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CIFAR-PITP
International Summer School on Numerical Methods for Correlated Systems in Condensed Matter

RQMP

UNIVERSITÉ DE SHERBROOKE

Éducation, Loisir et Sport Québec

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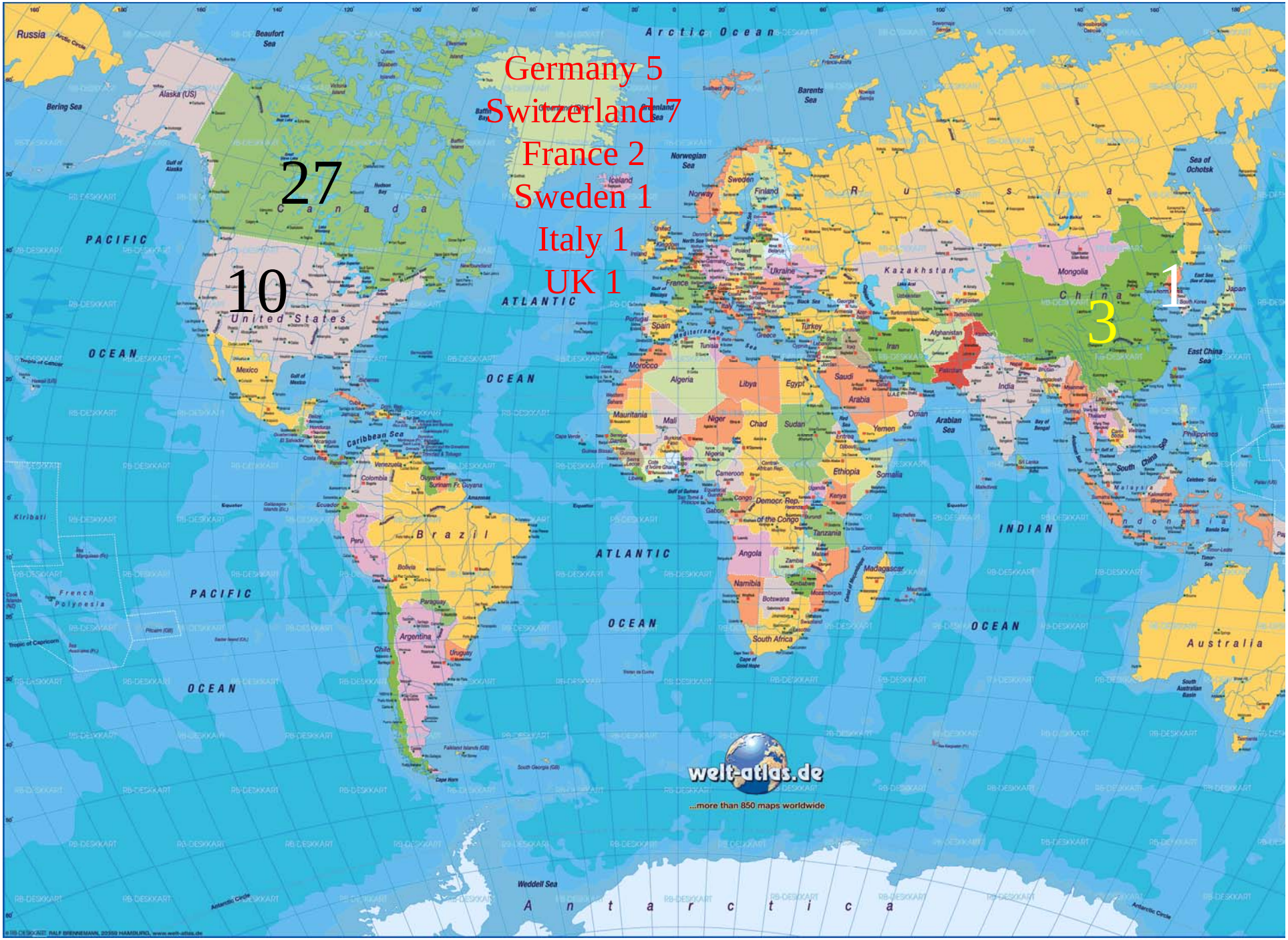
Germany 5
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France 2
Sweden 1
Italy 1
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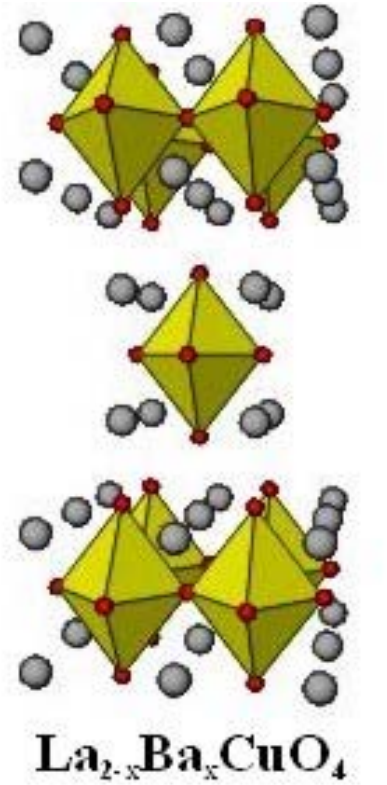
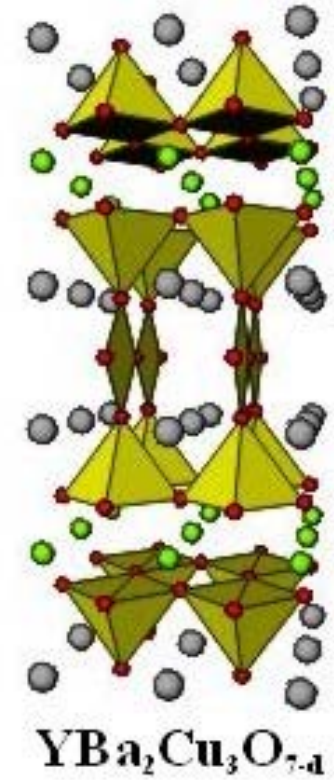
welt-atlas.de
...more than 850 maps worldwide

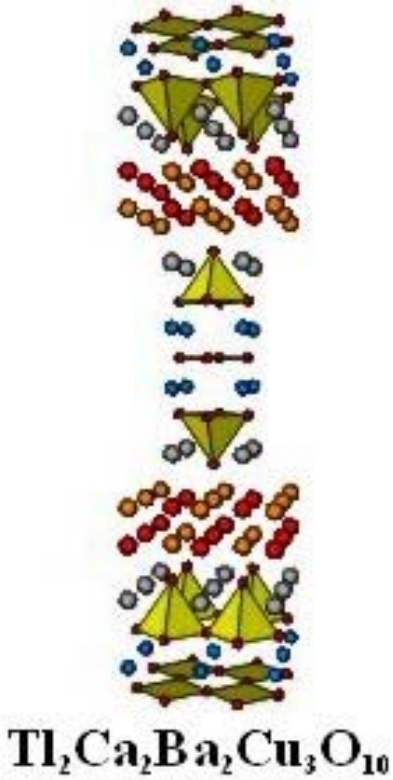
Condensed systems



$La_{2-x}Ba_xCuO_4$



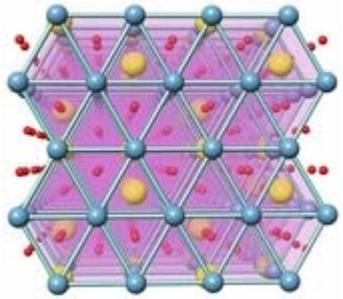
$YBa_2Cu_3O_{7-d}$

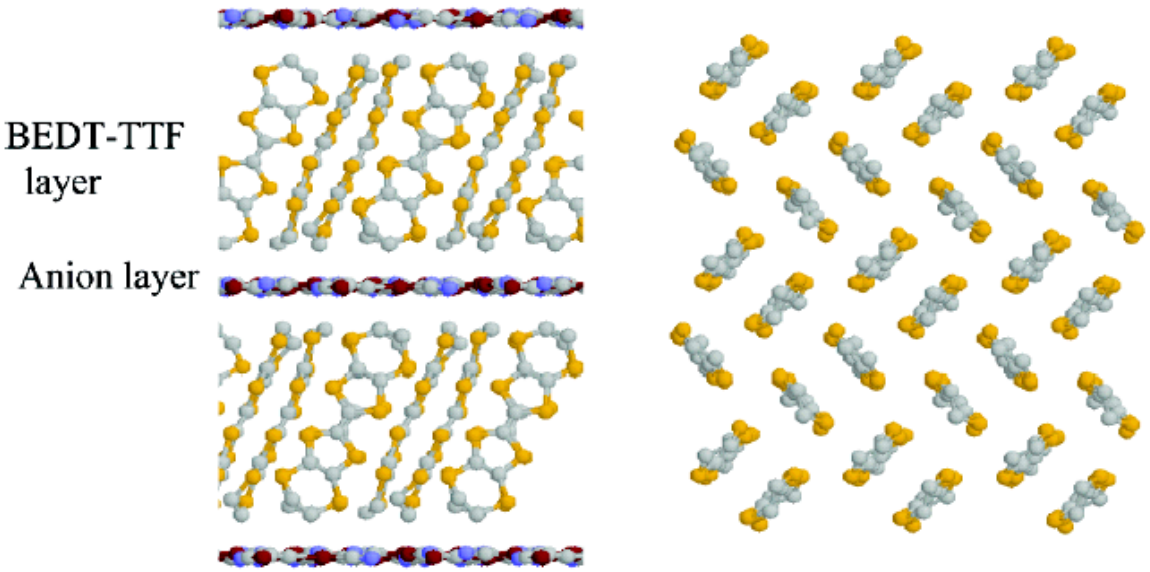


$Tl_2Ca_2Ba_2Cu_3O_{10}$

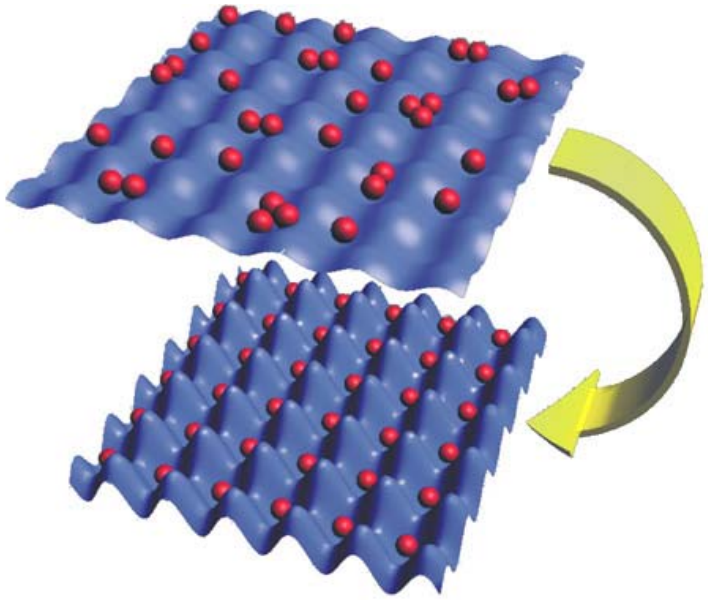
- High-temperature superconductors

- Cobaltates





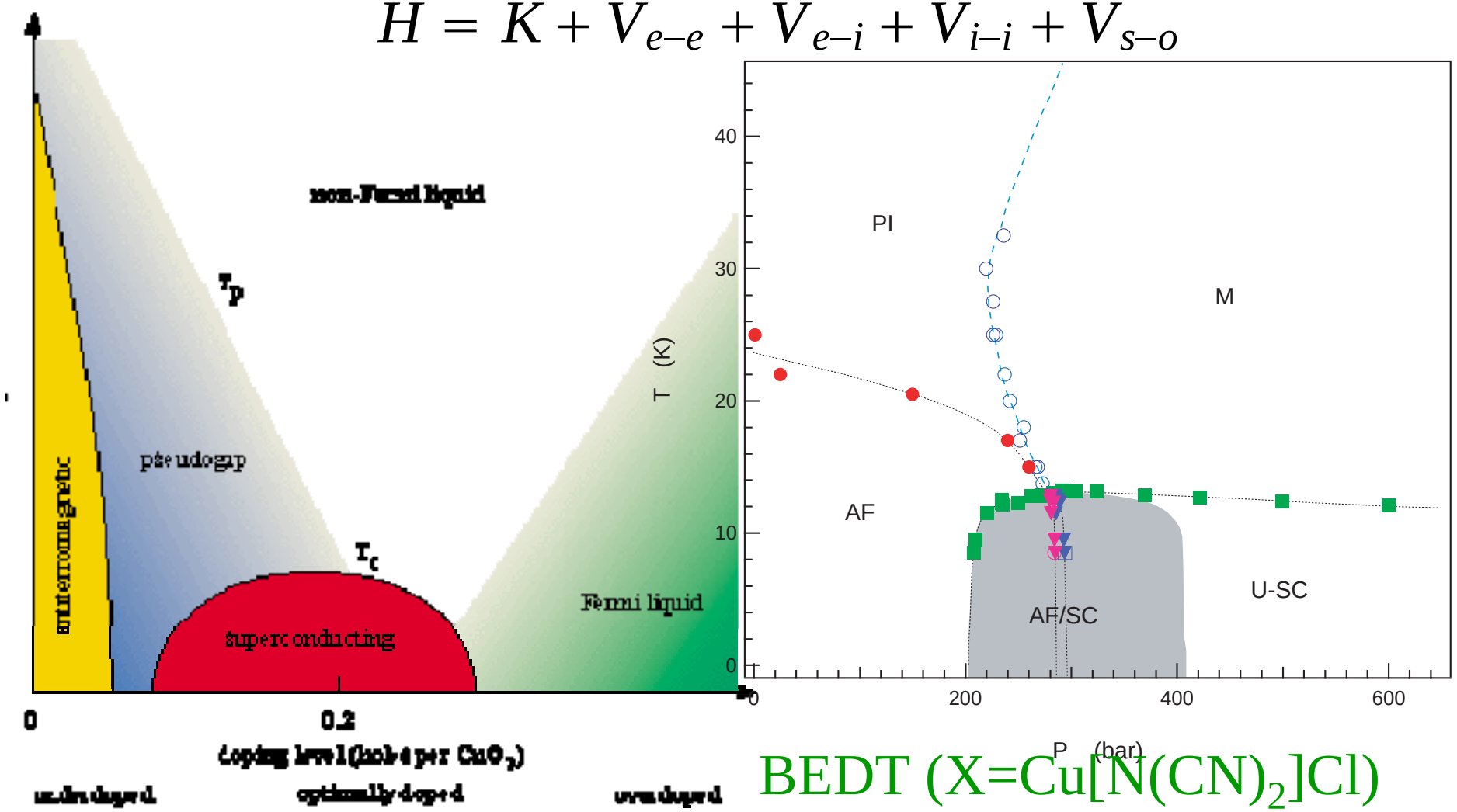
- Organics



- Cold atoms in optical lattices

The theory of everything

$$H = K + V_{e-e} + V_{e-i} + V_{i-i} + V_{s-o}$$



Battlogg and Varma,
Physics World, Feb. 2000

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

S. Lefebvre et al. PRL **85**, 5420 (2000),

P. Limelette, et al. PRL 91 (2003)

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The theory of everything

$$H = K + V_{e-e} + V_{e-i} + V_{i-i} + V_{s-o}$$

- 10-1000 eV vs 10 meV (3-5 orders of magnitude)

Réseau Québécois de Calcul de Haute Performance

The theory of everything

$$H = K + V_{e-e} + V_{e-i} + V_{i-i} + V_{s-o}$$

- 10-1000 eV vs 10 meV (3-5 orders of magnitude)
- Broken symmetry (lattice)
- Born-Oppenheimer approximation
- DFT
- Effective low energy Hamiltonian

Obtain « best » one-particle basis

- Hohenberg-Kohn theorem
- Kohn-Sham equations
- Exchange-correlation potential (s-p)
  - Michel Côté
  - Matthias Ernzerhof
  - Xiavier Gonze
- LDA + U

abinit.org

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Effective Hamiltonians (d-f)

- Hubbard
- t-J
- Anderson
  - André-Marie Tremblay

Solve Effective (or model) Hamiltonian

- Monte Carlo methods
  - Matthias Troyer
- QMC evaluation of Green function (Worm)
- Stochastic series expansion
  - Massimo Boninsegni
- Exact diagonalization
  - David Sénéchal
- Density Matrix Renormalization group
  - Steve White
  - Uli Schollwöck (Time dependence, Quantum Information)
- Numerical Renormalization group
  - Uli Schollwöck
- Continuous-time Quantum Monte Carlo
  - Philipp Werner

ALPS Matthias Troyer

DMFT

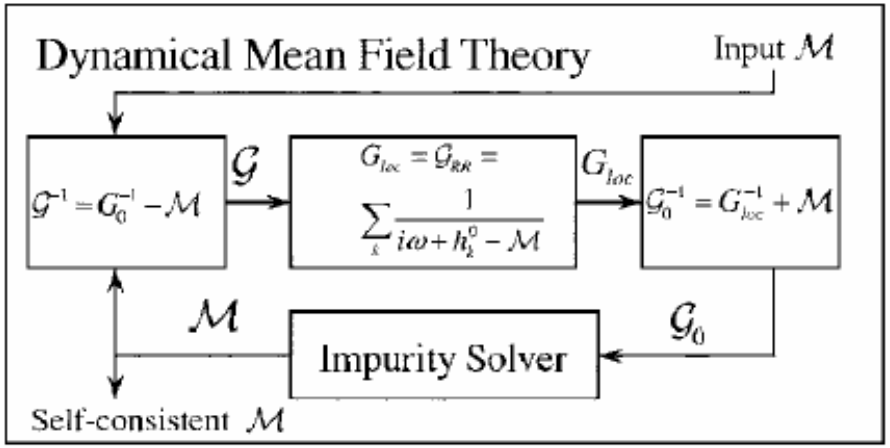


FIG. 5. Illustration of the self-consistent cycle in DMFT. Starting from a bath function, the impurity solver delivers a local M, which in turn defines a Kohn-Sham Green's function G defined for all R and R'. Only the diagonal part of the Kohn-Sham Green's function is important for the self-consistency condition which gives G_{loc}, which in turn provides the new bath function closing the iteration loop.

Kotliar et al. RMP (2006)

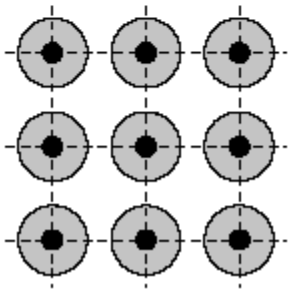
Variational cluster perturbation theory and DMFT as special cases of SFT

M. Potthoff *et al.* PRL **91,** 206402 (2003).

DCA, Jarrell et al.

Savrasov, Kotliar, PRB (2001)

DMFT



Georges Kotliar, PRB (1992).
M. Jarrell, PRL (1992).
A. Georges, *et al.* RMP (1996).

$$\sum_{\omega_n}\sum_{\mu\nu}\left[\frac{N}{N_c}\left(\frac{1}{G^{-1}_{0\mathbf{t}'}-\Sigma'(i\omega_n)}\right)_{\mu\nu}\right.$$
$$\left.-\sum_{\tilde{\mathbf{k}}}\left(\frac{1}{G^{-1}_{0\mathbf{t}}(\tilde{\mathbf{k}})-\Sigma'(i\omega_n)}\right)_{\mu\nu}\right]\frac{\delta\Sigma'_{\nu\mu}(i\omega_n)}{\delta\mathbf{t}'}=0.$$

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Quantum Cluster methods

- Variational Cluster Approximation
- Cellular Dynamical Mean-Field Theory
  - David Sénéchal
  - Gabi Kotliar
- Dynamical Cluster Approximation + Hirsch-Fye algorithm
  - Mark Jarrell
- Continuous-time Quantum Monte Carlo
  - Philipp Werner

LDA+DMFT

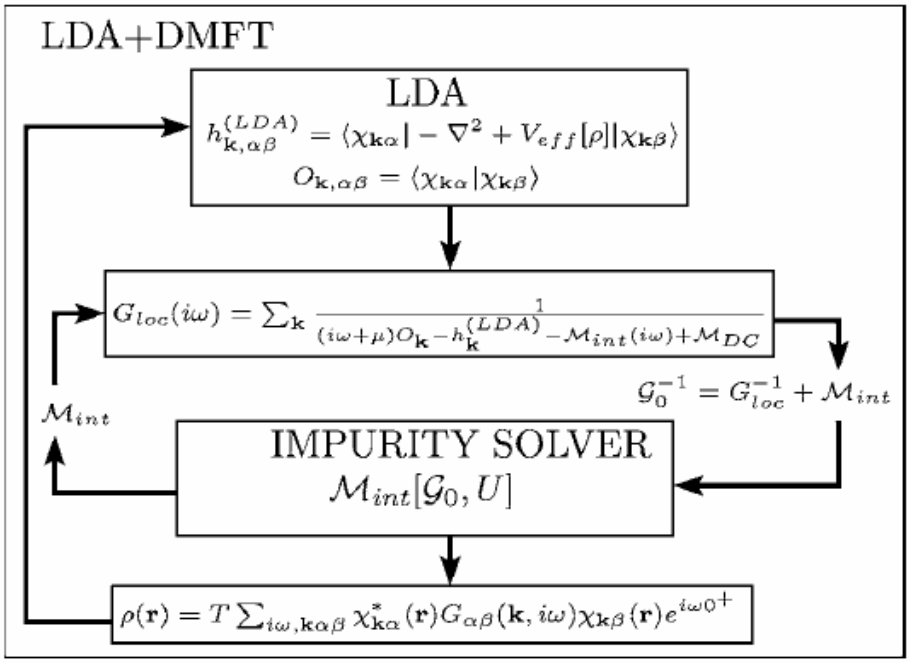


FIG. 9. Illustration of the self-consistent cycle in spectral density-functional theory within the LDA+DMFT approximation: the double iteration cycle consists of the inner DMFT loop and outer (density plus total energy) loop.

Kotliar et al. RMP (2006)

A unified perspective

- Inversion method
  - Gabi Kotliar
    - Exchange-correlation potential
    - Luttinger-Ward or Baym Kadanoff functional
    - Spectral density functional
- Self-Energy functional

Kotliar et al. RMP (2006)

A unified perspective

- Inversion method

TABLE I. Parallel between the different approaches, indicating the physical quantity which has to be extremized, and the field which is introduced to impose a constraint (constraining field). BL and AL correspond to the band and atomic limit reference systems, respectively.

Method	Physical quantity	Constraining field
Baym-Kadanoff	$G_{\alpha\beta}(\mathbf{k},i\omega)$	$\Sigma_{\mathrm{int},\alpha\beta}(\mathbf{k},i\omega)$
DMFT (BL)	$G_{\mathrm{loc},\alpha\beta}(i\omega)$	$\mathcal{M}_{\mathrm{int},\alpha\beta}(i\omega)$
DMFT (AL)	$G_{\mathrm{loc},\alpha\beta}(i\omega)$	$\Delta_{\alpha\beta}(i\omega)$
LDA+DMFT (BL)	$\rho(r)$, $G_{\mathrm{loc},ab}(i\omega)$	$V_{\mathrm{int}}(r)$, $\mathcal{M}_{\mathrm{int},ab}(i\omega)$
LDA+DMFT (AL)	$\rho(r)$, $G_{\mathrm{loc},ab}(i\omega)$	$V_{\mathrm{int}}(r)$, $\Delta_{ab}(i\omega)$
LDA+U	$\rho(r)$, n_{ab}	$V_{\mathrm{int}}(r)$, λ_{ab}
LDA	$\rho(r)$	$V_{\mathrm{int}}(r)$

Guest speakers

- Electron-Phonon interactions
  - Mona Berciu
- Ab Initio Molecular Electronics
  - Hong Guo

Overall view

Model Hamiltonians

Direct ED, QMC, SSE, Worm, NRG, DMRG

Quantum Clusters CPT, VCA, DCA, CDMFT

Final exam

- Friday June 6
- Take home is possible (but not recommended).

Groups for hands-on training and posters

- Today 13:30, first time.

- Group 1 and week 1: Ali to Joseph (30)
- Group 2 and week 2: Julien to Zhanyu (28)

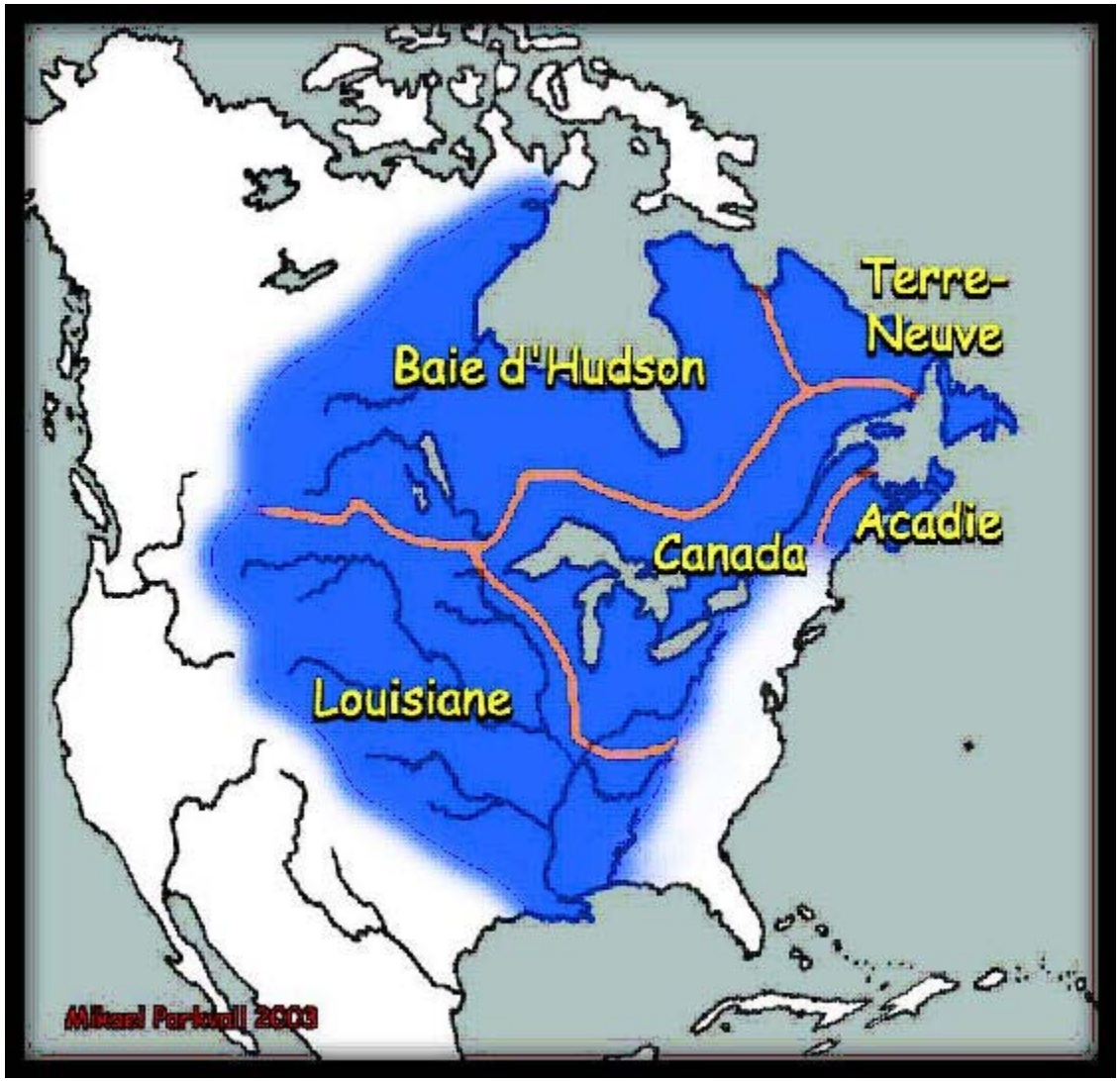
- CAUTION: Times not always the same.

Registration

- Tuesday: Passport or birth certificate
  - 13:00 A to D
  - 13:15 E to J
  - 13:30 K to P
  - 13:45 Q to Z

Québec 1608-2008

- Self-organized process



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