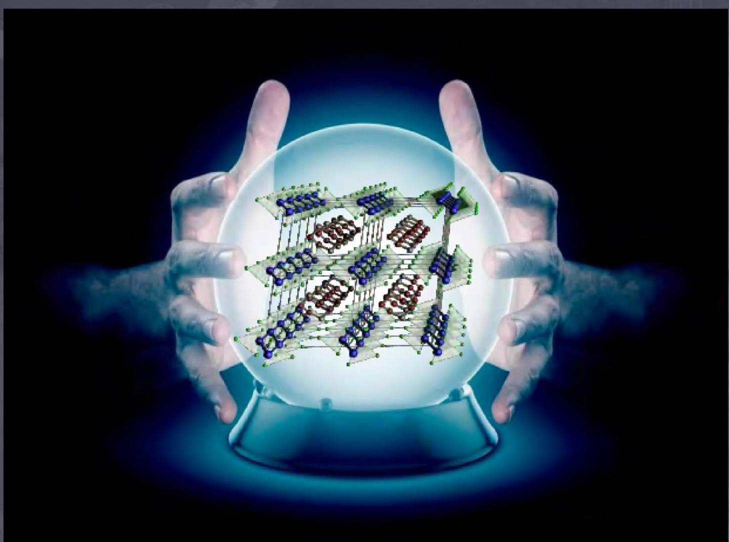
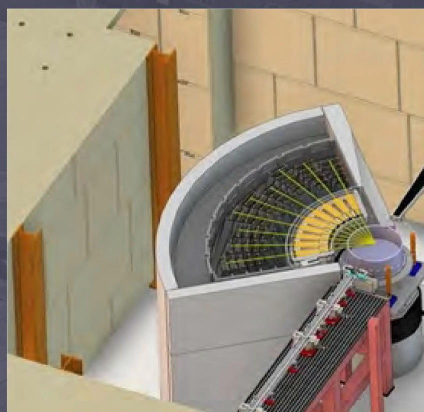
(BIFROST @ ESS)





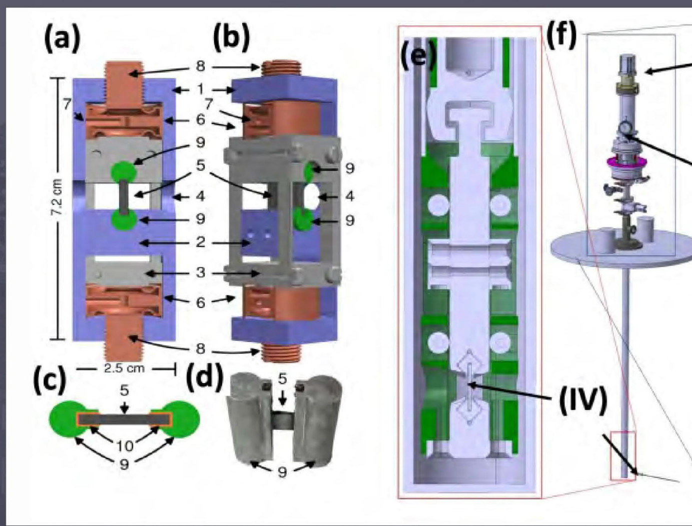
ni-axial Pressure Setup

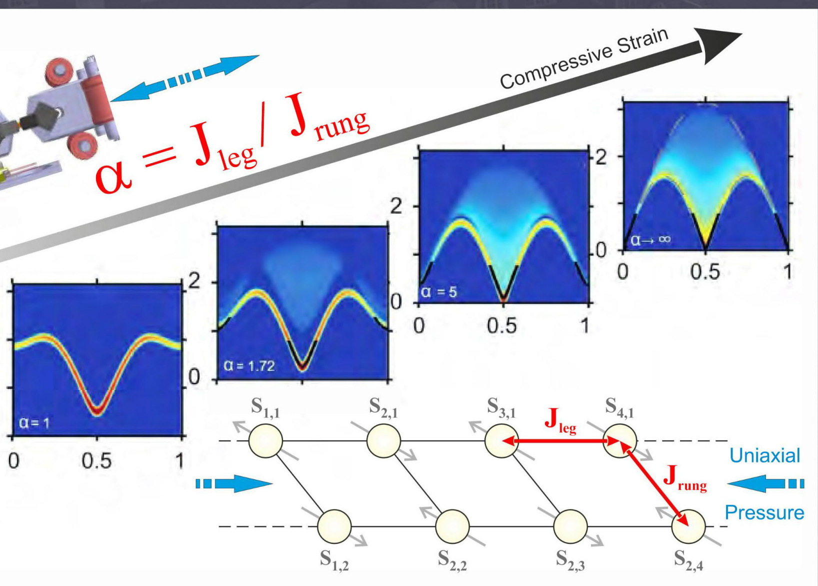
PAUL SCHERRER INSTITUT PSI

ent of novel sample environment for neutron
ttering with PSI, Chalmers, Uni. Zurich.

nge of pressure, both compressive/tensile
wn to 1.5 K and under magnetic field.

perational for XRD at PETRA III/P21 and
ned for neutrons at PSI (ND, INS, SANS).



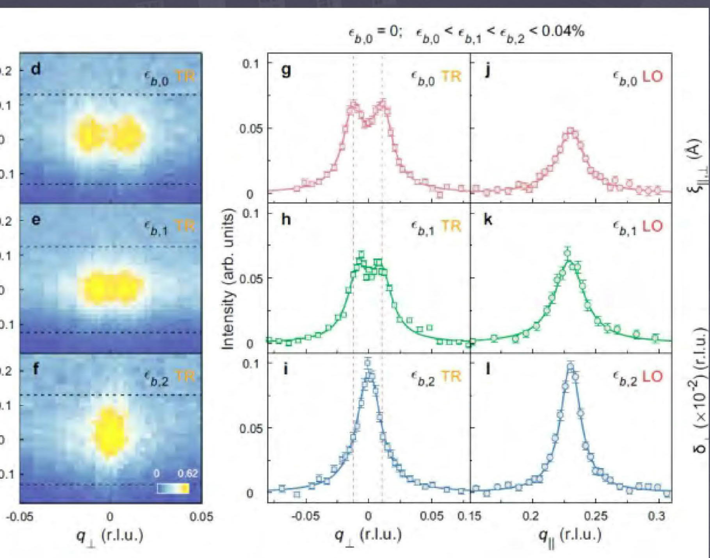


- Such setup allow us to apply press
individual crystallographic lattice d
- Can be used to break rotational sy
and/or tune specific magnetic exch
parameters (interactions J / J'...)
- Open up for systematic tuning of e
ladder from "strong leg" to "strong
without the need for chemical dop
risk of chemical disorder.

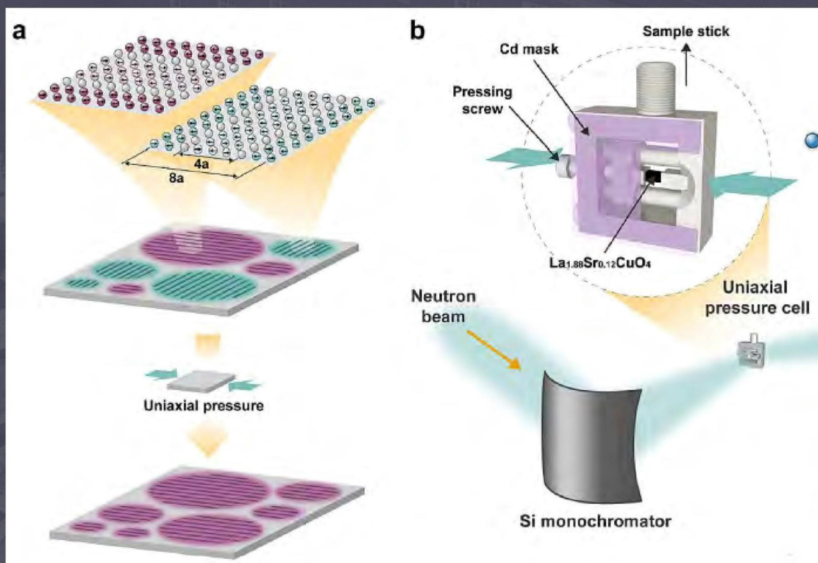
High-temperature Superconductors - Neutrons + X-rays

he new possibilities for systematic studies using uni-axial strain has already allowe
d long-standing scientific questions e.g. within high-temperature cuprate supercon

the strengths of neutrons (INS @ ILL) and x-rays (RIXS @ SLS) with uni-axial strai
ied that charge (CDW) and spin (SDW) degrees of freedom are coupled, possibly fo
nodulated superconducting order parameter (pair density wave, PDW, state).



e Communications 13, 1795 (2022)



Nature Communication Physics (2022) - Ac

Organic Materials DataBase (OMDB)

that focus on specifically organic materials (other DB
mainly for inorganic materials).

(.cif-files)comes from the Crystallographic Open
(COD)

wo modeling routes:

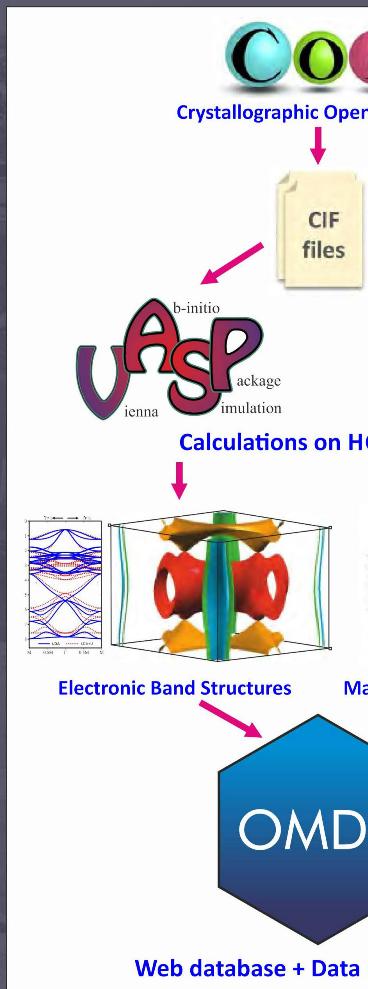
onic Properties (established)

etic Properties/Excitations

ully open access (~50'000 materials) please visit:

https://omdb.mathub.io/

t also links OMDB with physical sample synthesis,
nents of both electronic (photons) and magnetic
band structures.



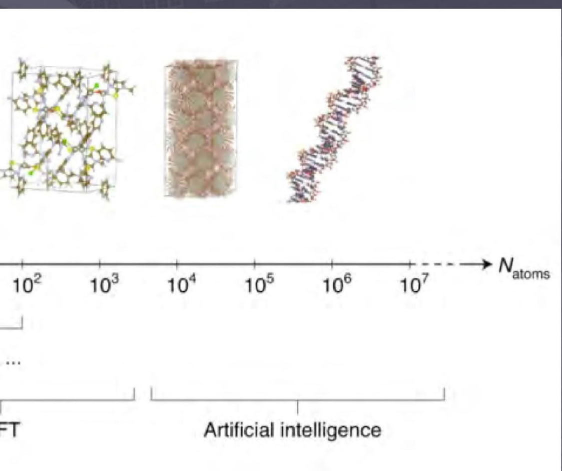
http://dx.doi.org/10.1371/jou

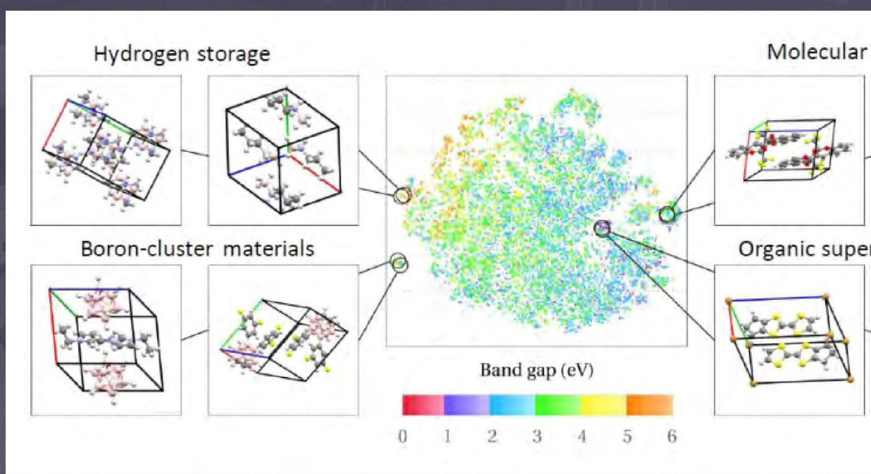
Search Tools and Machine Learning

o contain a set of advanced search tools find e.g. find materials with similar b

tools 15 potential new orgainic superconductors we found as well as
ion of strongly interacting organic semimetals.

Machine Learning (ML) tools have also been implemented to allow for high th
of physical properties of materials.



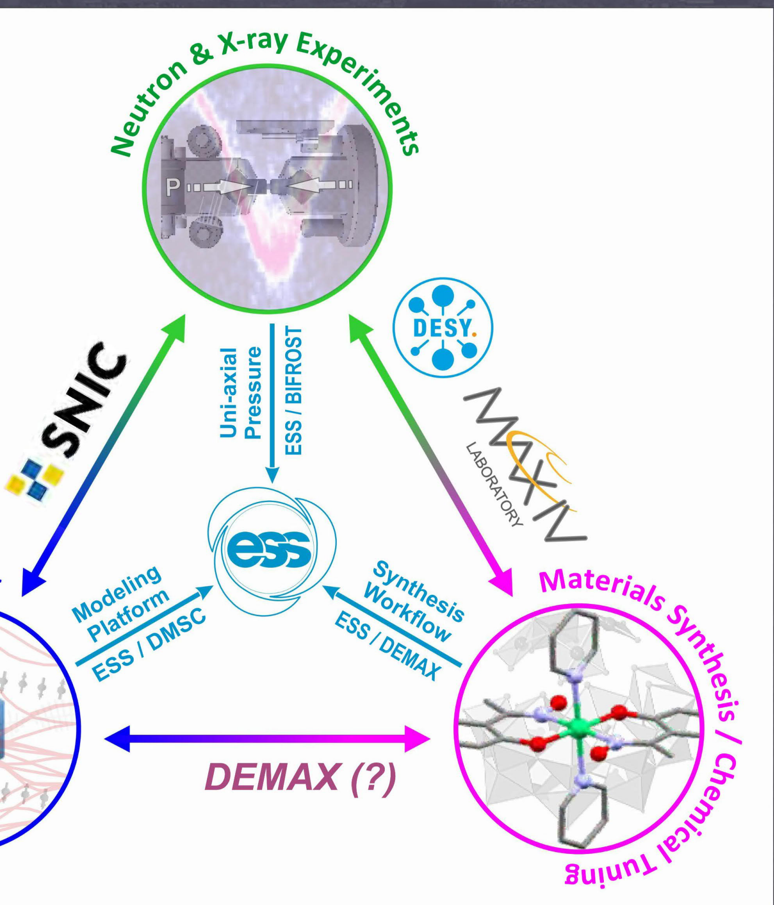


hoorn, Balatsky, Nature Physics (2021)

Olsthoorn, et al., Adv. Quantum Tech. (201

Ready for User Operation 2027

Ecosystem Around ESS/MAX IV



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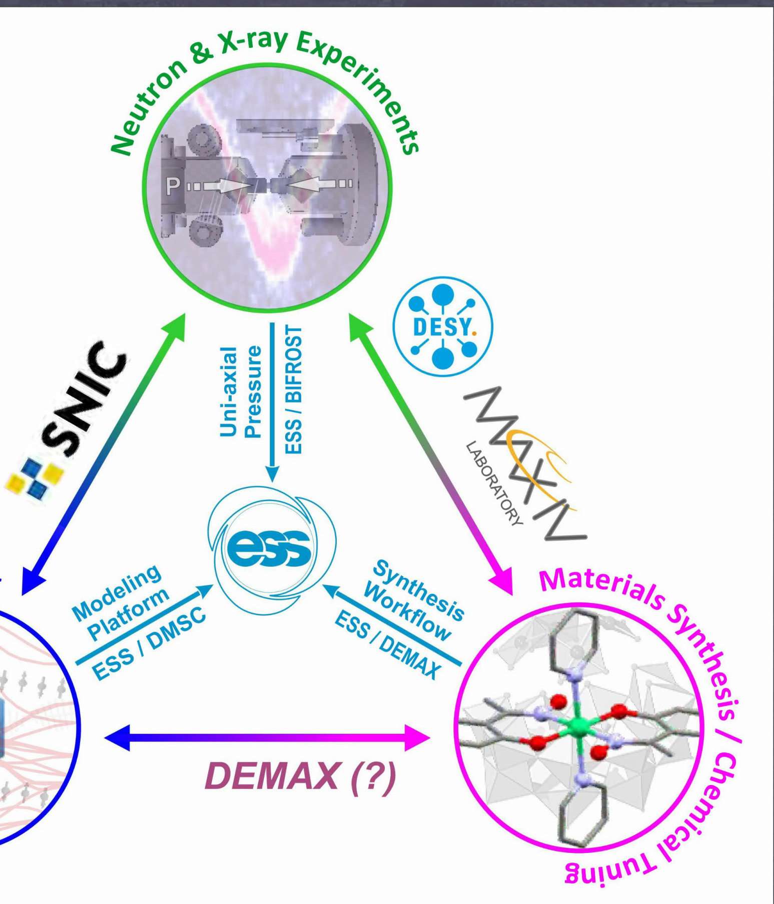

- Swedish graduate school in neutro
- SSF funding for 40 PhD students (2
- Open/Free course catalogue


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PSI
University of Zurich UZH
RWTH AACHEN UNIVERSITY
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