

# Theory @ IFP

## AG Toschi & AG Held



Dr. Georg Rohringer



Thomas Schäfer



Elias Assmann



Dr. Jan Tomczak



Patrik Gunacker



Dr. Marco Battiato



Ciro Taranto



Dr. Patrik Thunström



Liang Si



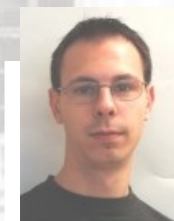
Dr. Zhicheng Zhong



Markus Wallerberger

### Recent/Current PAs

Monika Stipsitz, Patrik Gunacker, Rainer Bachleitner, Tin Ribic, Stefan Donsa, Lukas Semmelrock, Georg Harrer, Lorenz Auzinger



Dr. Angelo Valli



Anna Galler

# AG Held: Research topics

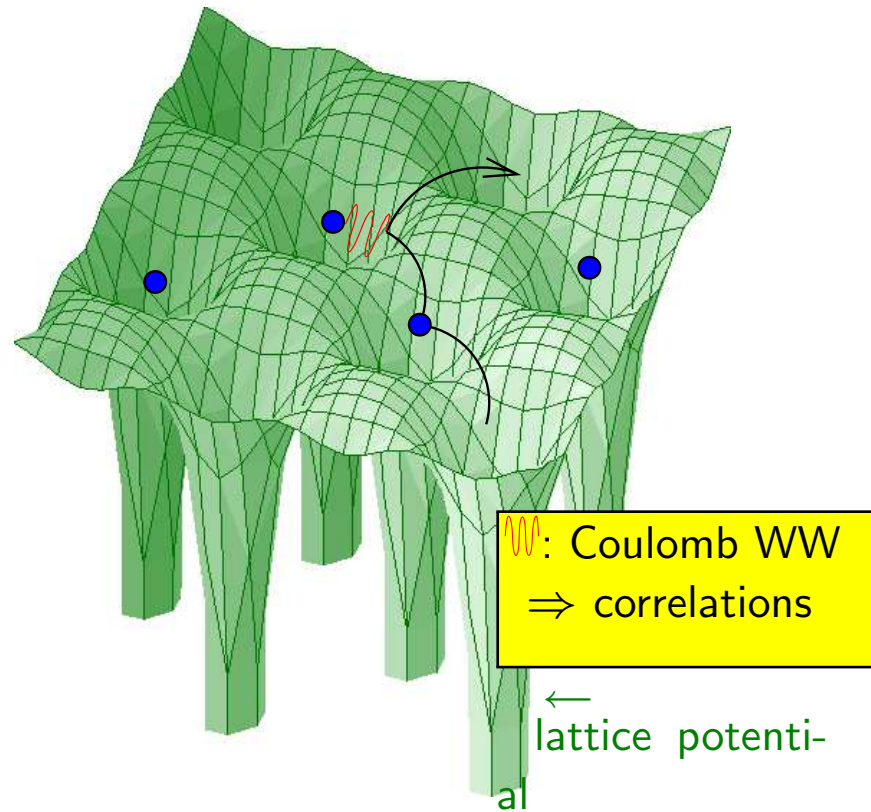
- computational materials science: **LDA+DMFT**
- quantum field theory:  **$D\Gamma A$**
- physics of strongly correlated electron systems:  
**thermoelectrics, kinks, QCP, heterostructures...**
- physics of nanoscopic systems:  
**NanoDMFT, decoherence, Kondo, RMT qdots...**

# Computational Materials Science

	LDA bandstructure theory	many body theory
+	<ul style="list-style-type: none"><li>● material specific</li></ul>	<ul style="list-style-type: none"><li>● many electron physics</li></ul>
-	<ul style="list-style-type: none"><li>● effective one-particle approach</li></ul>	<ul style="list-style-type: none"><li>● model Hamiltonian</li></ul>

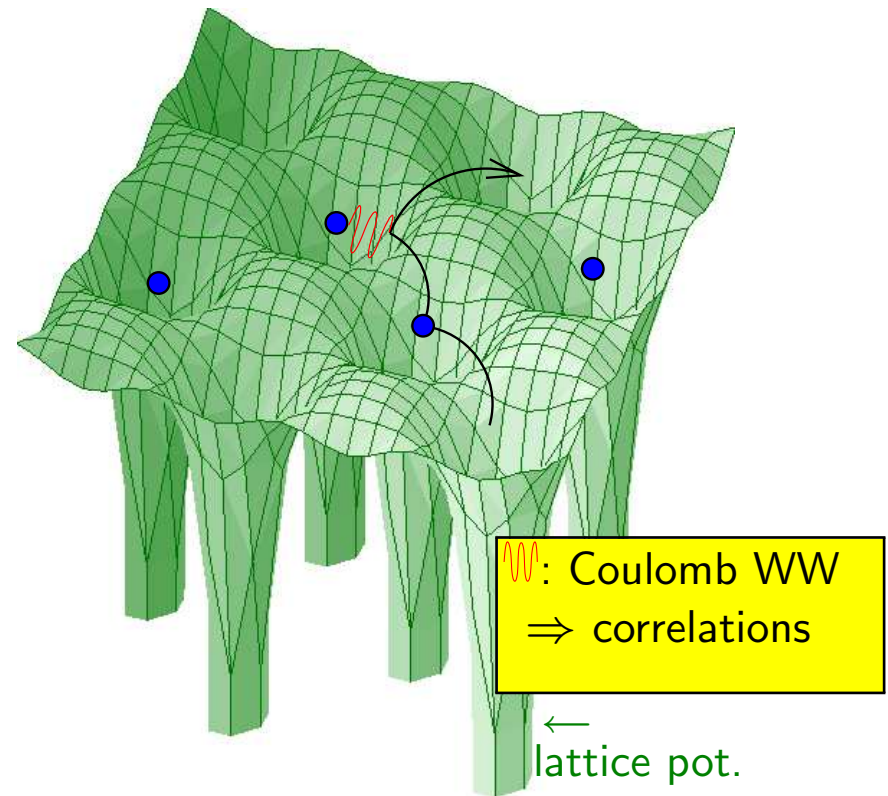
# Computational Materials Science

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# Computational Materials Science

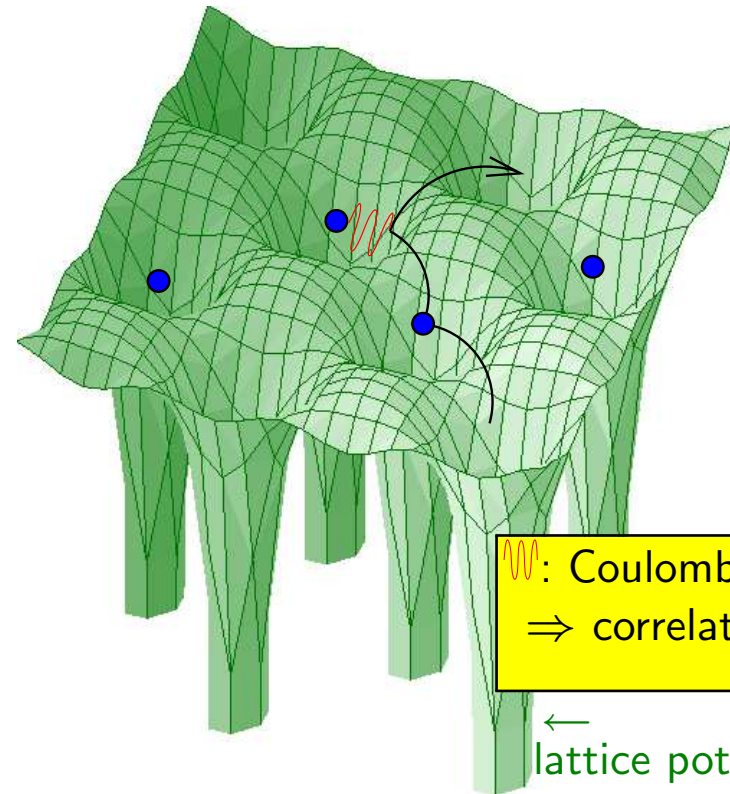
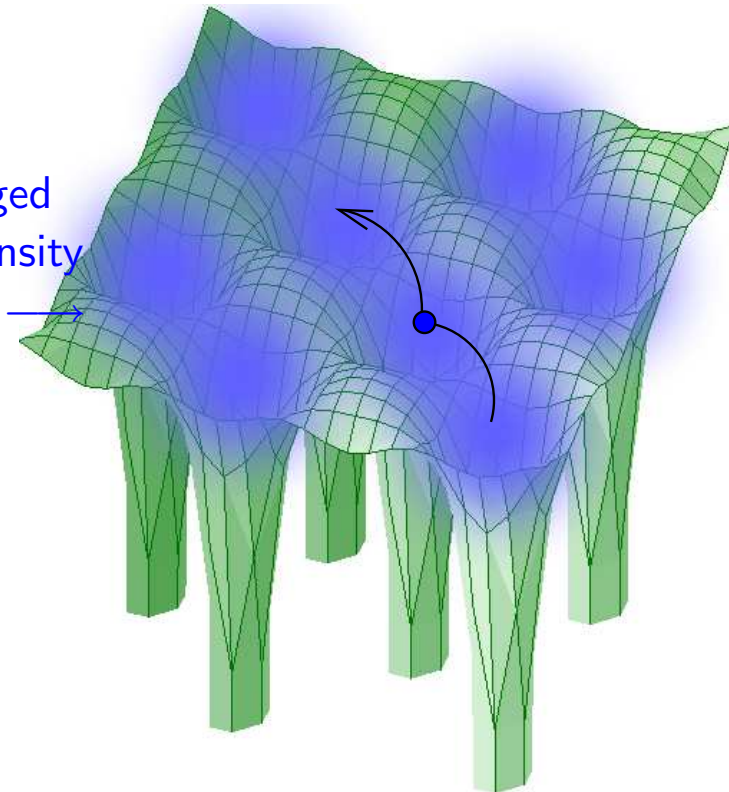
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# Computational Materials Science

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time averaged  
electron density



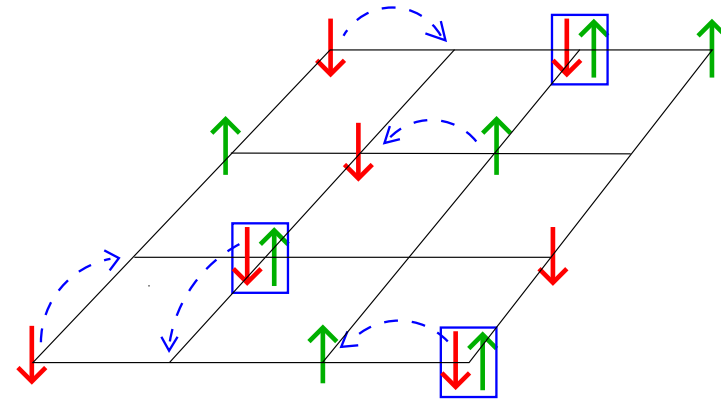
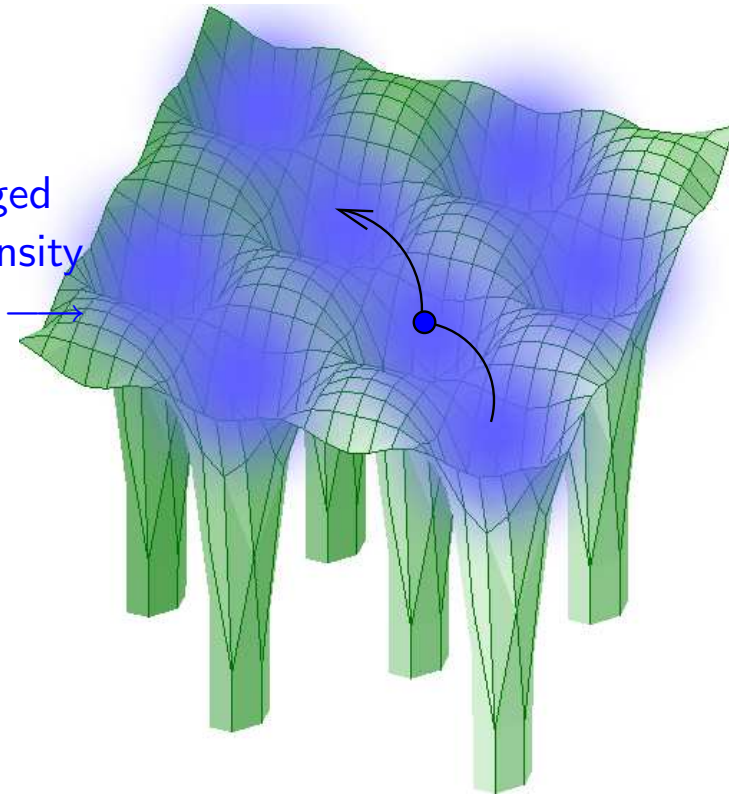
⤿: Coulomb WW  
⇒ correlations

←  
lattice pot.

# Computational Materials Science

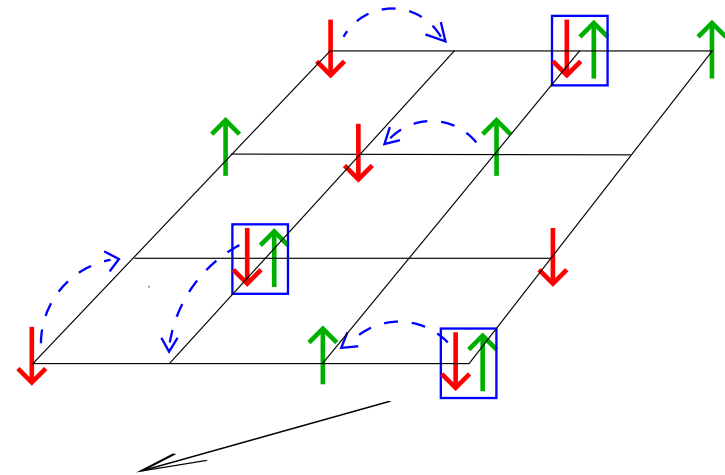
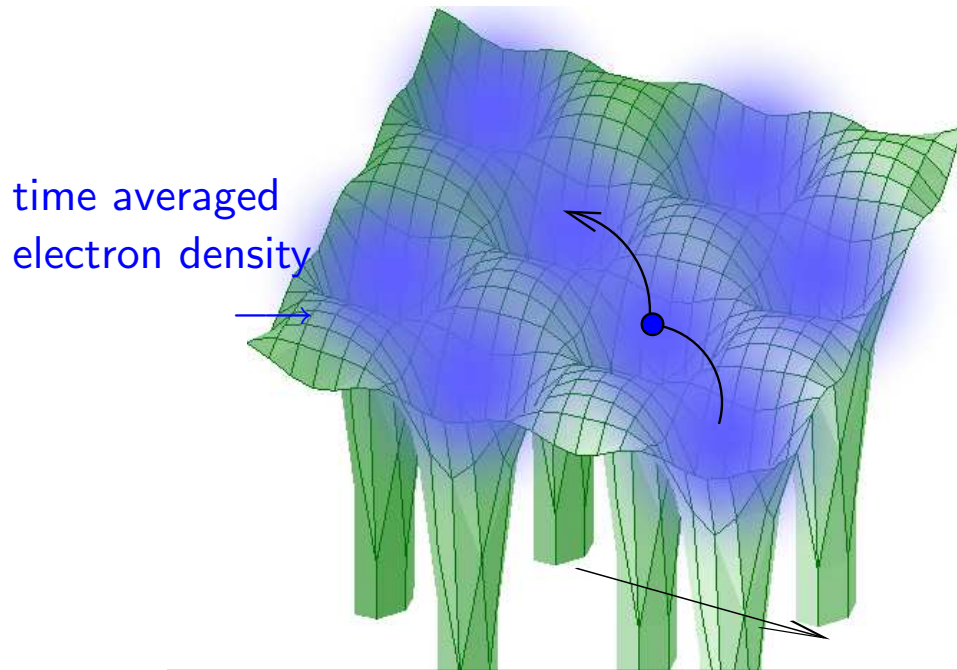
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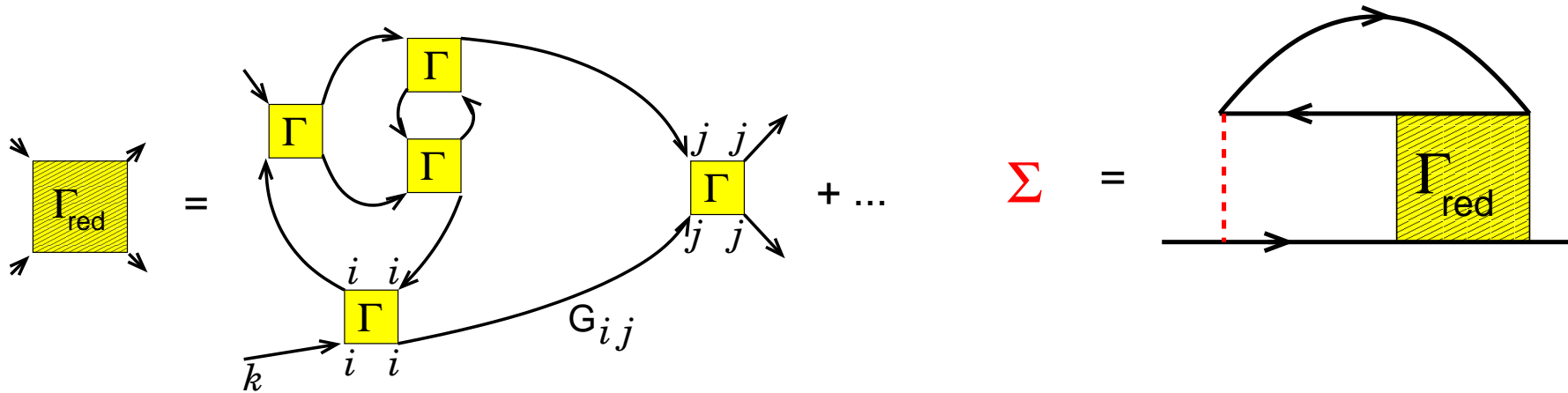
Local density approximation (LDA) + dynamical mean field theory (DMFT):  
realistic calculation of strongly correlated materials



# Quantum Field Theory for Solids

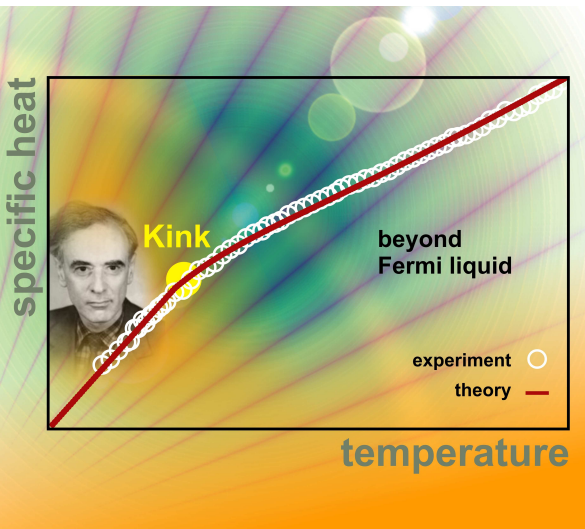
## Development of new methods

e.g. dynamical vertex approximation (D $\Gamma$ A), 1PI functional

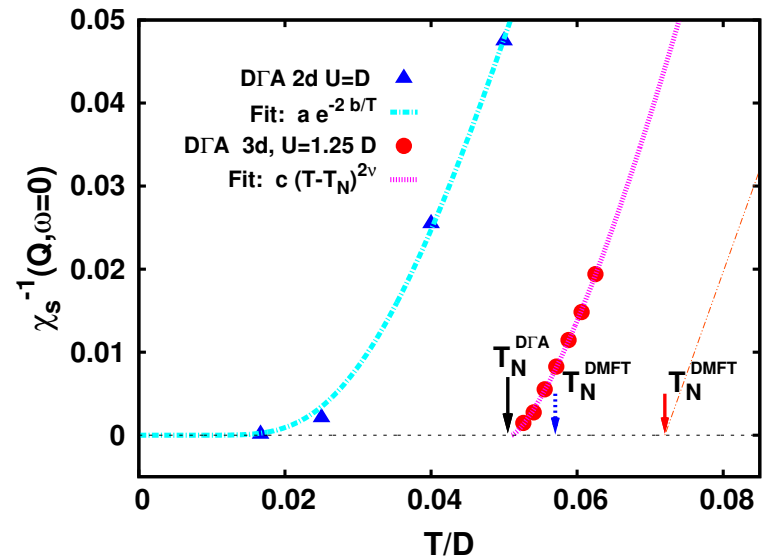
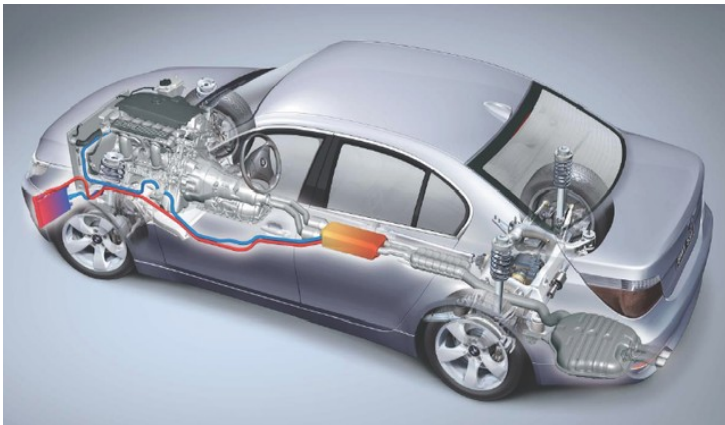


- Magnons
- Quantum criticality
- High temperature superconductivity

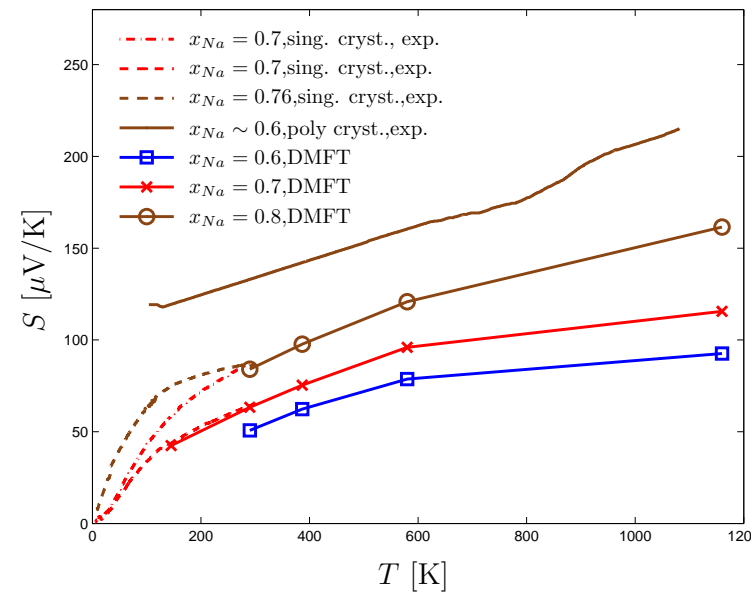
# Physics of correlated electron systems



## Kinks

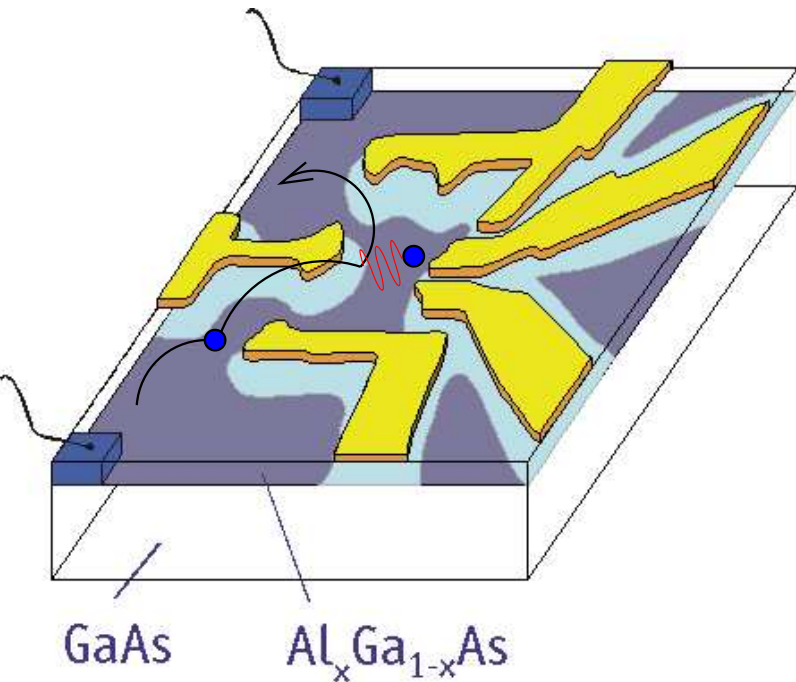


## Criticality Hubbard model



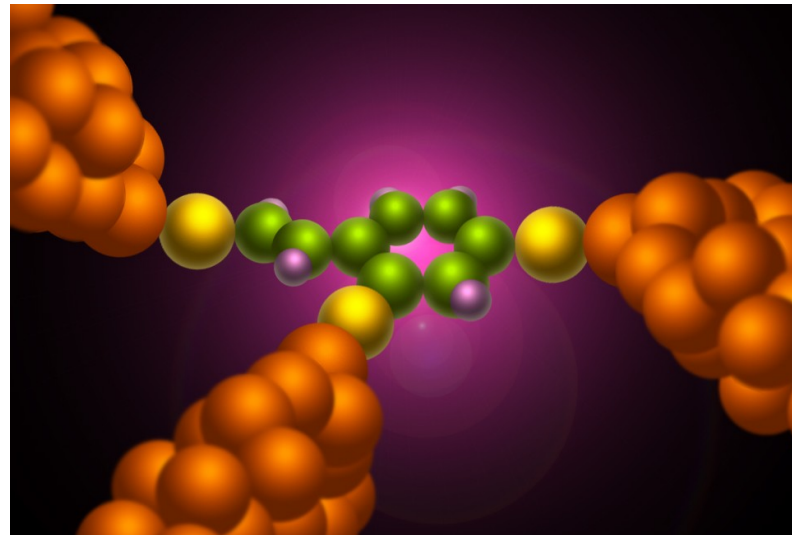
## Thermoelectrics (here $Na_xCoO_2$ )

# Physics of nanoscopic systems



decoherence, Kondo effect,  
random matrix theory in [qdots](#)

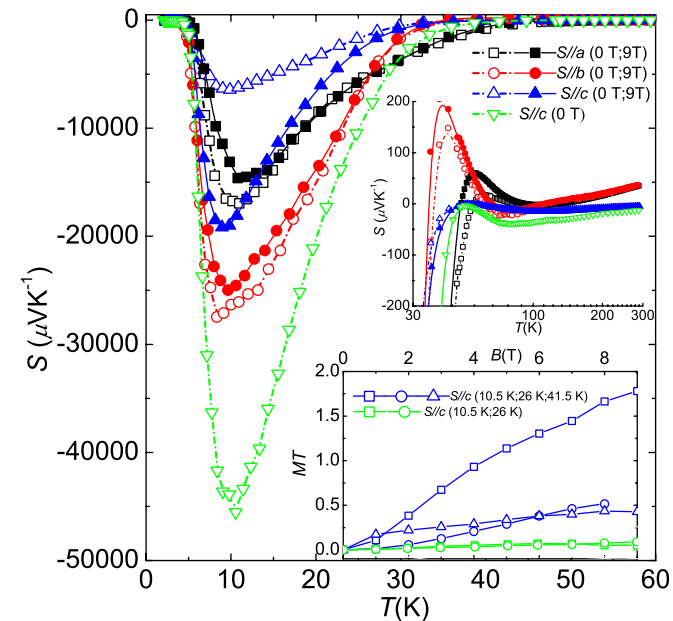
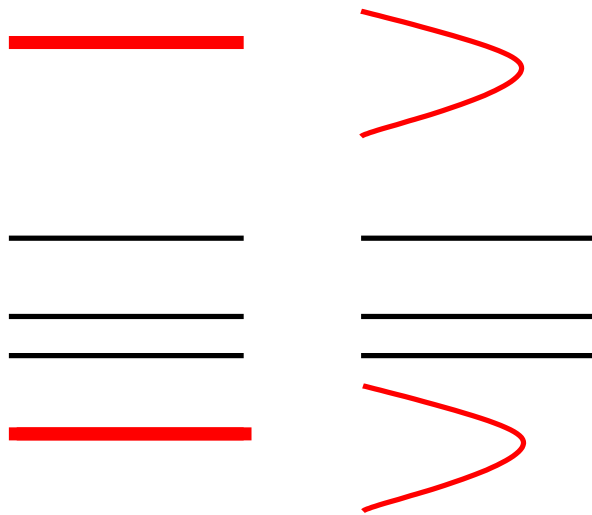
[NanoDMFT](#) for coupled quantum dots,  
macromolecules, clusters on surfaces ...



# Topic 1 (PA): Thermoelectricity – Boltzmann equation

Festkörpertheorie

Puzzling large thermopower in  $\text{FeSb}_2$



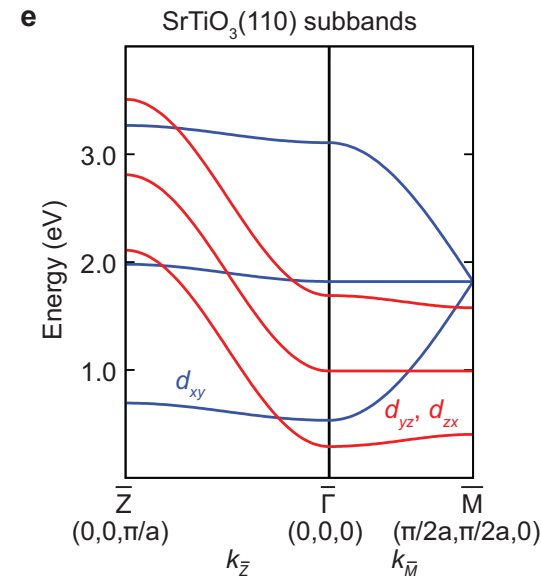
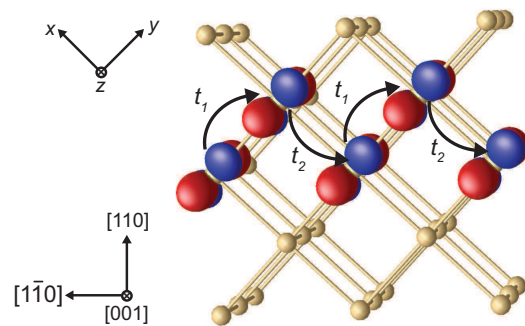
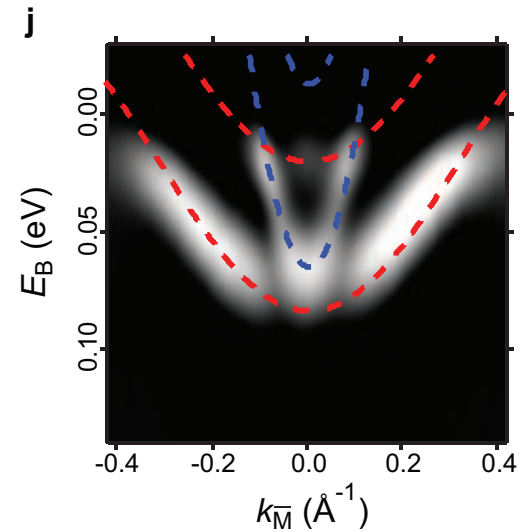
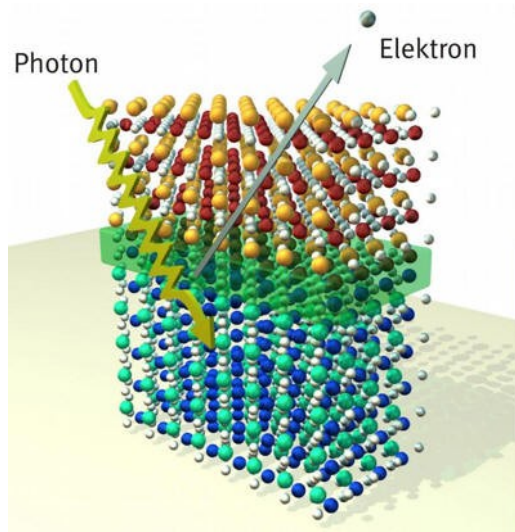
Modelling thermopower by semiconducting gap plus in-gap states include **finite bandwidth** in Boltzmann equation

Prerequisite: good theory skills, C, FORTRAN or mathematica

Supervisor: Battiato, Tomczak

# Topic 2 (PA): Ferromagnetism in (110) heterostructures

Festkörpertheorie



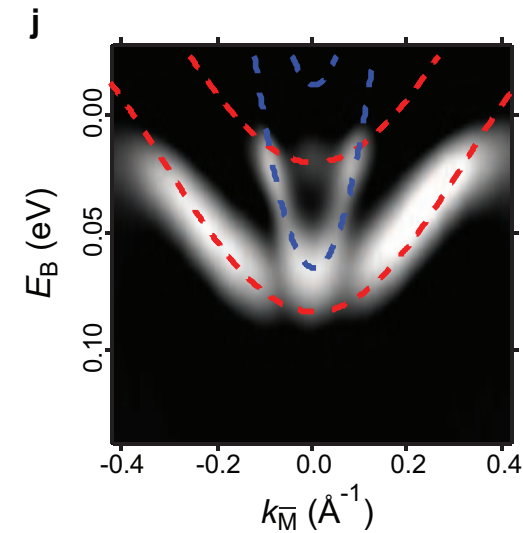
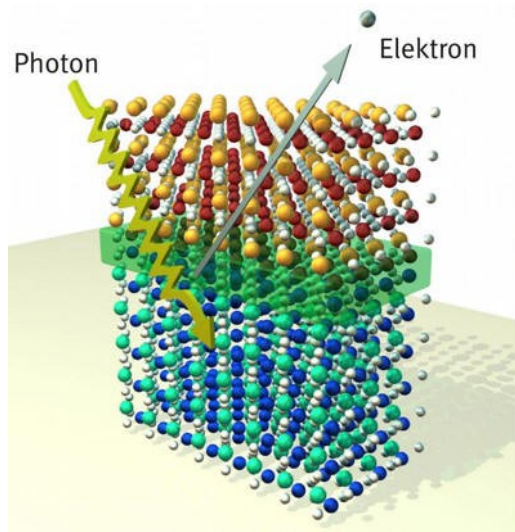
Analysis of **tight binding** model (from LDA) correlations by **Hartree-Fock**

Prerequisite: good theory skills

Supervisor: Zhong, Held

# Topic 3 (PA): Spin-orbit coupling

Festkörpertheorie



Analysis of **tight binding** model (from LDA)

modelling correlation effects by **Hartree-Fock**

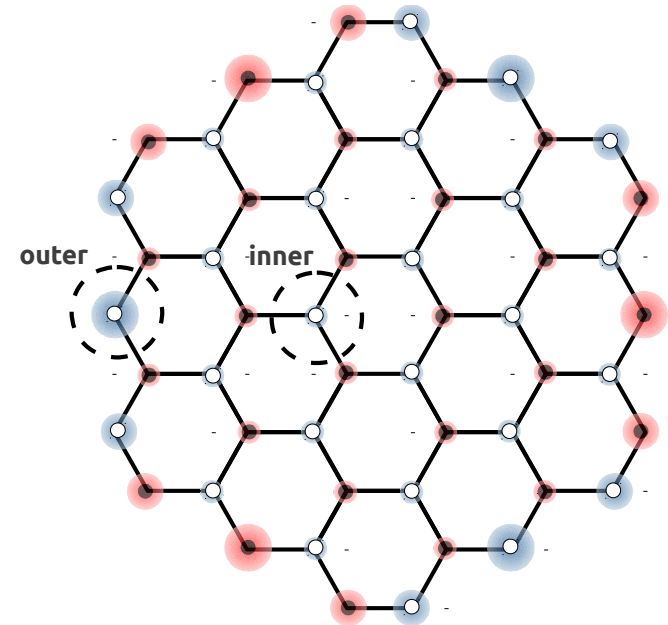
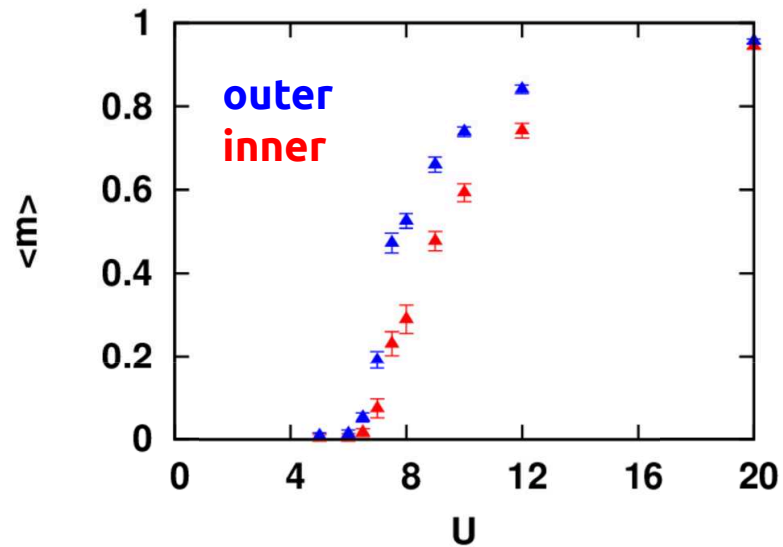
$$H = H_{\text{tightbinding}} + \zeta LS + \sum_{i\alpha\sigma, \alpha'\sigma'} U n_{i\alpha\sigma} \langle n_{i\alpha'\sigma'} \rangle \quad (1)$$

Prerequisite: good theory skills

Supervisor: Zhong, Held

# Topic 4 (PA): Magnetism in graphene nanoflakes

Computational Materials Science



## Dynamical mean field theory

Tight binding model correlations by Hartree-Fock

Prerequisite: good theory skills, FORTRAN, C or python

Supervisor: Valli, Held