International summer school on Computational Quantum Materials 2018

Québec 1608-2008

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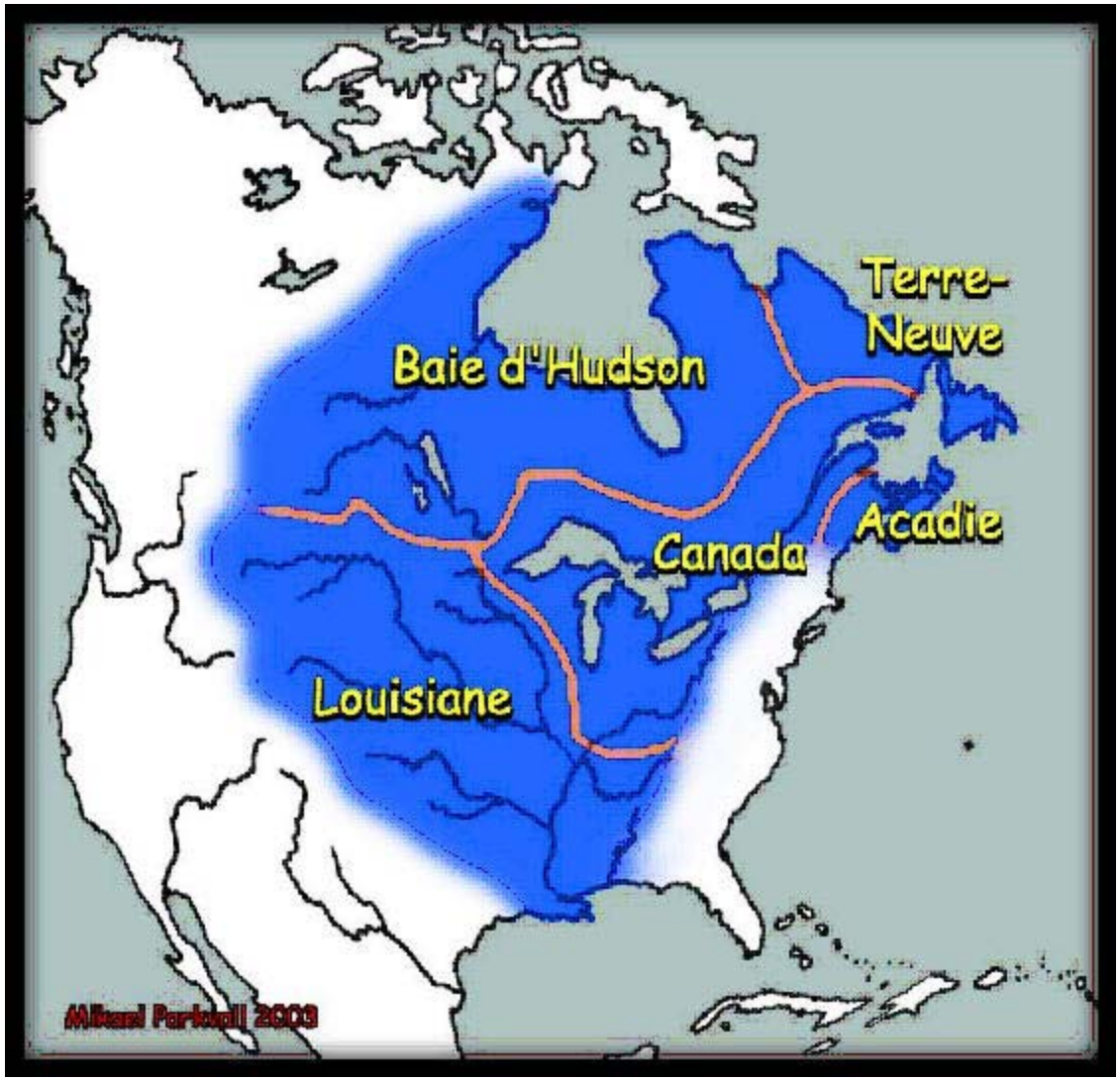


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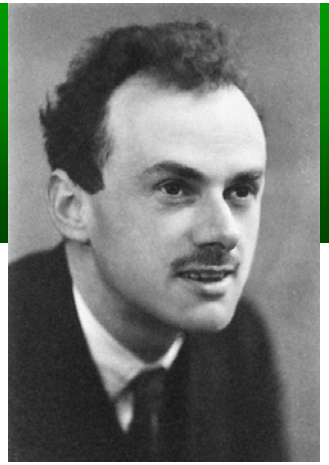
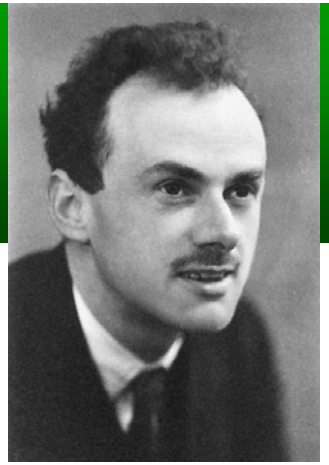
Total: 57
welt-atlas.de
...more than 850 maps worldwide

Dirac



- The underlying physical laws necessary for the mathematical theory of a large part of physics and the whole of chemistry are thus completely known, and the difficulty is only that the exact application of these laws leads to equations much too complicated to be soluble.

Dirac



- It therefore becomes desirable that **approximate practical methods of applying quantum mechanics should be developed, which can lead to an explanation of the main features of complex atomic systems without too much computation.**
  - *Proceedings of the Royal Society of London. Series A, Containing Papers of a Mathematical and Physical Character, Vol. 123, No. 792* (6 April 1929)

The theory of everything

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

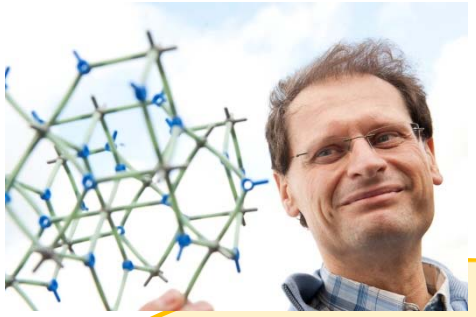
- 10-1000 eV vs 10 meV (3-5 orders of magnitude)

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
- Density functional theory (DFT)
- Methods for effective low energy Hamiltonian (DMFT, GW)
- Beating Moore's law: better algorithms

Overview



Ab initio
Abinit
Wien2k
Comsuite

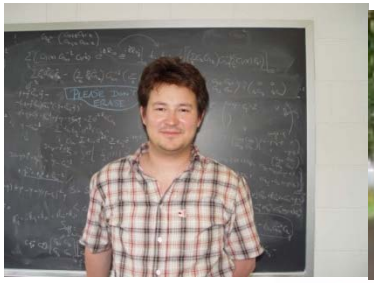
GW
DMFT
Monte Carlo
TRIQS
Analytic cont.

Models
Hubbard model
Anderson impurity





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Obtain « best » one-particle basis

- Hohenberg-Kohn theorem
- Kohn-Sham equations
- Exchange-correlation potential (s-p)
- LDA + GW
  - Michel Côté
  - Rignanese, Gian-Marco

abinit.org

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Best one-particle basis

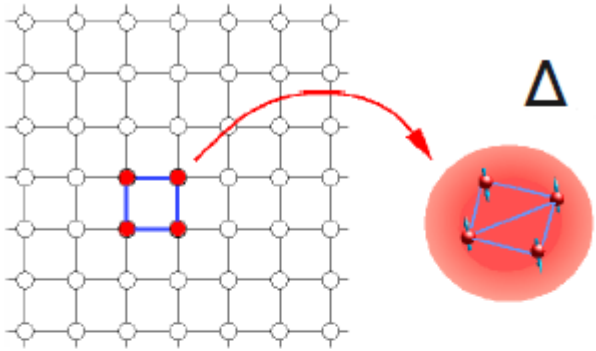
- Topological insulators (spin orbit)
  - Ion Garate
- LDA+DMFT (Wien2k)
  - G. Kotliar
  - K. Haule
- Analytic continuation
  - D. Bergeron

Many-body and Effective Hamiltonians (d-f)

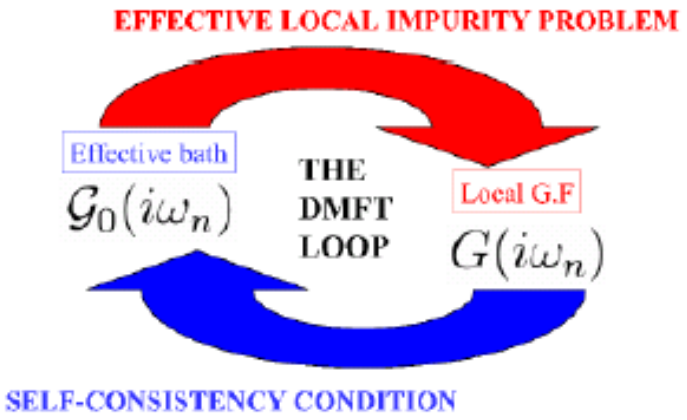
- Hubbard
  - André-Marie Tremblay

DMFT

-David Sénéchal



$$Z = \int \mathcal{D}[\psi^\dagger, \psi]\, e^{-S_c - \int_0^\beta d\tau \int_0^\beta d\tau' \sum_{\mathbf{K}} \psi^\dagger_{\mathbf{K}}(\tau)\Delta_{\mathbf{K}}(\tau,\tau')\psi_{\mathbf{K}}(\tau')}$$



REVIEWS

Maier, Jarrell et al., RMP. (2005)

Kotliar *et al.* RMP (2006)

AMST *et al.* LTP (2006)

Gull *et al.* RMP (2011)

-

$$\Delta(i\omega_n) = i\omega_n + \mu - \Sigma_c(i\omega_n) - \left[\sum_{\tilde{k}} \frac{1}{i\omega_n + \mu - t_c(\tilde{k}) - \Sigma_c(i\omega_n)}\right]^{-1}$$

Solve Effective (or model) Hamiltonian

- Monte Carlo methods
  - Mauro Iazzi
- QMC evaluation of Green function (Worm)
  - Adrian Del Maestro
- Stochastic series expansion
  - Roger Melko
- Exact diagonalization and quantum cluster methods
  - David Sénéchal
- Continuous-time Quantum Monte Carlo
  - Philipp Werner

ALPS Michele Dolfi

Solve Effective (or model) Hamiltonian

- Density Matrix Renormalization group
  - Miles Stoudenmire
  - Uli Schollwöck (Time dependence, Quantum Information)
- Further insights from Quantum Information PEPS, Fermionic tensor networks
  - Roman Orus

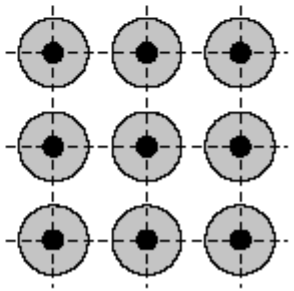
Variational cluster perturbation theory and DMFT as special cases of SFT

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).

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

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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

Overall view

Model Hamiltonians

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

Quantum Clusters CPT, VCA, DCA, CDMFT

LDA+DMFT

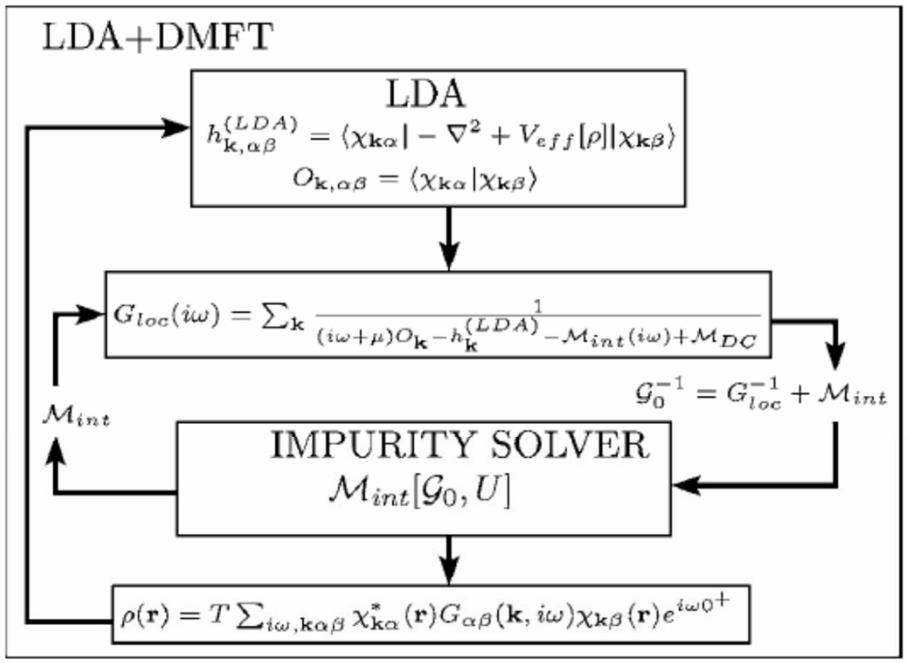


FIG. 9. Illustration of the self-consistent cycle in spectral density-functional theory within the LDA+DMFT approximation: the double iteration cycle consists of the inner DMFT loop and outer (density plus total energy) loop.

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)

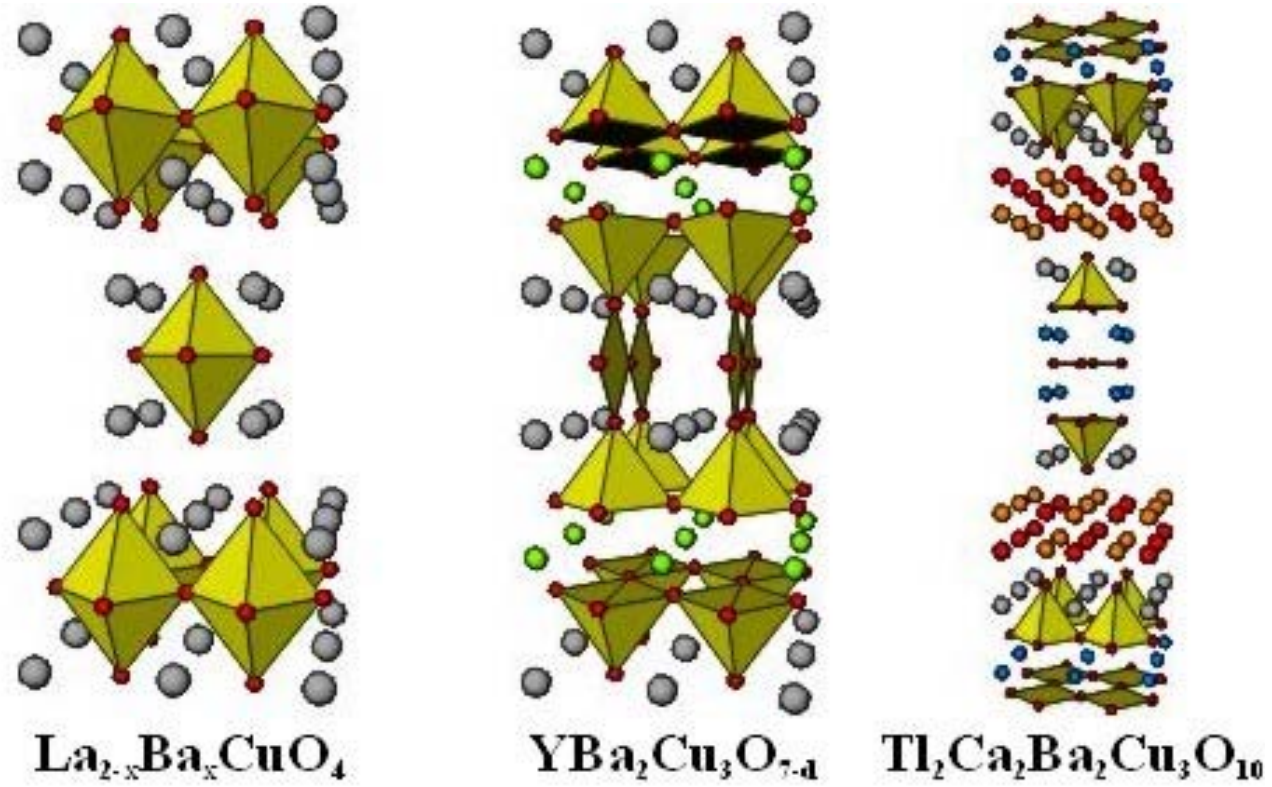
A unified perspective

- Inversion method

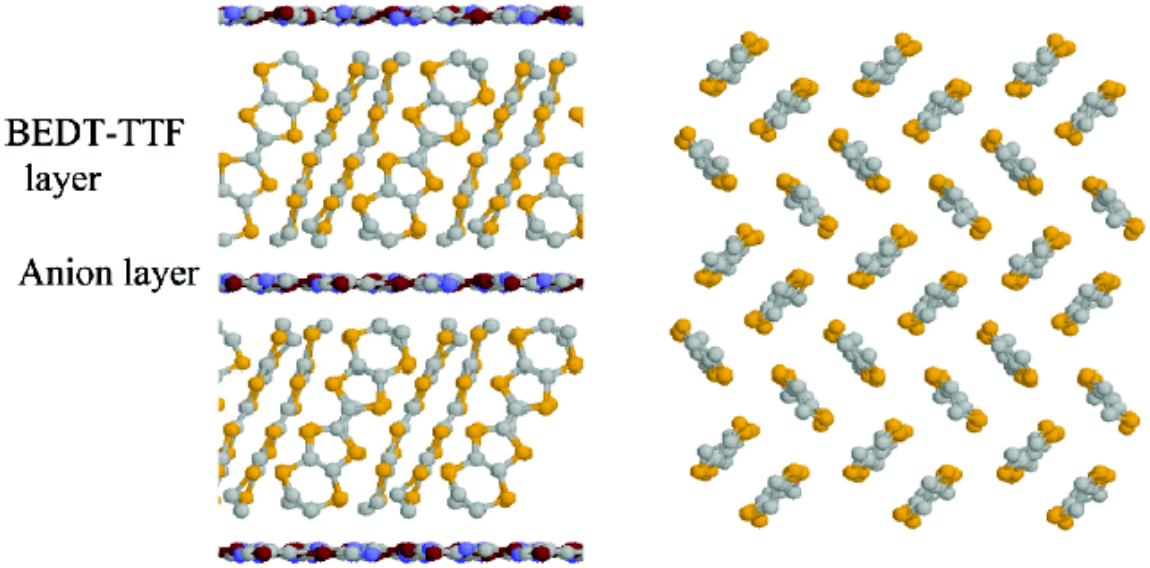
TABLE I. Parallel between the different approaches, indicating the physical quantity which has to be extremized, and the field which is introduced to impose a constraint (constraining field). BL and AL correspond to the band and atomic limit reference systems, respectively.

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	$\rho(r)$	$V_{\mathrm{int}}(r)$

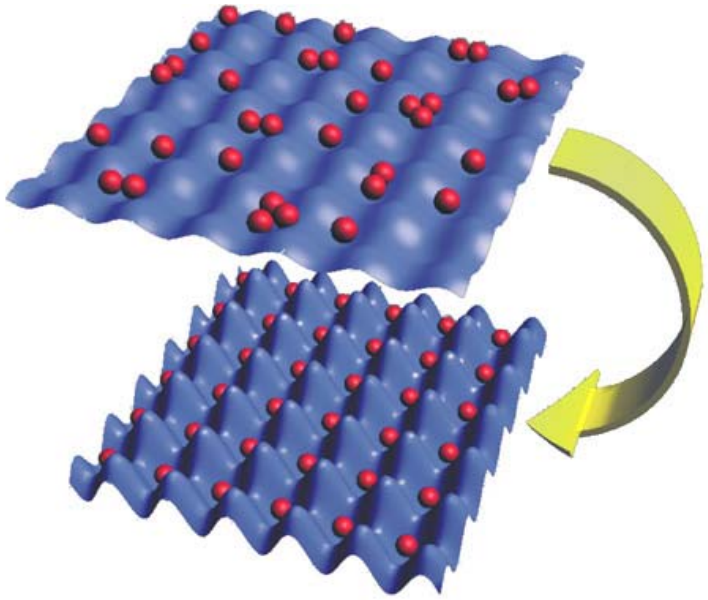
Quantum Materials



- High-temperature superconductors



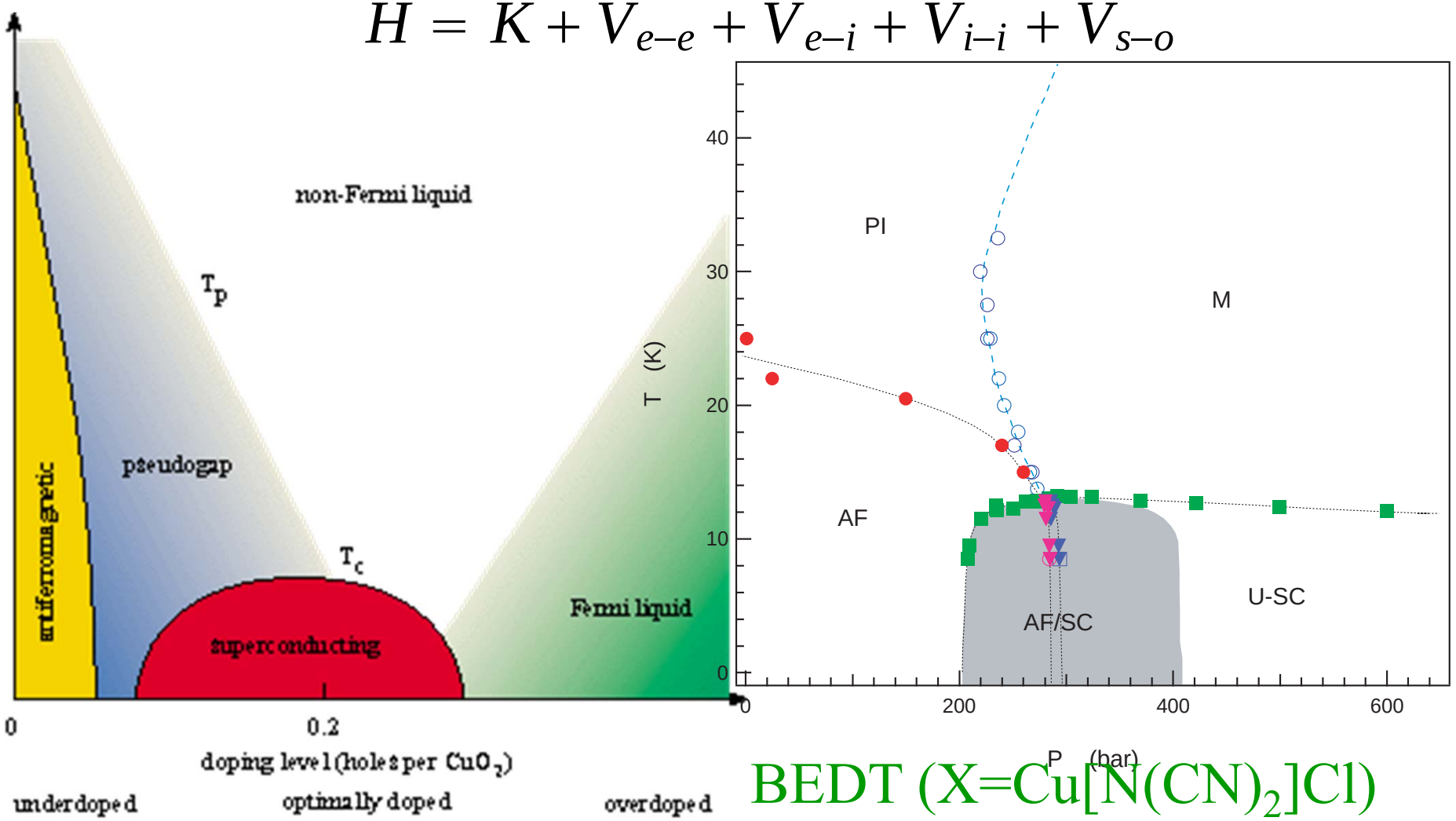
- Organics



- 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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Local computing infrastructure

Thanks: Michel Barrette, David Sénéchal

- 4 servers with the following
- 2 AMD EPYC 7301 2.1GHz (30/32 cores visibles)
- 256GB RAM (200GB visible)
- 400GB disk
- CentOS 7.5 Linux OS
- Gbit Ethernet local network

POSTERS

- Set them up for the whole school.
- Preceeded by « poster advertisement »
  - Today, 14:00
- Special times:
  - Monday May 28, 14h00 to 15h00
  - Tuesday May 29, 14h00 to 15h30
- But will be posted during the whole school

Final exam

- Thursday night June 7
- Friday morning June 8
- Marks:
  - Multiple Choice 50%
  - One homework on Abinit 25%
  - One homework on TRIQS 25%
- YOU CAN STILL REGISTER TODAY

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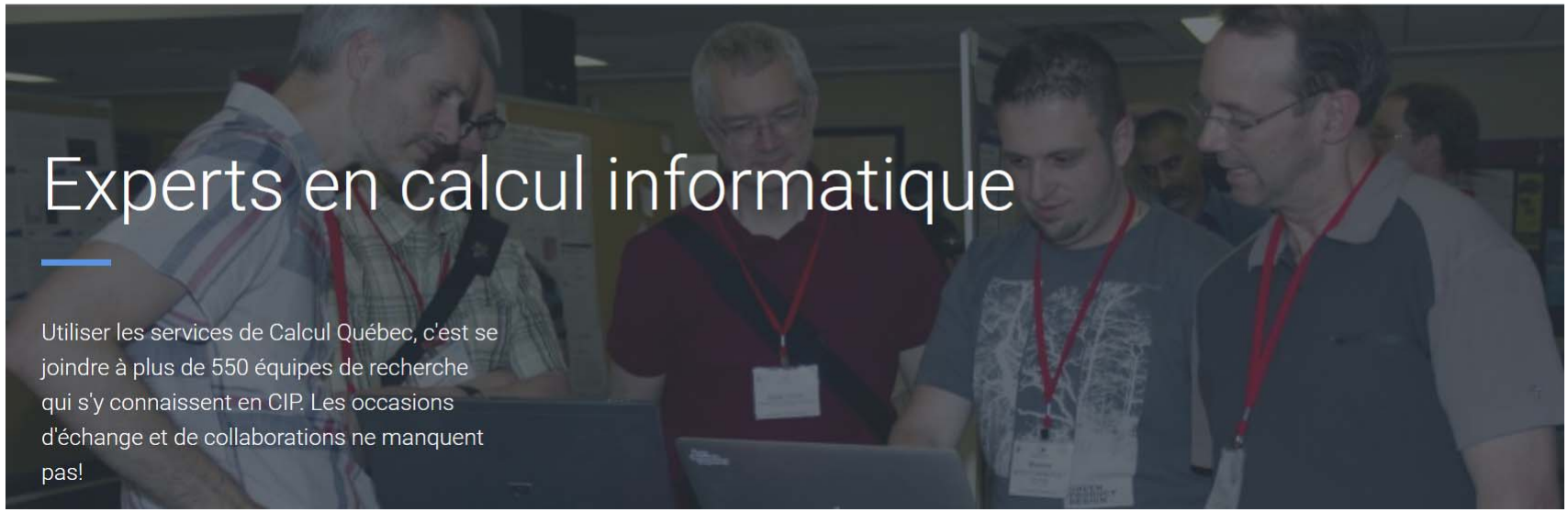

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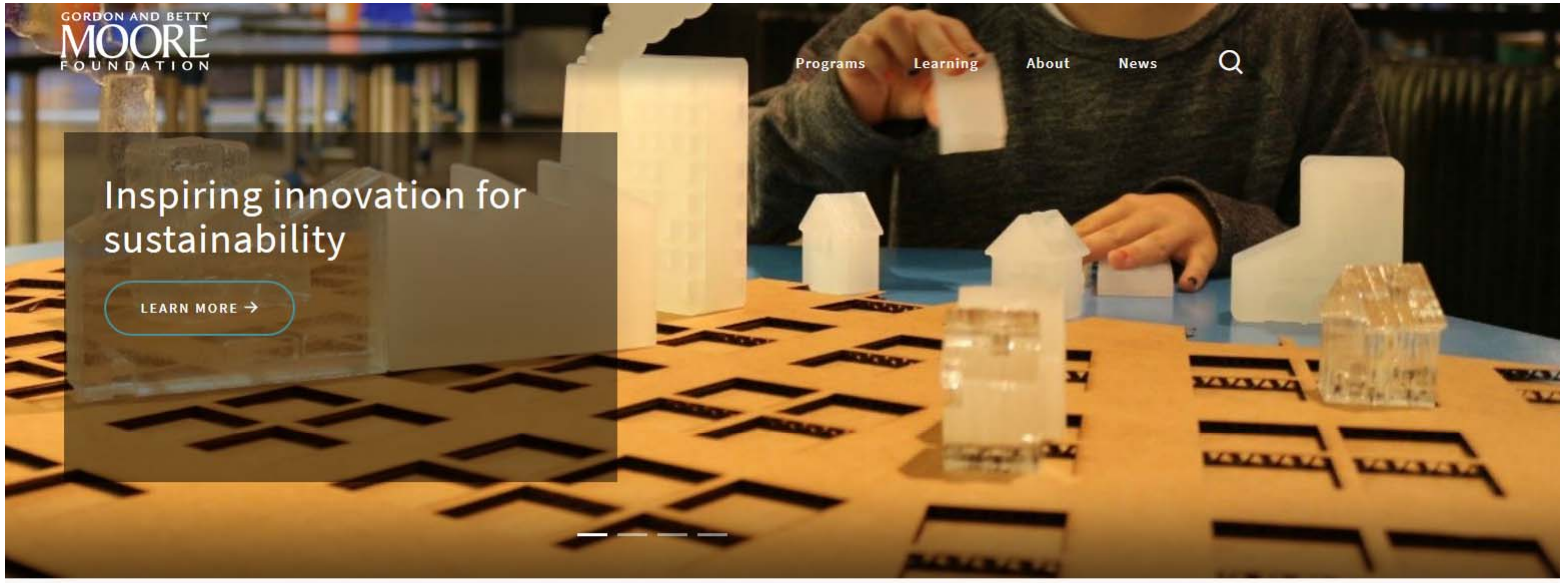

Our mission

Gordon and Betty Moore established the foundation to create positive outcomes for future generations. In pursuit of that vision, we foster path-breaking scientific discovery, environmental conservation, patient care improvements and preservation of the special character of the San Francisco Bay Area.

SCIENCE | ENVIRONMENTAL CONSERVATION | PATIENT CARE | THE BAY AREA

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Sponsors

The Institut quantique of Université de Sherbrooke is a unique research centre, the result of strong international collaborations and concerted actions in quantum materials, quantum information and quantum engineering.

FIND OUT MORE

[VOULEZ-VOUS EN FAIRE PARTIE?]

CANADA FIRST RESEARCH EXCELLENCE FUND

APOGÉE CANADA FONDS D'EXCELLENCE EN RECHERCHE

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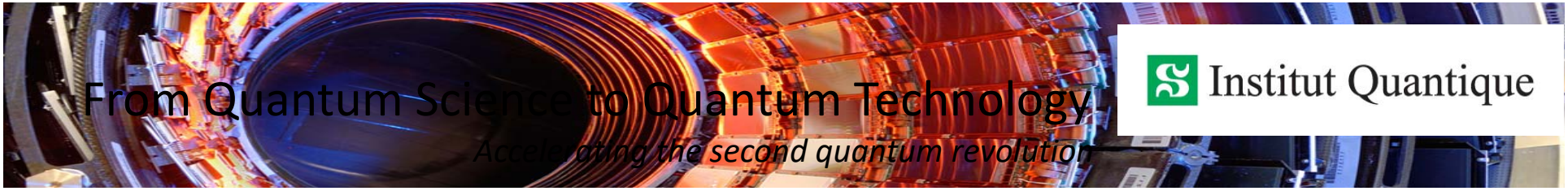

Université de Sherbrooke, through the Canada First Research Excellence Fund, is launching an ambitious **33.5M$** research program to become a key player in the second quantum revolution of the 21st century.

Bring quantum science to the next level by fostering a unique synergy between quantum information, quantum materials and electrical engineering

-

Recruit the best talent of physicists and engineers to exploit groundbreaking discoveries and go ***from quantum science to quantum technology***

Partnerships

Strengthen their **existing** and build **future** partnerships and collaborations with high-tech companies and established research centres, which are pushing the boundaries of quantum-based research, to put Université de Sherbrooke in an excellent position on the world stage.

Contact us

We are looking for motivated individuals and interested parties to be part of this exciting adventure.

SubventionApogee@usherbrooke.ca

Institut Quantique

From Quantum Science to Quantum Technology

Institut Quantique

Accelerating the second quantum revolution

From quantum science to quantum technology *Initiative* is an ambitious **40M$** research program at the interface of quantum information sciences, quantum materials and quantum engineering.

Quantum sciences is at a stage that it is ready to yield technologies with transformative impact on our society

We offer a world-class research environment where the best talent of physicists and engineers
can work together on groundbreaking research, exchanging ideas, and technology development

Through partnerships with established research centres and high-tech companies, pushing the boundaries of quantum-based research, we will accelerate the second quantum revolution and move from **Quantum Science to Quantum Technology**

Contact us

We are looking for motivated individuals and interested parties to be part of this exciting adventure.

SubventionApogee@usherbrooke.ca

Institut Quantique