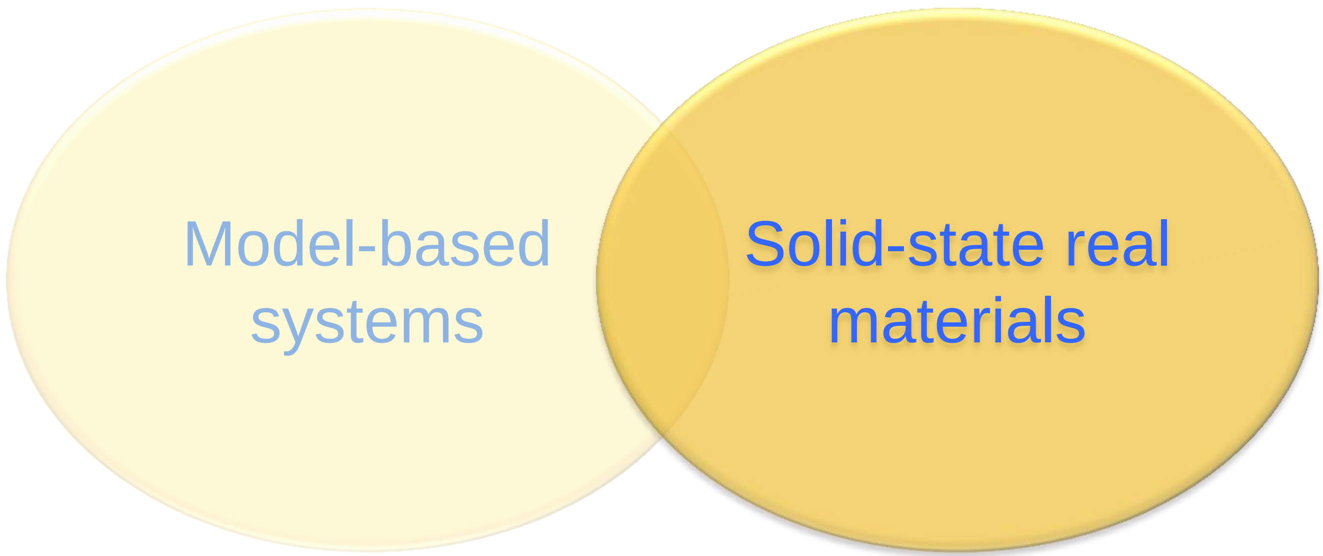
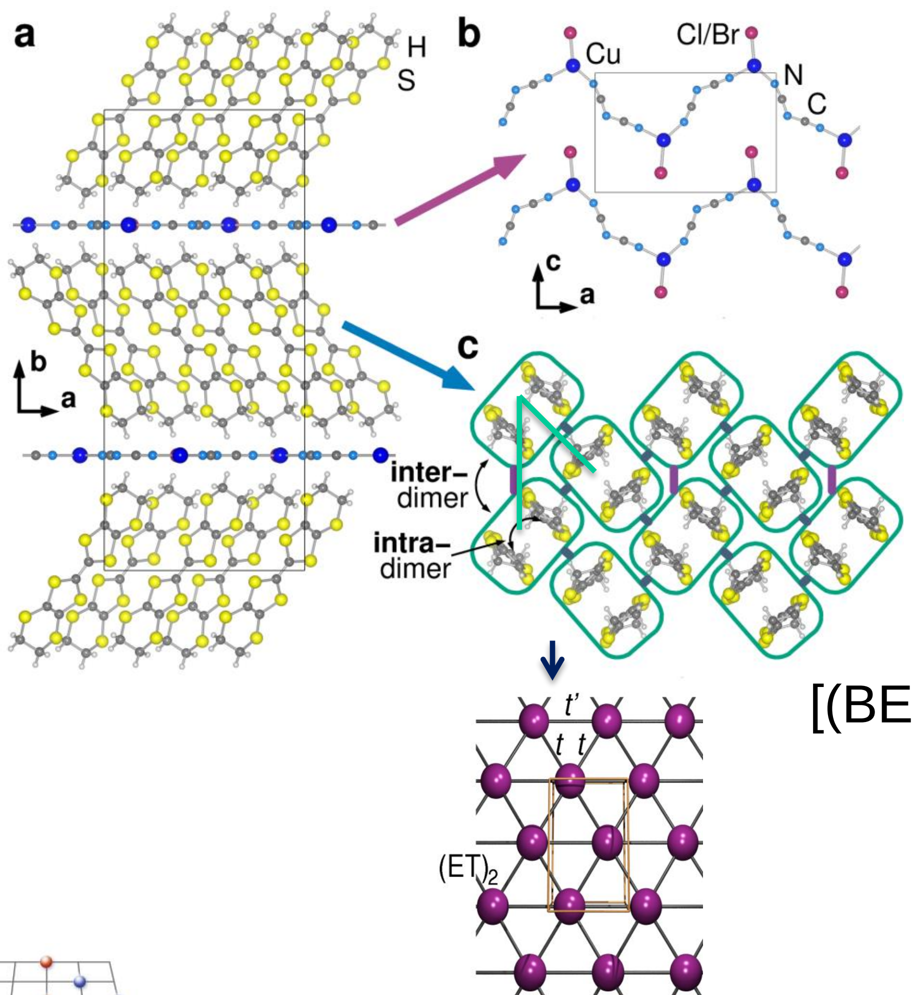
Cooperative Phenomena



Mott transition

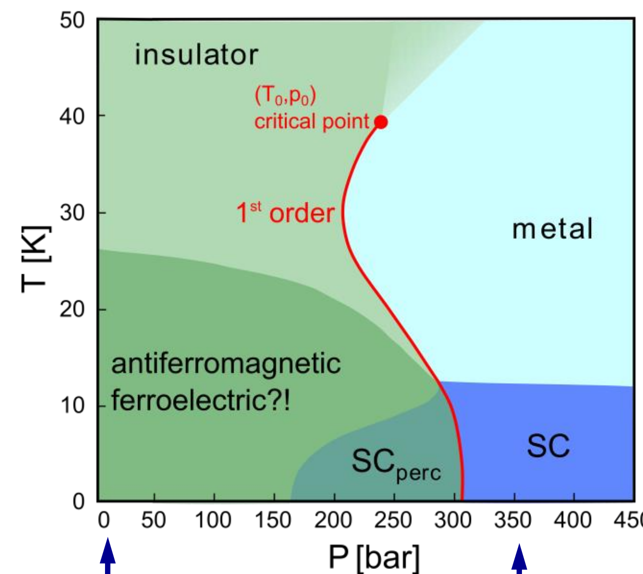
κ- (BEDT-TTF)$_2$X



X$^-$

[(BEDT-TTF)$_2$]$^+$

„ET“



X = Cu[N(CN)$_2$]Cl Cu[N(CN)$_2$]Br

- Mott transition :
  metal - insulator

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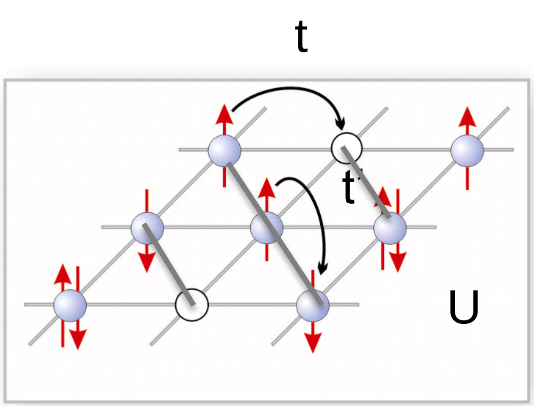
Frankfurt / Kaiserslautern / Mainz

Mott transition: correlated phases

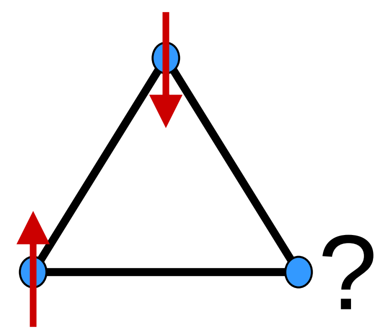
correlated phases:

- Mott insulator & criticality at T_0
- spin liquid / anomalous magnetic states
- multiferroics
- superconductivity
- novel phases



effects of:

- pressure t/U (control)
- temperature (control)
- interaction with lattice (electron-phonon)
- frustration
- disorder



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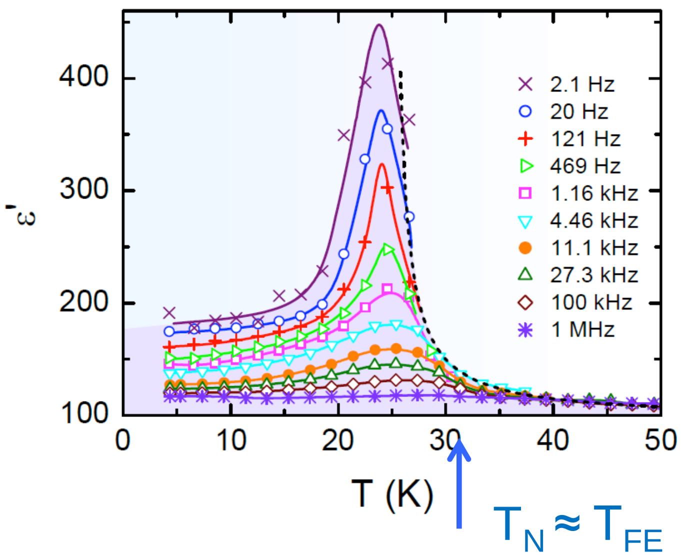
Mott transition and anomalous states nearby

B11 **B6**

P. Lunkenheimer,
U Augsburg

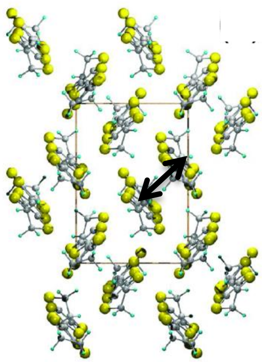
Multiferroicity – electric-dipole-driven magnetism

κ-$(ET)_2Cu[N(CN)_2]Cl$ – first multiferroic charge-transfer salt !



Nature Mater. **11**, 755 (2012)

IEEE Trans. Mag. **6**, 2700107 (2014)

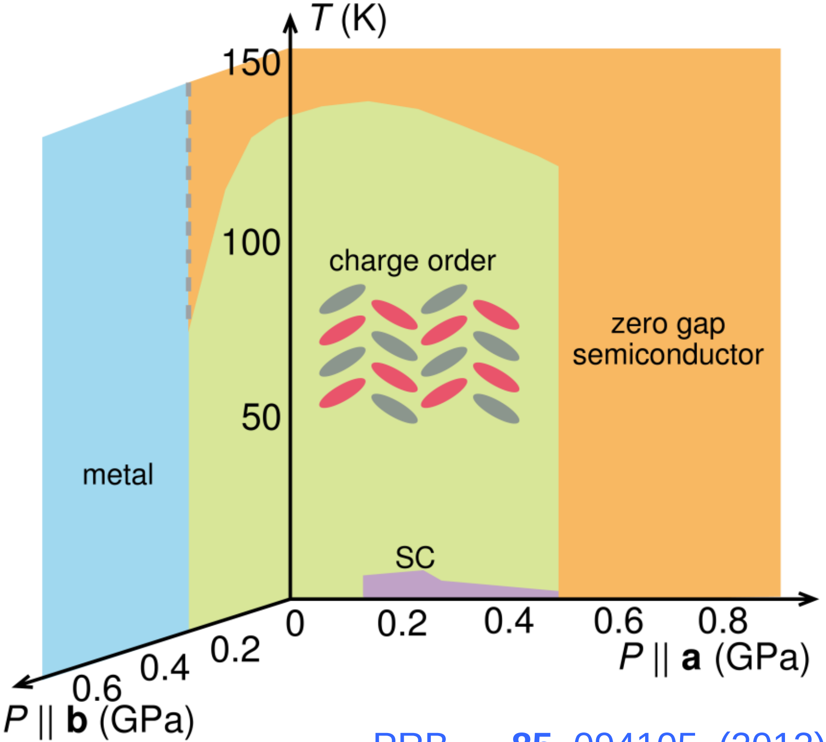


Next:

- investigate order-parameter coupling
- dielectrics under pressure, fluctuation spectroscopy
- ab initio density functional theory simulations. Dielectric response
- spin-charge-lattice coupling → phonon anomalies ?

Mott transition and anomalous states nearby

α- $(ET)_2I_3$ under strain: From charge-ordered insulator to correlated Dirac metal



PRB **85**, 094105 (2012)

PNAS **111**, 5106 (2014)

signatures of ferroelectric order

arXiv:1407.0339

Next:

- monitor the phase transitions under pressure/strain
- dielectrics under pressure, fluctuation spectroscopy
- ab initio DFT calculations at finite pressure/ van der Waals corrections / dielectric function
- extended Hubbard model (correlations)

Mott transition & criticality

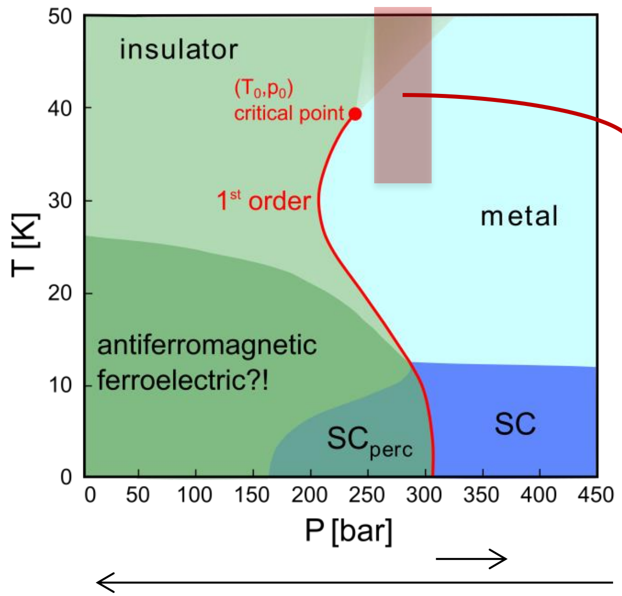
First thermodynamic measurement on Mott criticality using a novel technique: Thermal expansion under gas pressure

B6

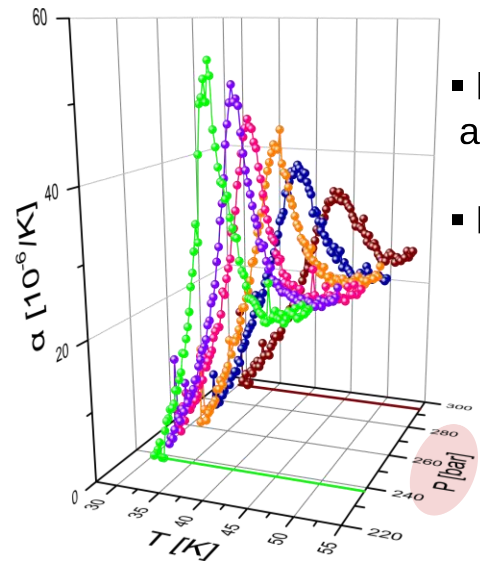
κ-$(ET)_2Cu[N(CN)_2]Cl$

$$\alpha = \frac{1}{l}\frac{\partial l}{\partial T}$$

Rev. Sci. Instrum. **83**, 085111 (2012)



U/t, cooling speed



- large lattice effects around the Mott transition
- highly pressure sensitive!

50 bar!

Next:

- solve controversy on universality class
  2D Ising ←→ unconventional Mott criticality
- investigate electron-phonon effects

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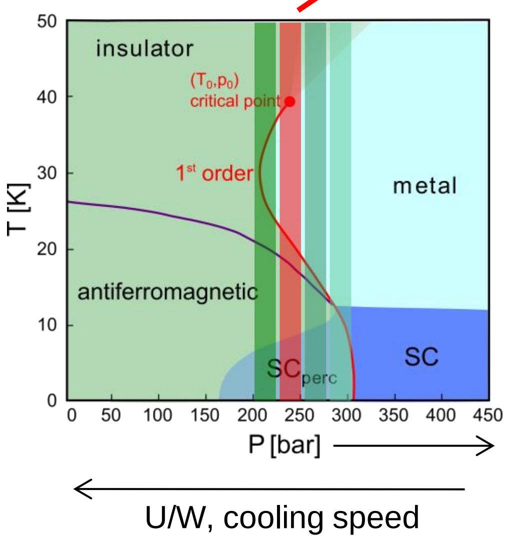
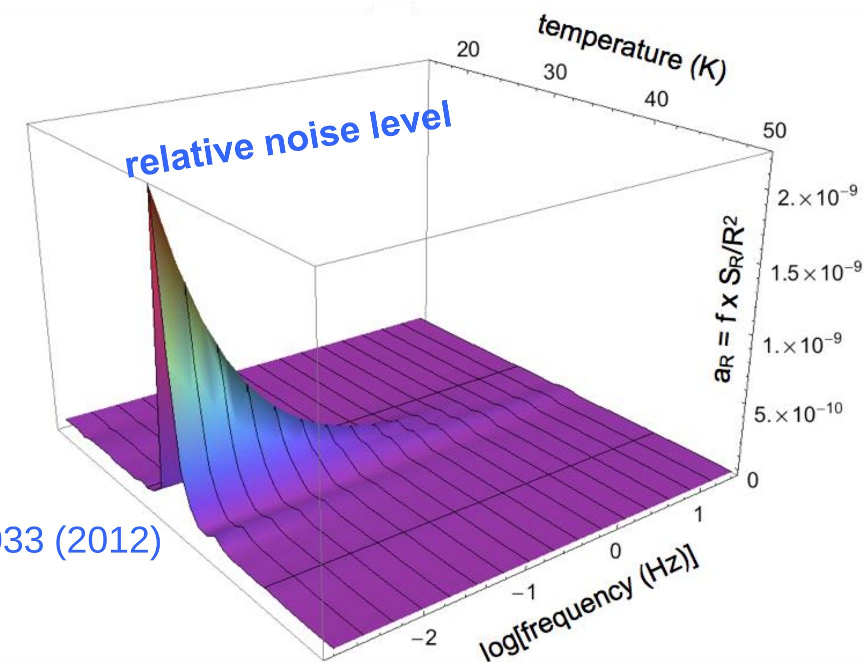
Mott transition & criticality



NJP **14**, 023033 (2012)



- critical slowing down of the order parameter (i.e. doublon density) fluctuations
- onset of non-Gaussian noise at the critical point

Next:

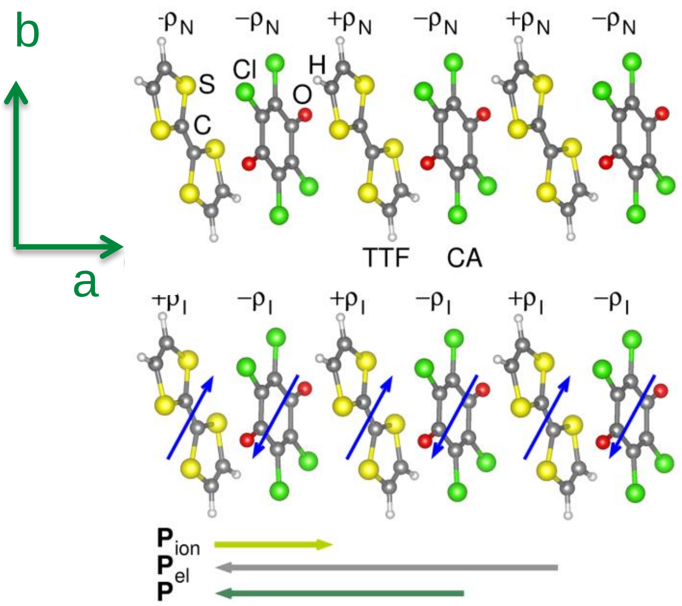
- investigate possible correlated fluctuations
- criticality as a function of magnetic field
- influence of disorder
- coupling to lattice

B11

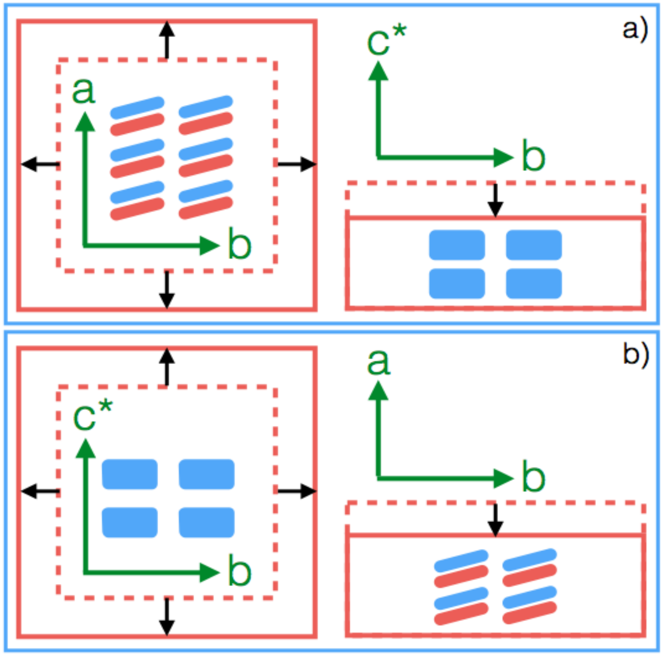
B6

Neutral-ionic transition

Electronically induced ferroelectricity in TTF-CA (tetrathiafulvalene-p-chloranil)



strain effects
on neutral-ionic
transition
and ferroelectricity



candidate for controlling polarization in the picosecond domain

Preliminary work on new CT

JACS **134**, 4694 (2012)

Mater. Res. Expr. **1**, 046303 (2014)

Phys. Chem. Chem. Phys. **17**, 4118 (2015)

Next:

- simulation uniaxial and biaxial strain effects by *ab initio* DFT
- calculation of spontaneous polarization: $P^{ion} + P^{el}$ (Berry phase approach)
- dielectric state of thin layers

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B9 **B2**

Quantum magnetism

Spin-phonon interaction and quantum criticality

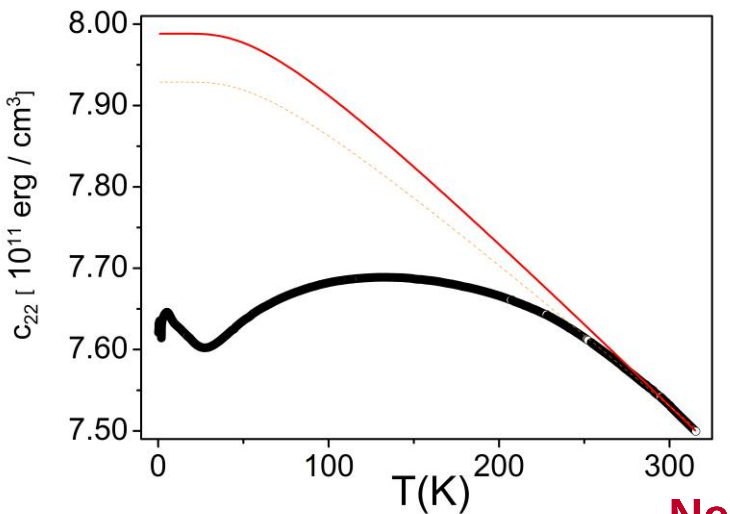
PRL **106**, 217201 (2011)

PRB **89**, 174427 (2014)

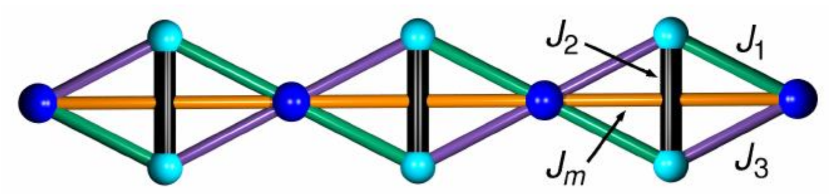
1D system

azurite: distorted diamond chain;

B1 **B2** **B3** **A10**



Next:



- exceptionally large magnetoelastic coupling constant: large $\partial J_2/\partial \varepsilon_b$

- perturbation theory-based calculations

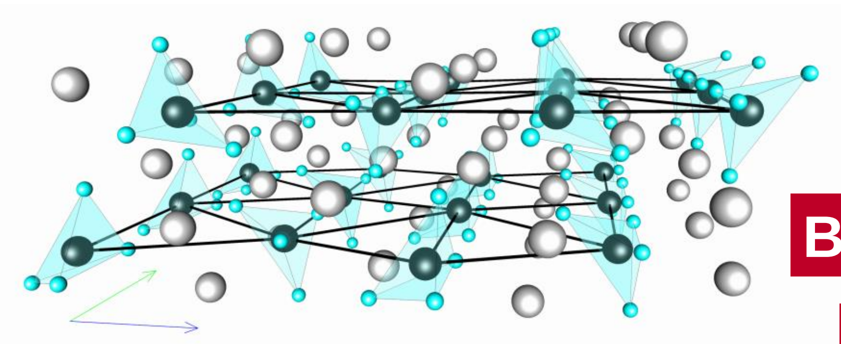
$\Rightarrow$ origin of the huge magneto-elastic coupling

$B13_N$

Quantum magnetism/ spin liquid phases

2D systems

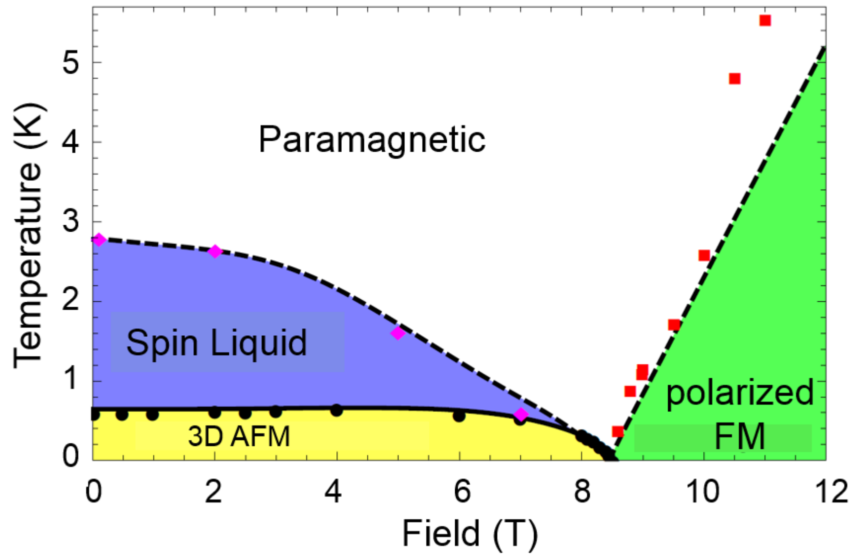
Cs_2CuCl_4: **triangular antiferromagnet**



Exchange parameters

B4 **B2** **B13$_N$**

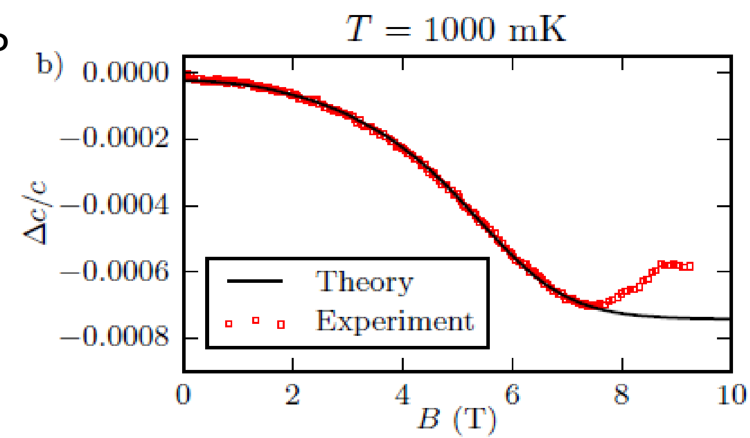
PRB **91**, 035124 (2015)



B1 **A8** PRB **91**, 041108(R) (2015)

Next:

- correlation functions for dilute Bose gas near QCP
  hard-core boson + fRG
- coupling hard core bosons ←→ lattice
- ultrasound near QCP
- non equilibrium



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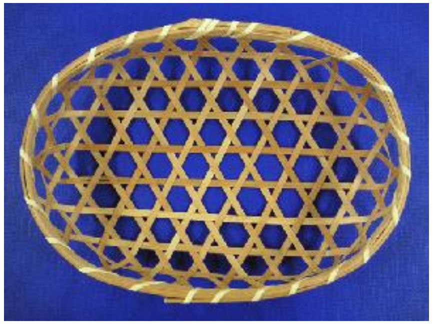
Quantum magnetism/ Kagome

Nature Comm. **5**, 4261 (2014)
PRL **111**, 147201 (2013)



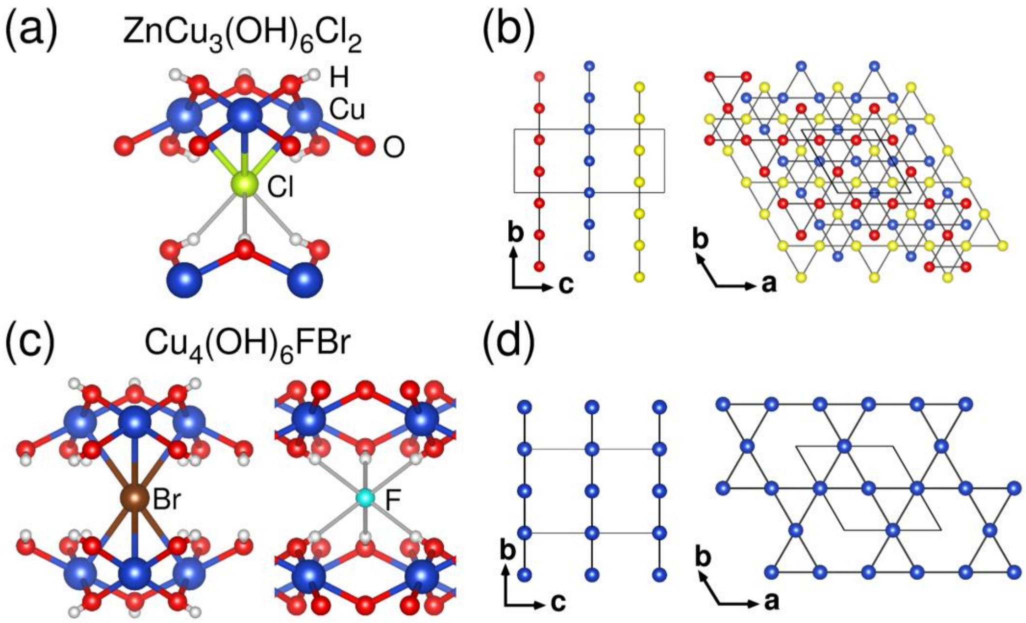
Next:

Exotic phases in frustrated Kagome systems:

Kagome lattices of spin ½ Cu

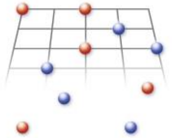
Herbertsmithite

Barlowite



- filling effects ?
- Dzyaloshinskii-Moriya
- interaction?
- correlation effects?
- lattice effects?

B1 **B2** **B3** **B4** **B13$_N$** **A5**



Theoretical Modelling

State-of-art and further development:

B2

***Ab initio* density functional theory,** projective Wannier functions, finite pressure structure prediction, genetic algorithm, molecular dynamics
Many-body methods: DMFT, VMC, exact diagonalization

B3

Quantum Monte Carlo simulations, coupled spin cluster approach, investigation of tunable frustrated systems, cross-dimensional transitions

A3

Dynamical mean field theory for inhomogeneous systems**,** projection operator approach

A5

Further extend of **DMRG** to 2D systems

A8

Functional **RG** method

B13$_N$

***Ab initio* Quantum Monte Carlo**, **perturbation theory** for spin systems

Ab initio Quantum Monte Carlo

B13$_N$

K. Foyevtsova / R. Valenti, Uni Frankfurt

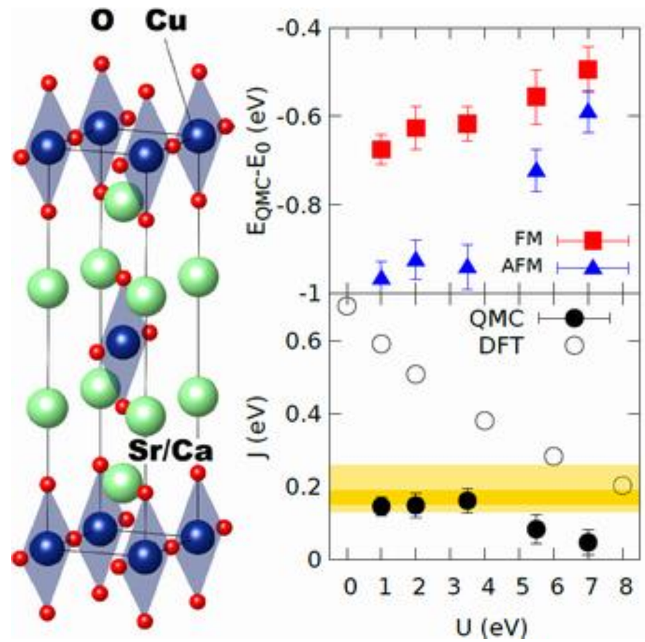
ab initio approach alternative to DFT

PRX **4**, 031003 (2014)

collaboration with
F. Reboredo, E. Dagotto

Example: Ca_2CuO_3

DFT → $D(\vec{R})$ Slater determinant (defines nodes) → **VMC** → $J(\vec{R})$ Jastrow factors → **DMC** → $\Phi_0(\vec{R})$ Ground state WF



Ceperley, Alder PRL **45**, 566 (1980)

Booth,Grüneis,Kresse,Alavi Nature **493**, 365(2013)

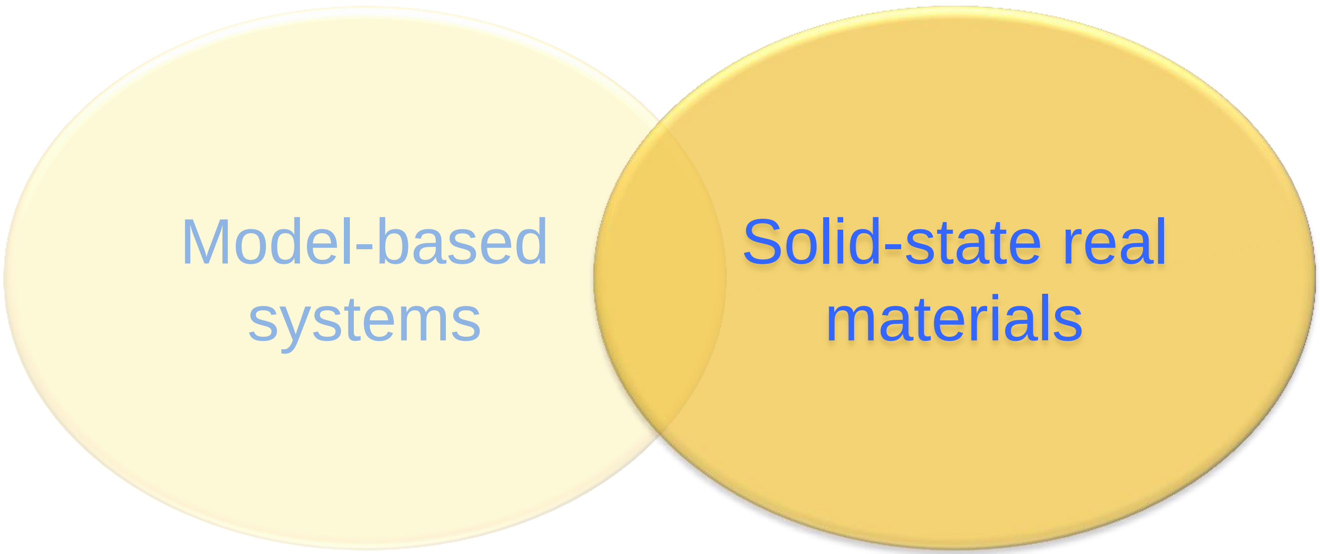
Next:

- benchmark the method
- spin superexchange couplings
- $Cs_2CuCl_{4-x}Br_x$, azurite,
- organic molecules

➢ Accurate *ab initio* treatment of many-body interactions
➢ High fidelity
➢ **Free from adjustable parameters**

A8 **B1** **B2** **B3** **B4** **B6**

Cooperative Phenomena



	Frankfurt am Main	Kaiserslautern	Mainz
Materials Design - Synthesis & Modelling	B1, B2, B4, B6,	A7, A9, A12	A10, B5, B8, B13N
Cooperative Phenomena	A3, A8, B1, B2, B4, B6, B9, B11	A5, A7, A9, A12, B3	A10, B5, B8, B12, B13N
Excitations & Interactions	A3, A8, B1, B2, B4, B6, B9, B11	A5, A7, A9, A12, B3	A10, B5, B8, B12, B13N