

# Local and Long-Range Correlations in Strongly Correlated Systems:

## Insights into Two-dimensional Systems of Adatoms on Surfaces from Self-Consistently Combined GW and Dynamical Mean Field Theory

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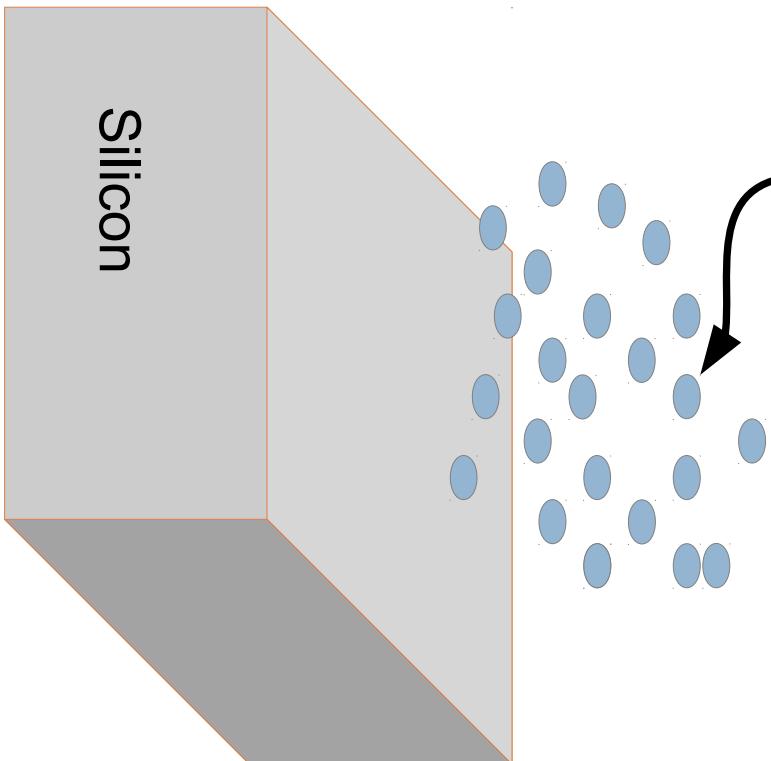


Paris, Nov 29th, 2013

# Ad-atoms on surfaces

Crystalline silicon sliced along the (111) direction  
Deposition of atoms on the surface

$X = \text{Pb, Sn, Si, C}$

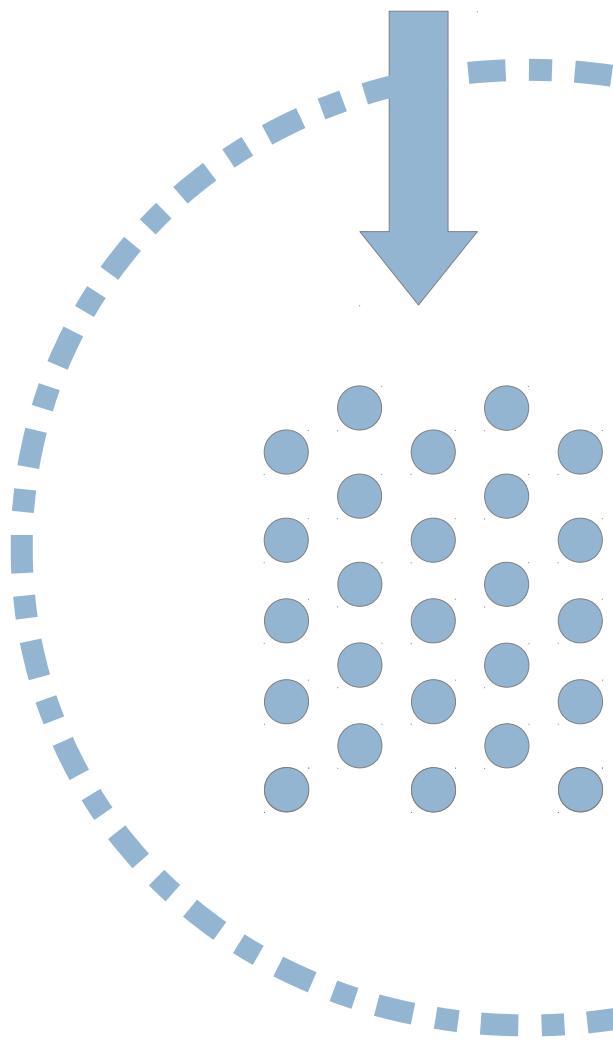
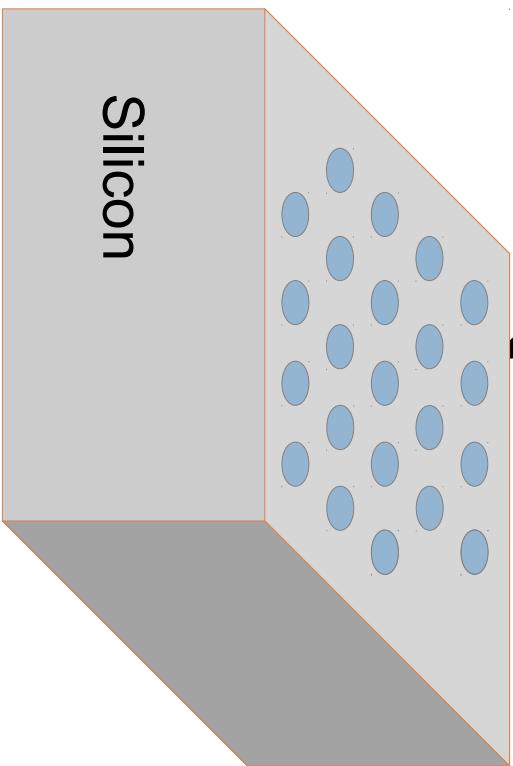


# Ad-atoms on surfaces

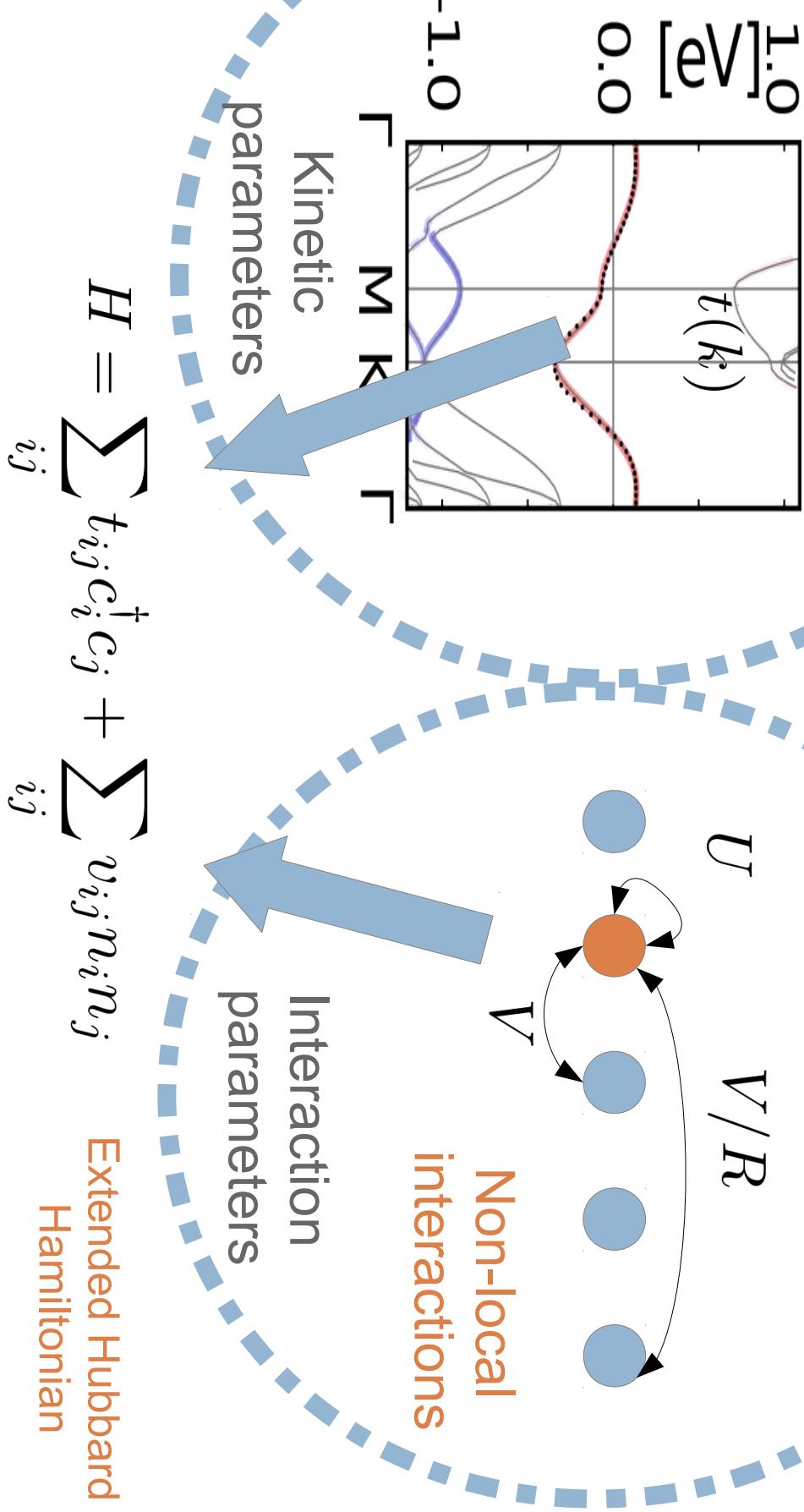
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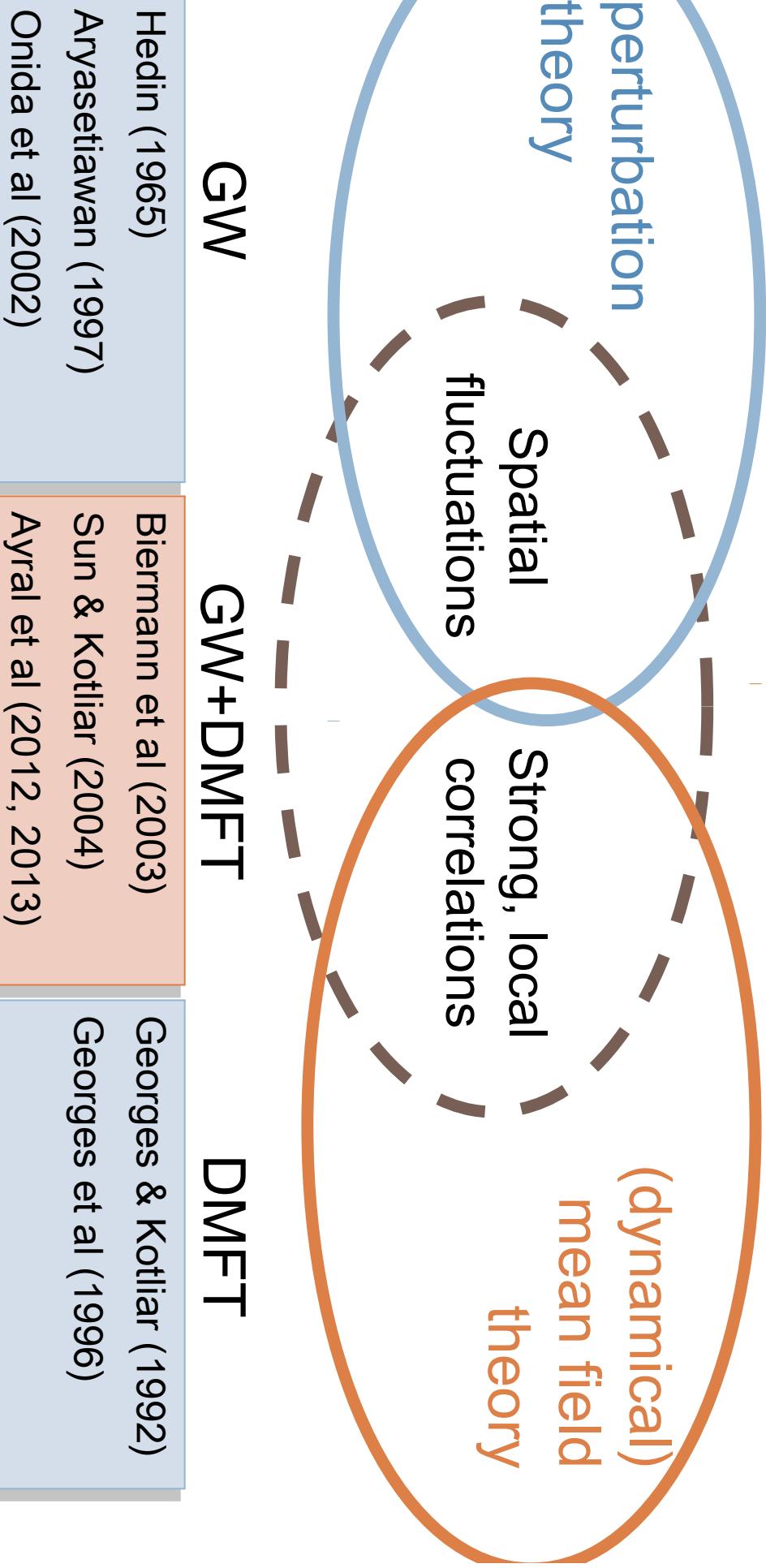
Effective description:  
2D triangular lattice of  
ad-atoms



# Effective Hamiltonian from the first principles



# A combined method for spatial fluctuations and strong local interactions



# Long-range correlations

Self-energy

$$\Sigma_{ij} = \Sigma_{loc} + G_{ij} W_{ij} (i \neq j)$$

Polarization

$$P_{ij} = P_{loc} + G_{ij} G_{ji} (i \neq j)$$

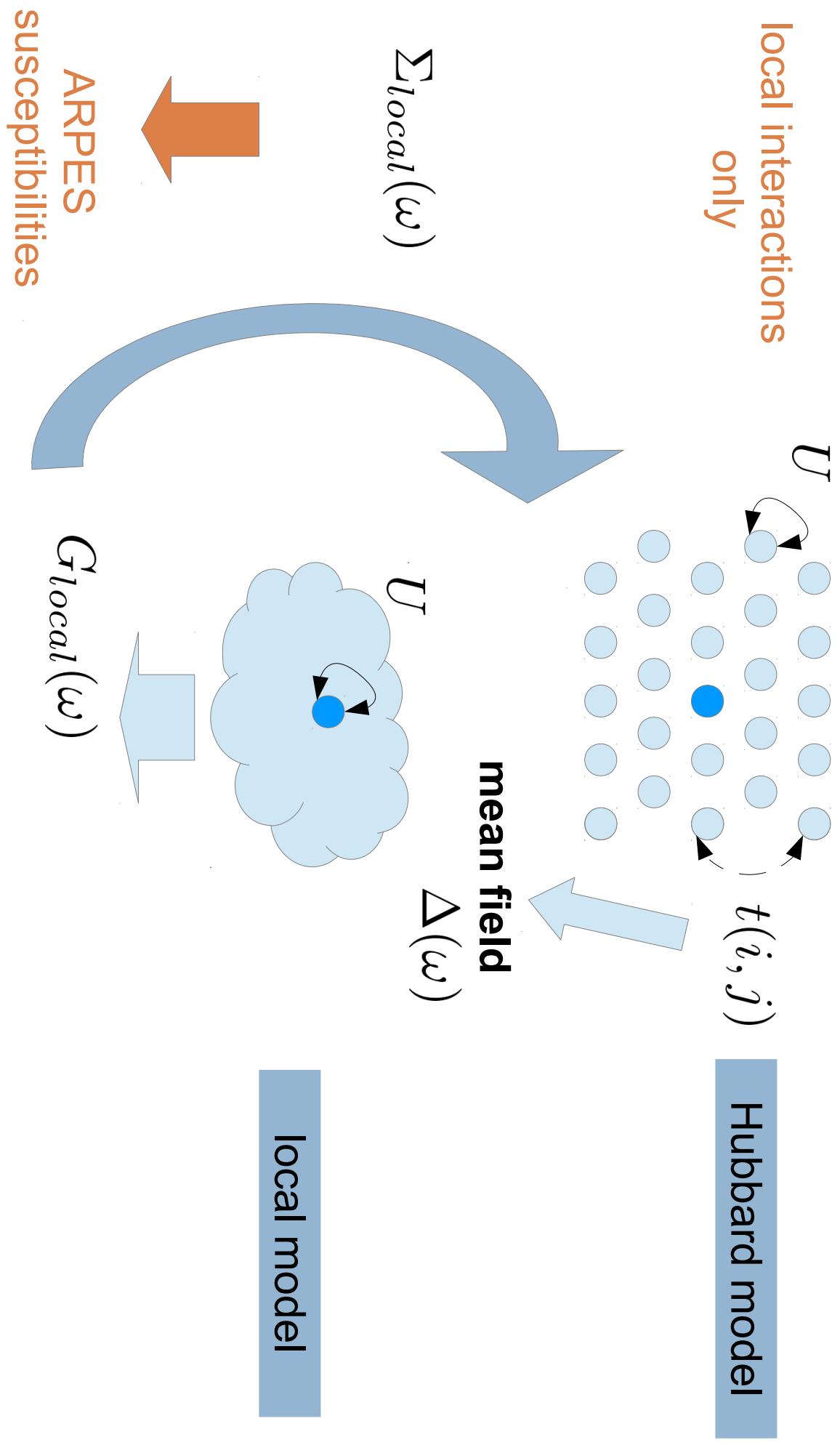
from solution of local  
impurity model

GW calculation  
on the lattice

Direct access to non-local charge susceptibility

$$\chi_{ij}(t - t') = \langle n_i(t) n_j(t') \rangle$$

# Dynamical mean field theory



# TRIQS ([ipht.cea.fr/triqs](http://ipht.cea.fr/triqs))

## a toolbox for many-body calculations



### Tour 4: Dynamical Mean Field Theory on a Bethe lattice

Requires `TRIQS` and the application `cthyb_matrix`

In the case of Bethe lattice the dynamical mean-field theory (DMFT) self-consistency condition takes a particularly simple form

$$G_{0,\sigma}^{-1}(i\omega_n) = i\omega_n + \mu - t^2 G_\sigma(i\omega_n).$$

Hence, from a strictly technical point of view, in this case the DMFT cycle can be implemented by modifying the previous single-impurity example to the case of a bath with semi-circular density of states and adding a python loop to update  $G_0$  as function of  $G$ .

Here is a complete program doing this plain-vanilla DMFT on a half-filled one-band Bethe lattice:

```
from pytriqs.gf.local import *
from pytriqs_operators import *
from pytriqs_arbive import *
import pytriqs.utility.mpi as mpi

# Set up a few parameters
u = 2.5
half_bandwidth = 1.0
chemical_potential = u/2.0
beta = 100
n_loops = 5

# Construct the CTQMC solver
from pytriqs_appliarity_solvers_cthyb_matrix import Solver
S = Solver(beta = beta, gf_struct = [ ('up',[1]), ('down',[1]) ])
# Initialize the Green's function to a semi circular
S.G <=> Semicircular(half_bandwidth)
```

#### Quick search

Go

Enter search terms or a module, class or function name.

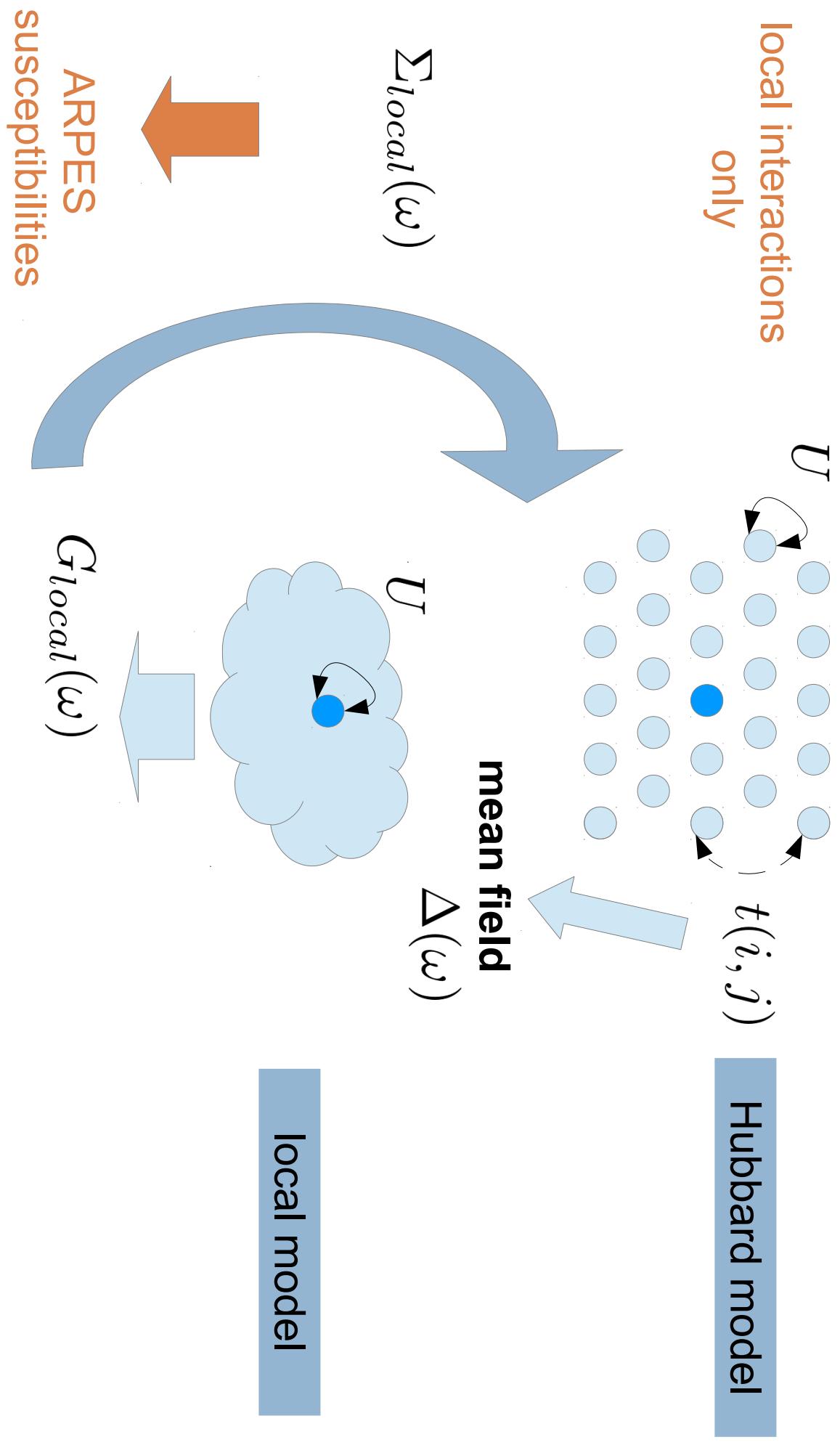
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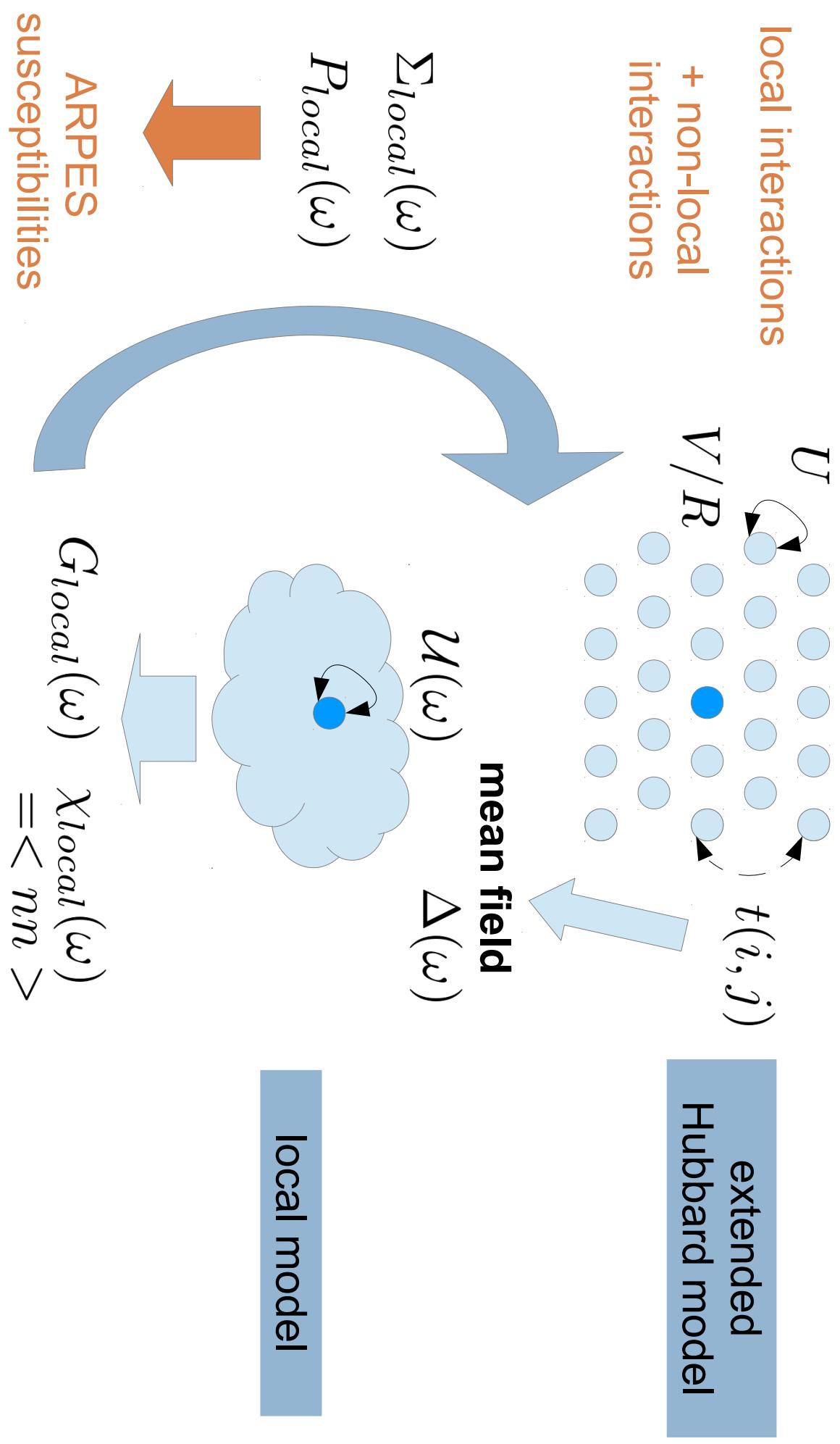
Previous topic  
Tour 3: Solving a quantum impurity model with QMC

Next topic  
Iterated perturbation theory: an more elaborate DMFT example

# Dynamical mean field theory



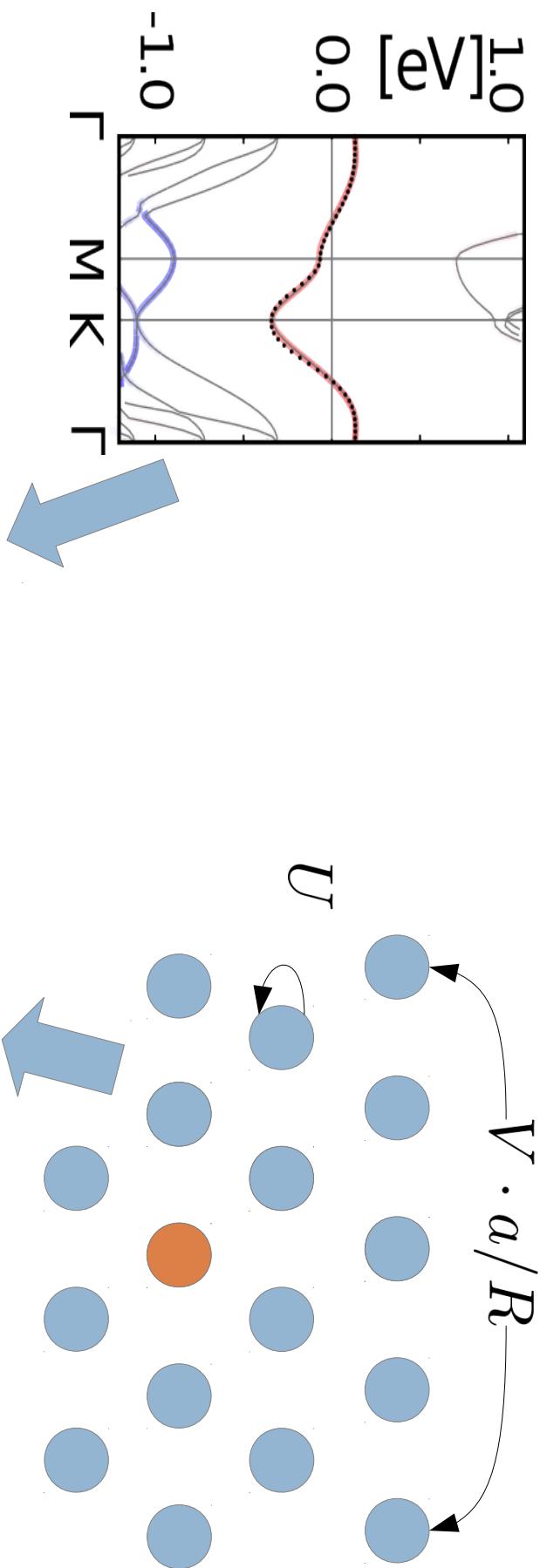
# Extended Dynamical mean field theory



# Back to ad-atoms on surfaces...

Tight-binding fit  
of LDA bandstructure

Interaction parameters  
from cRPA



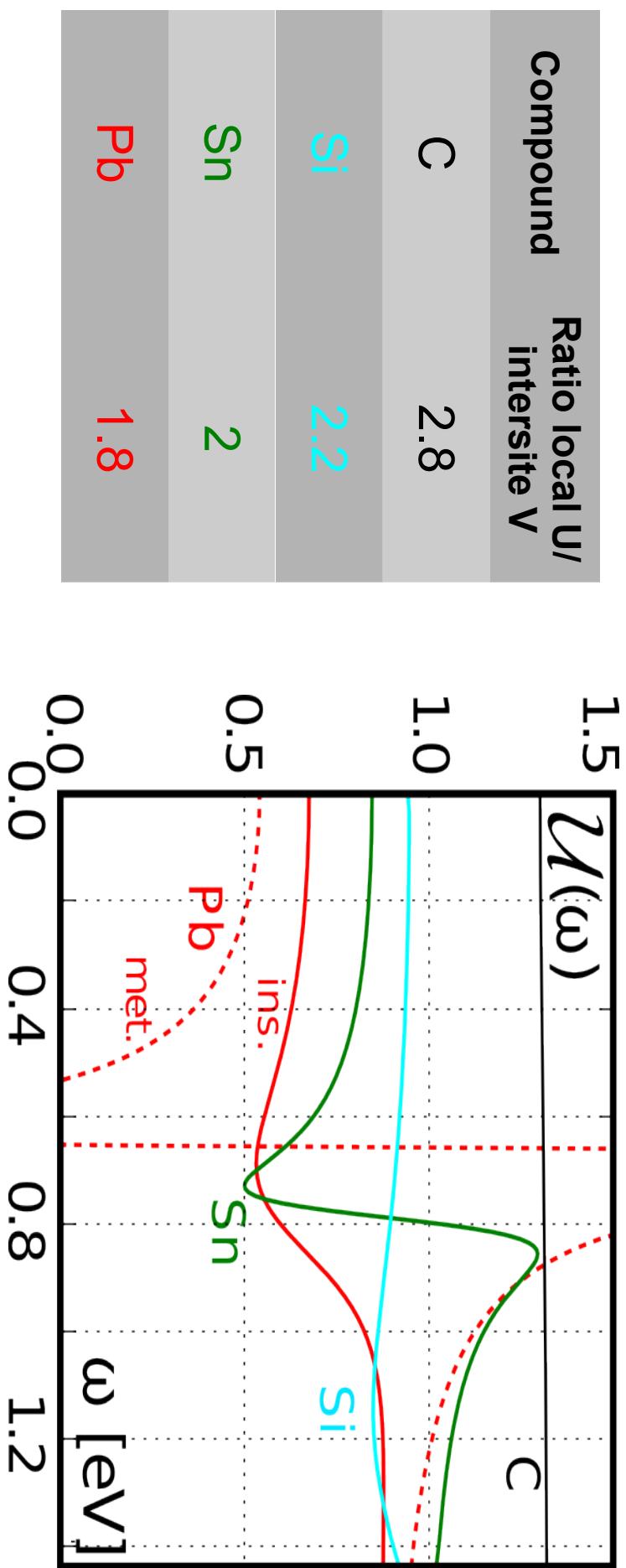
half-filled

$$H = \sum_{ij} t_{ij} c_i^\dagger c_j + \sum_{ij} v_{ij} n_i n_j$$

See also  
Schuwalow et al (2010)

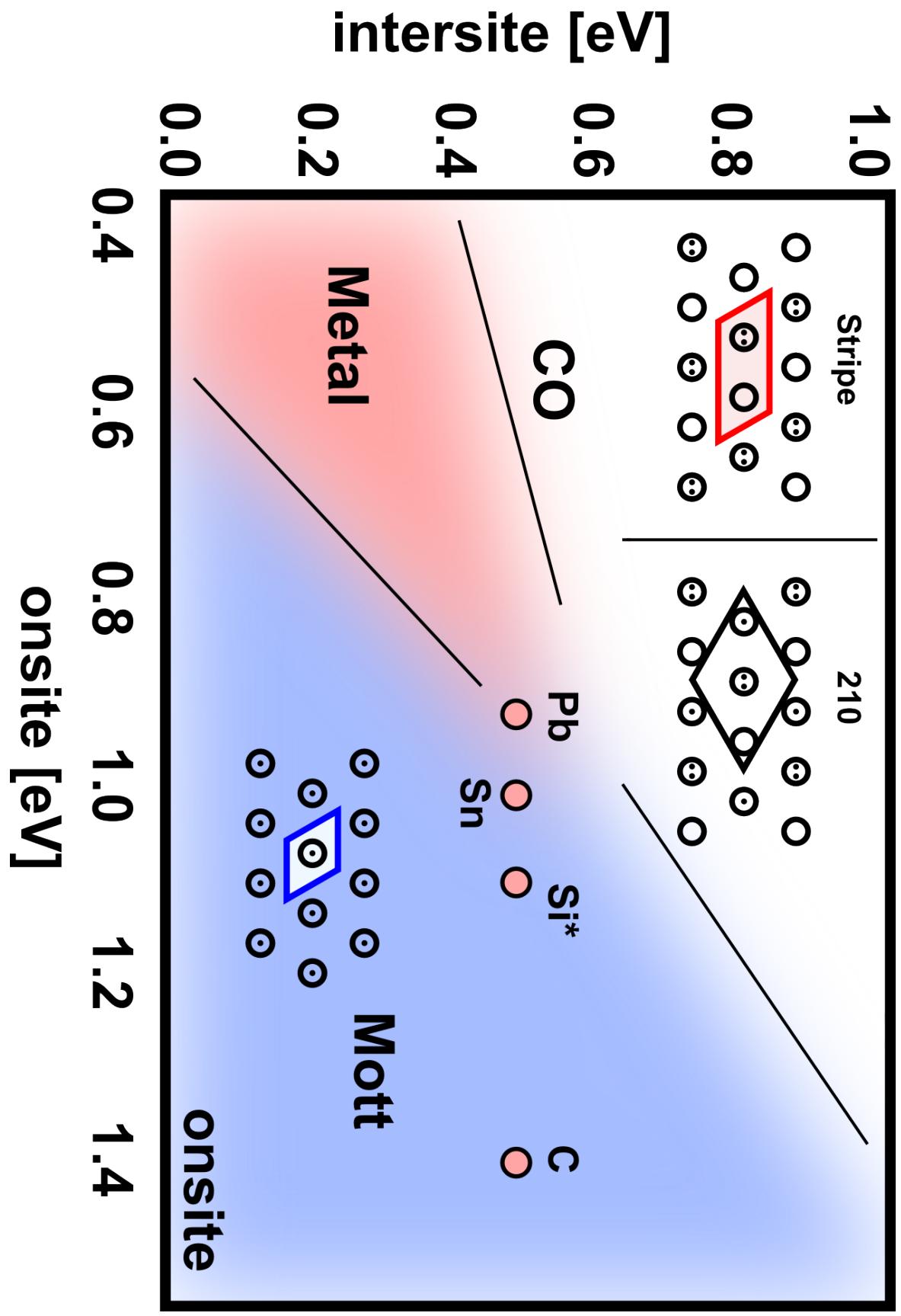
# Self-consistent dynamical interactions from long-range screening

$$U\delta(R) + V \cdot a/R \longrightarrow U(\omega)\delta(R)$$

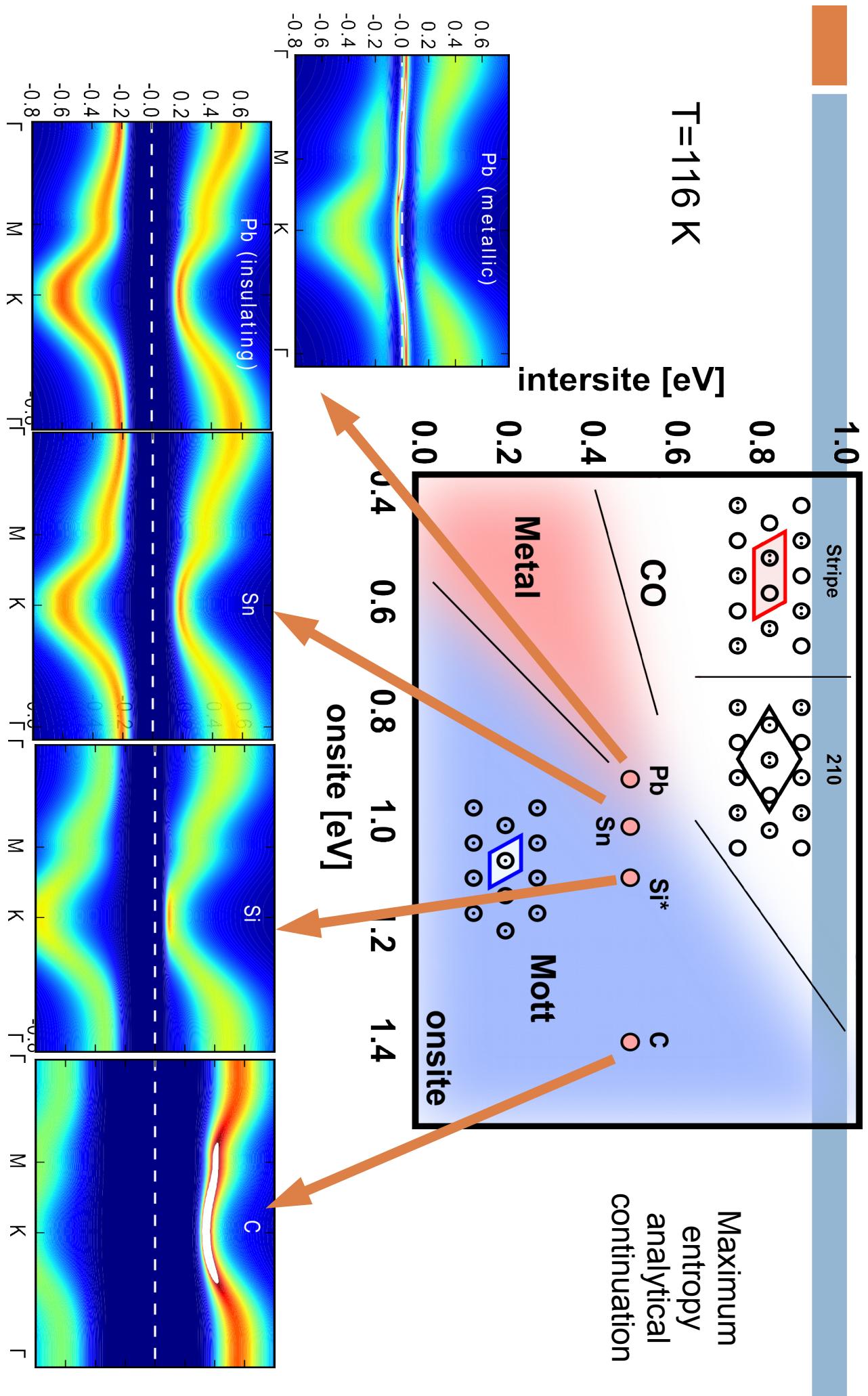


The larger the non-local interactions, the more retarded the local interactions

# Phase diagram from GW+DMFT



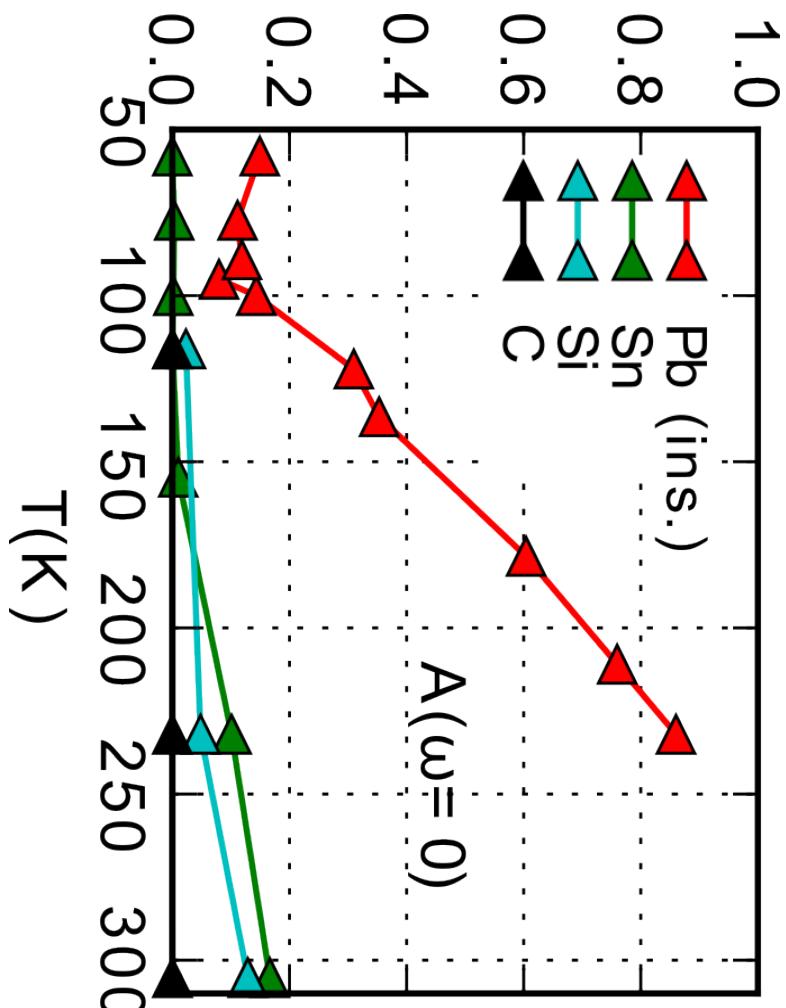
# ARPES spectra



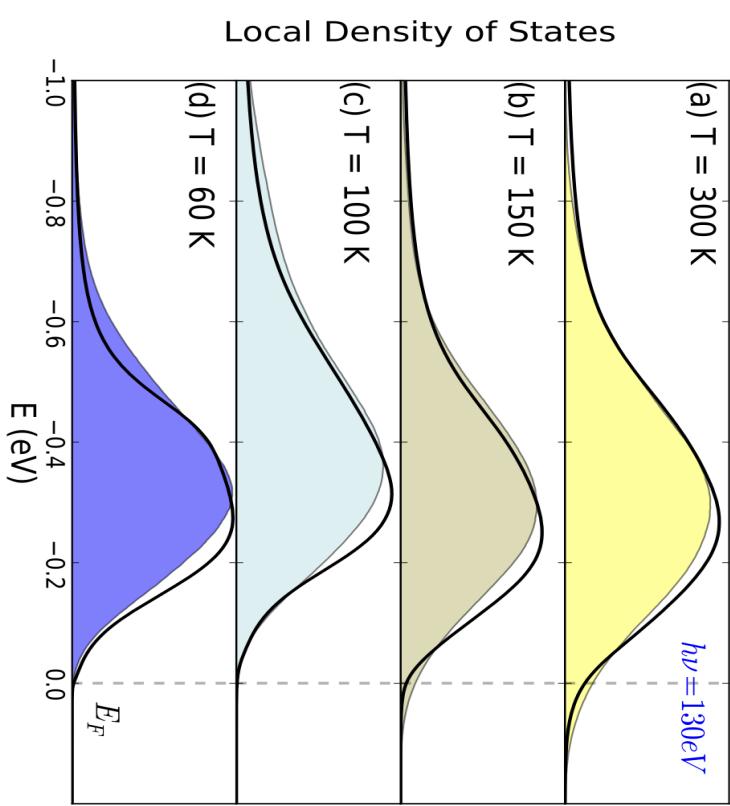
# ARPES spectra:

theory and experiments

Temperature dependence  
of spectral weight at Fermi level



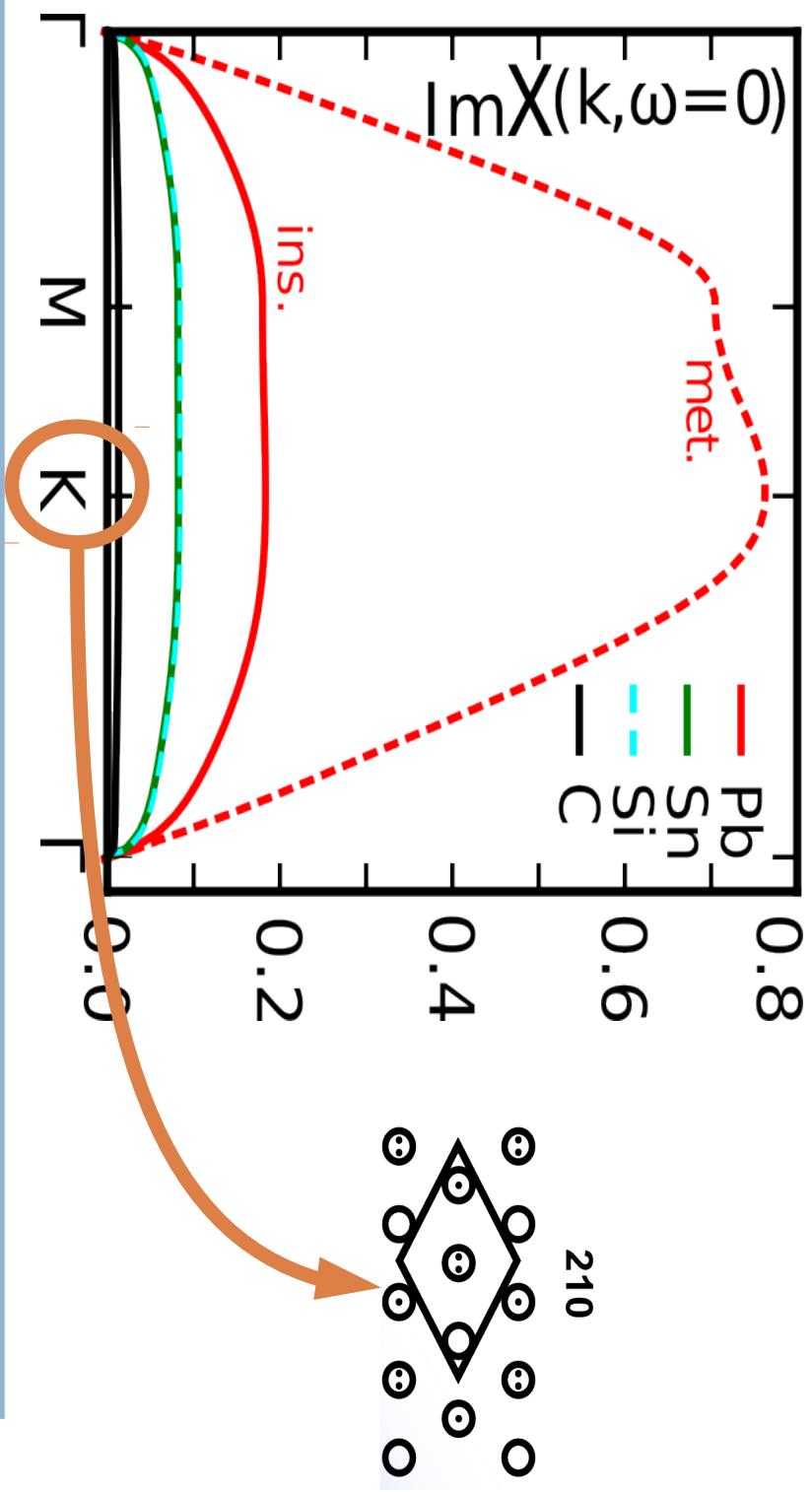
Photoemission results for  
**Sn** on Si (color)



# Charge-Ordering

Momentum-resolution of charge-charge correlation function  
Insights into nature of charge-order

Static charge-  
charge  
correlation  
function



3x3 ordered phase observed in **STM** (Pb/Si)  
(Slezak et al, PRB 1999)

# Conclusions

- Combination of **perturbative, but non-local** description of screening (GW)...
- ... with **non-perturbative, but local** description of strong correlations (DMFT)
- Treatment of **strong and/or long-ranged** interactions
- Insights into **charge-ordering**
- **Momentum structure** of charge susceptibilities

Merci pour votre attention

