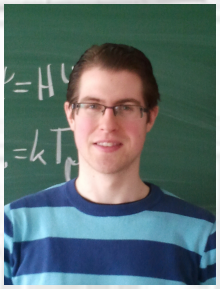
Master theses & project works

AG Toschi & AG Held


Tin Ribic


Thomas Schäfer


Agnese Tagliavini


Dr. Jan Tomczak

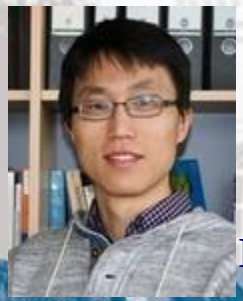

Patrik Gunacker


Dr. Marco Battiato


Petra Pudleiner


Dr. Patrik Thunström


Liang Si


Dr. Gang Li


Markus Wallerberger

Current MAs

Nikolaus Berlakovich, Michael Weis, Josef Kaufmann

Recent PAs

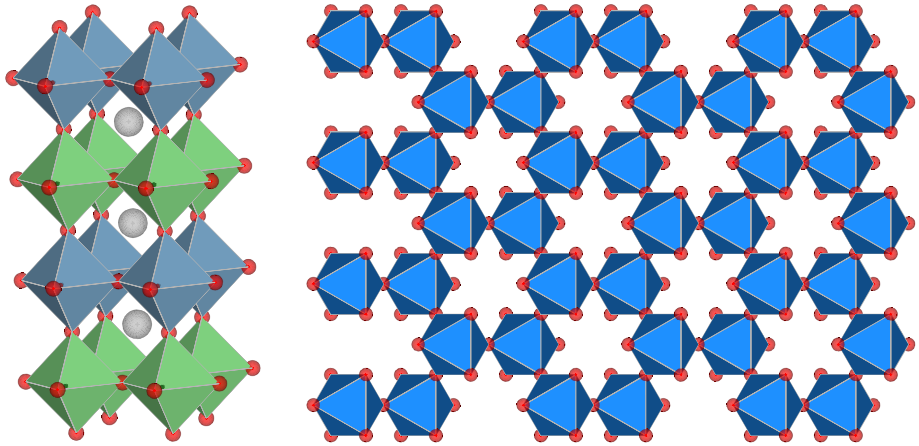
Matthias Pickem, Felix Hörbinger, Benedikt Hartl, Tobias Reisch, Marie-Therese Philipp, Bejamin Klebel, Paul Semmelrock

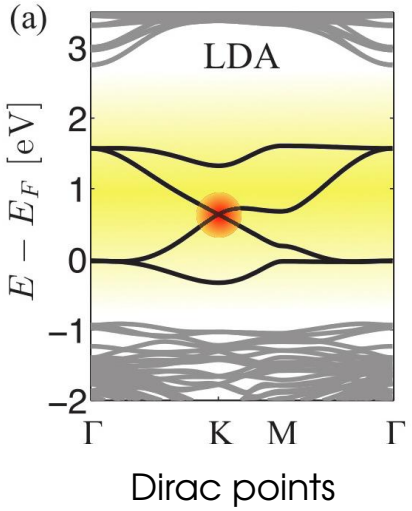

Dr. Oleg Janson


Anna Galler

Topic 1: Topology – hexagonal layers

New research area: Transition metal oxide heterostructures





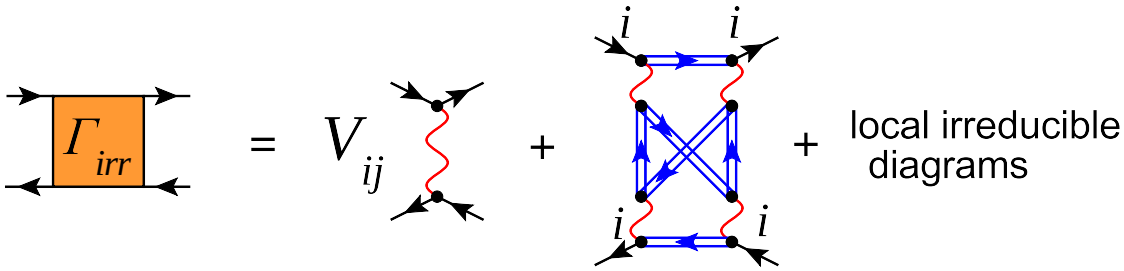
(111) surface, 2 layers → hexagonal lattice → Dirac points

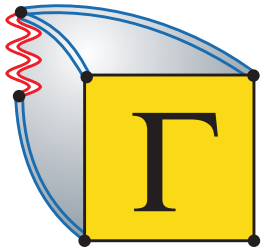
Density functional theory (DFT) + dynamical mean field theory (DMFT) for materials with hexagonal layers – analysis of topological properties

Prerequisite: good theory skills and physical understanding

Supervisors: Held (held@ifp.tuwien.ac.at), Janson

Topic 2: Ab initio dynamical vertex approximation (DΓA)





ERC project

includes GW (exchange), DMFT (correlations), and non-local correlations beyond

Materials calculations and/or program development

Start: summer 2016

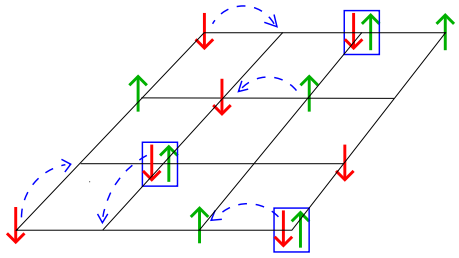
Prerequisite: quantum field theory, good physical understanding

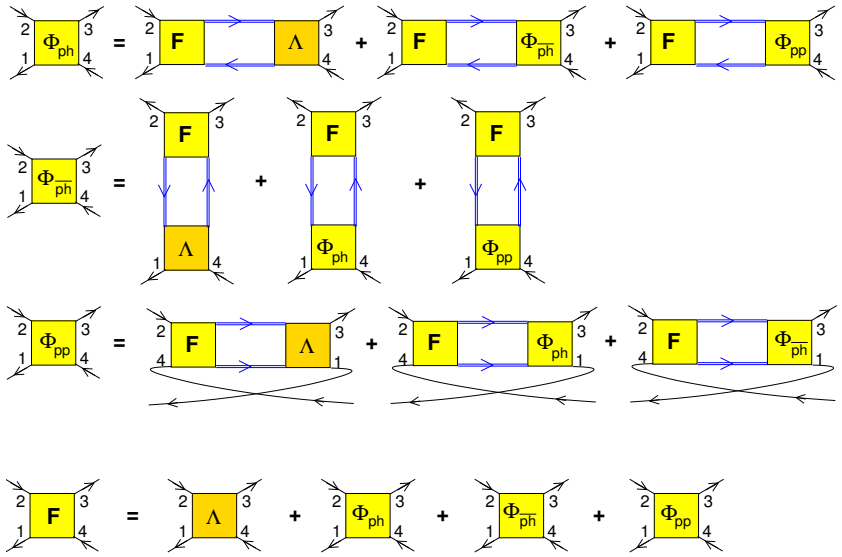
Supervisors: Held (held@ifp.tuwien.ac.at), Tomczak, Galler, Thunström

Topic 3: Full parquet DΓA for Hubbard model

Hubbard model with t, t'

$$H = \sum_{ij\sigma} t_{ij} c^\dagger_{i\sigma} c_{j\sigma} + U \sum_i c^\dagger_{i\uparrow} c_{i\uparrow} c^\dagger_{i\downarrow} c_{i\downarrow}$$





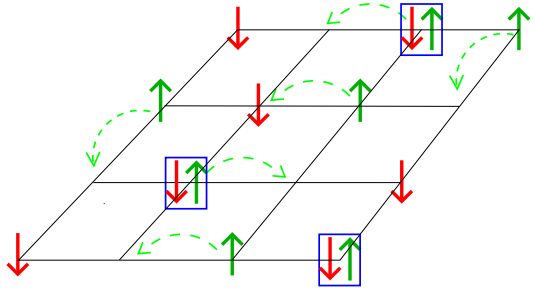
Dynamical vertex approximation (DΓA) with full parquet calulation: Hubbard model with t', physics of cuprates

Prerequisite: quantum field theory

Supervisors: Held (held@ifp.tuwien.ac.at), Li, Pudleiner

Topic 4: Falicov-Kimball model

$$H = \sum_{ij} t_{ij} c^\dagger_{i\uparrow} c_{j\uparrow} + U \sum_i c^\dagger_{i\uparrow} c_{i\uparrow} c^\dagger_{i\downarrow} c_{i\downarrow}$$



Master, Ph.D. thesis Ribic: Analytical calculation of n-particle vertex

Tasks:

- corrections due to 3-particle vertex
- $\Sigma(\omega)$ at real frequencies

Prerequisite: quantum field theory

Supervisors: Held (held@ifp.tuwien.ac.at), Ribic

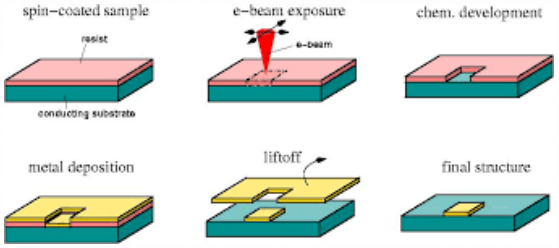
Project 1:
Mobile Molecular Orbitals

Waltzing Atoms

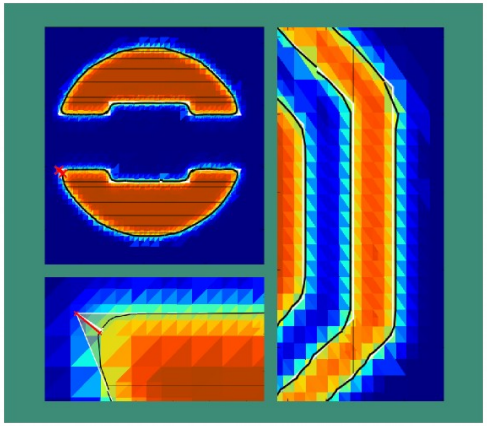
- Waltzing Atoms is an educational app to learn chemistry & physics
- Goal: Develop an efficient algorithm to visualize molecular orbitals on web & mobile.
- Questions: How to approximate many-electron physics on a molecule to get majority of molecules isosurfaces right?
  Starting Point: electron-negativity
- Technology: web and mobile technology, web-interfaces (can be learned during project)
- Company: 3DataX GmbH & Co KG
  Lambrechtgasse 3 1040 Vienna
  Contact: office@waltzingatoms.com

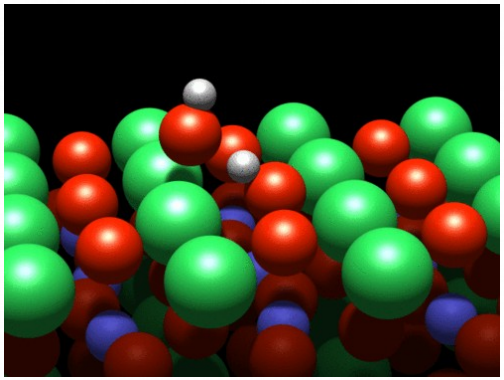
Project 2:
Energies of Surface Layers for electron-beam nano-lithography

Waltzing Atoms



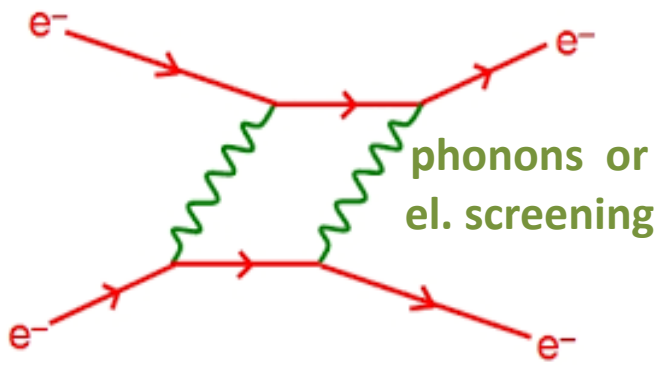
- 3DataX develops a simulator for e-beam nano-lithography (semi-conducting industry)
- Goal: Develop an automatized way to determine the work function of top layers in computer chip mask materials
- Questions: Depending on depth, how quickly do surface energies morph to bulk properties? How strong is this behavior dependent on the material? Starting Point: WIEN2k super-cell calculations
- Technology: WIEN2k, web-GUI and interface (can be learned during project)
- Company: 3DataX GmbH & Co KG
  Lambrechtgasse 3 1040 Vienna
  Contact: office@waltzingatoms.com



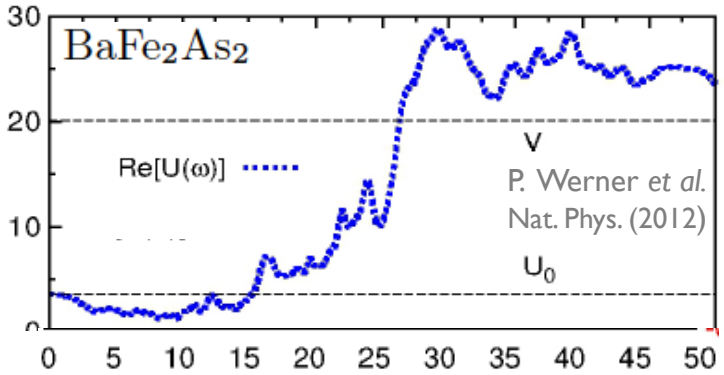


MA/DA: Implementation of $U(\omega)$ in the quantum Monte-Carlo (w2dynamics) code

MOTIVATION: Current version of **w2dynamics** (our DMFT imputity solver) allows *only* calculations with **static** electron interaction $U(\omega) = U$. **BUT,** *in general* ...



$$U(\omega) \neq U$$



GOALS: Extension of **w2dynamics** to include also the case of $U(\omega)$**:** a preliminary implementation for the simplest case can be used as a starting point.

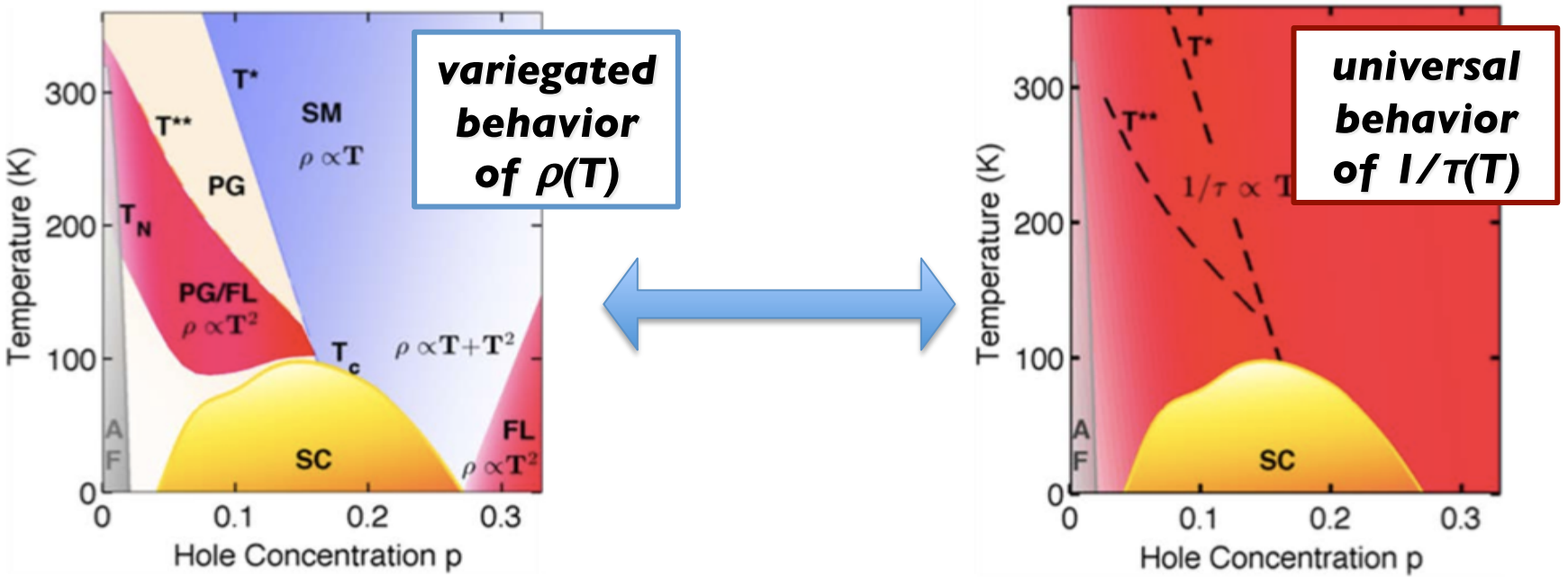
PHYSICS APPLICATIONS: (second part of MA) several:
from correlated surfaces/heterostructure, to Fe-based superconductors.

PREREQUISITES: good programming skills, CMS, QFT, and/or this VO may help

SUPERVISION: **Toschi**, Tomczak, Held (& cooperation UniWürzburg: Sangiovanni)

MA/DA: The „puzzling“ scattering rate of high-Tc cuprates

MOTIVATION: unexpected new, experimental estimate of an **universal electronic scattering rate** in high-Tc supercondicting cuprates (N. Barisic‘s group, here @ IFP)



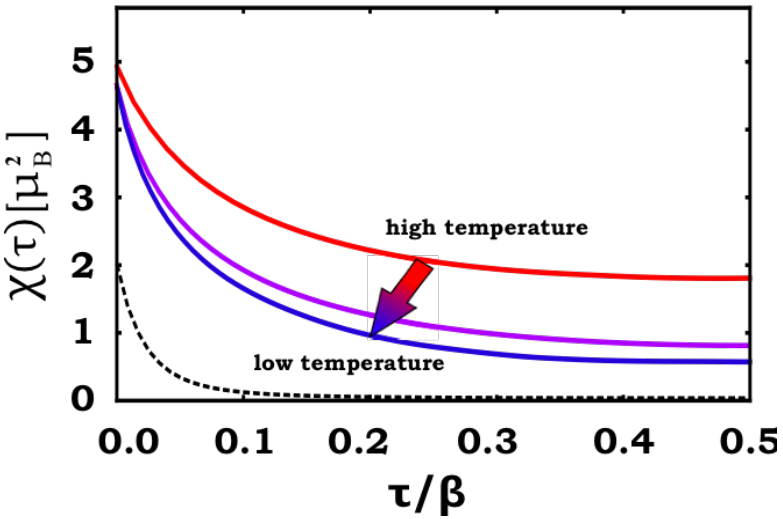
GOALS: theoretical investigation of the phenomenon**:** Direct calculation of electron self-energy in DMFT & beyond (DΓA). Derivation of the expressions for resistivity and Hall coefficient in DMFT/DΓA, and their implementation in the algorithm.

PREREQUISITES: solid theoretical background, CMS or QFT, and/or this VO

SUPERVISION: **Toschi**, Schäfer (coll. with : Tomczak, Held and –maybe- N. Barisic)

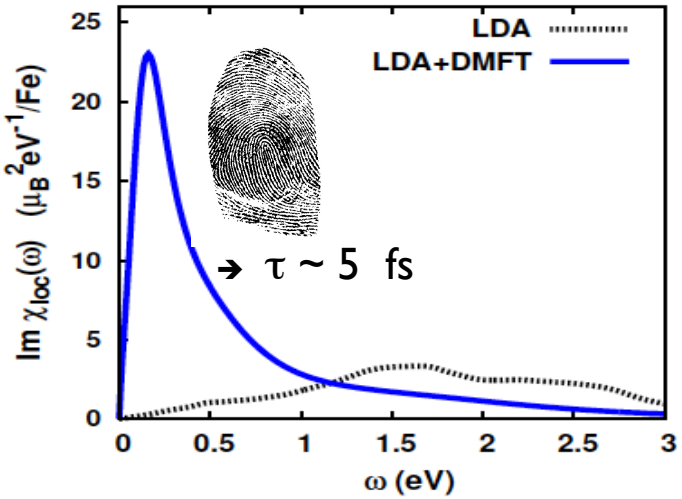
MA/DA: Detecting the time scales of the spin dynamics

MOTIVATION: Dynamic spin susceptibilties yield crucial information about the presence/absence of **local magnetic moments** and their **time/energy scales.**
BUT such infos need to be „disentangled“ in the numerics (often in imaginary time).



on real

frequencies



GOALS: analytical modellization of χ(t) on real-time axis (w. one /more time-scales), characterization of its general properties on both real/frequency domains

➔ **rules of thumb** to detect time-scales from data

PHYSICS APPLICATIONS: 2-orbital systems, Fe-based superconductors.

PREREQUISITES: good theory background, e.g. QFT, and/or this VO (o. ae.)

SUPERVISION: **Toschi** (possible cooperation with Würzburg: G. Sangiovanni)