Determinant Monte Carlo algorithms for dynamical quantities in fermionic systems

Alice Moutenet, Wei Wu and Michel Ferrero
École polytechnique, Collège de France

We express the partition function as a series in the interaction (here *U*):

$$Z = \sum_n Z_n U^n$$

Diagrammatic MC algorithm: write Z_n as a sum of Feynman diagrams:

$$Z_n = \underbrace{\int \mathrm{d}x_1 \dots \mathrm{d}x_n}_{\text{MC sampling}} \overbrace{\sum_{\text{Feynman diagrams } \mathcal{F}}}^{\text{accumulation}} \mathcal{F}(x_1, \dots, x_n) = \int \mathrm{d}x_1 \dots \mathrm{d}x_n \, \det(x_1, \dots, x_n)$$

What about dynamical quantities (Green's function, self-energy, …)?

$$G_n = \int \mathrm{d}x_1 \dots \mathrm{d}x_n \sum_{\text{conn. Feynman diagrams } \mathcal{F}} \mathcal{F}(x_1, \dots, x_n)$$

R.Rossi, PRL 119, 045701 (2017)

$$\Sigma_n = \int \mathrm{d}x_1 \dots \mathrm{d}x_n \sum_{\text{1PI Feynman diagrams } \mathcal{F}} \mathcal{F}(x_1, \dots, x_n)$$

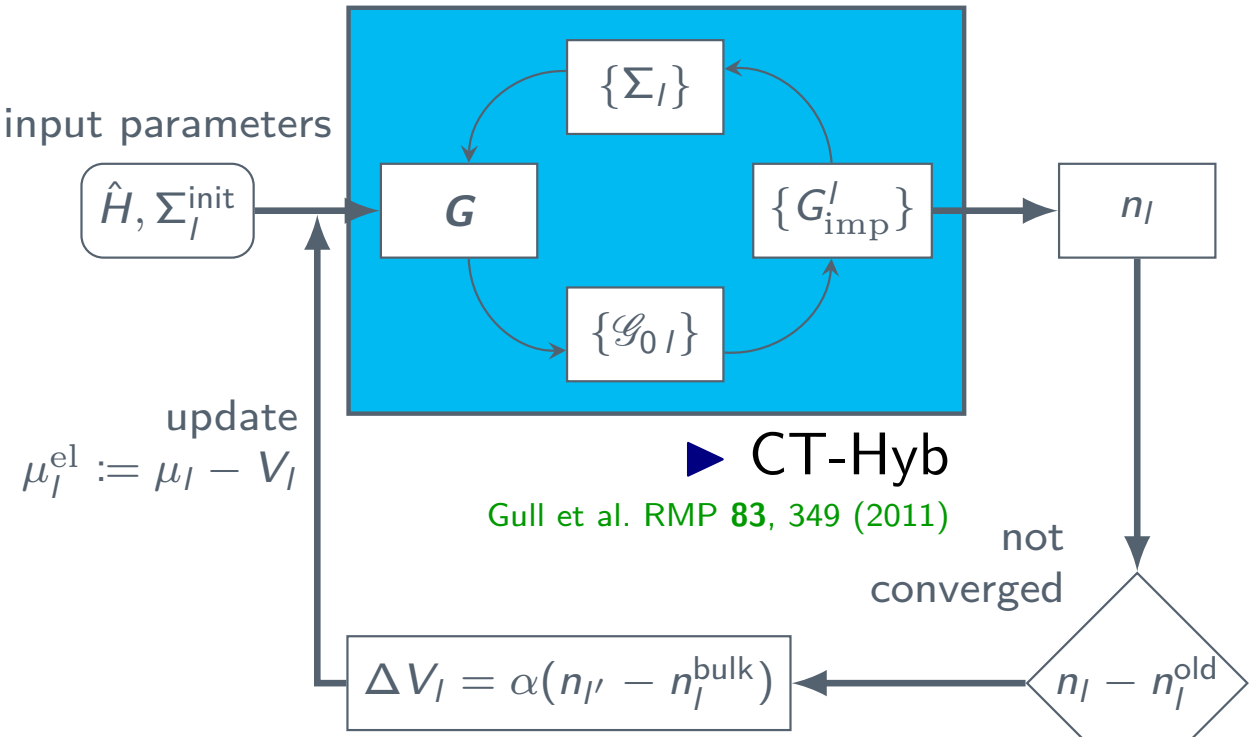
A. Moutenet et al., PRB 97, 085117 (2018)

Charge reconstruction in magnetic heterostructures

Andreas Weh, Augsburg University, Germany

- Hubbard model
- r-DMFT

Kotliar & Vollhardt PT **57**, 3, 53 (2004)
Potthoff & Nolting PRB **60**, 7834 (1999)
Pairault et al. EPJB **16**, 85-105 (2000)



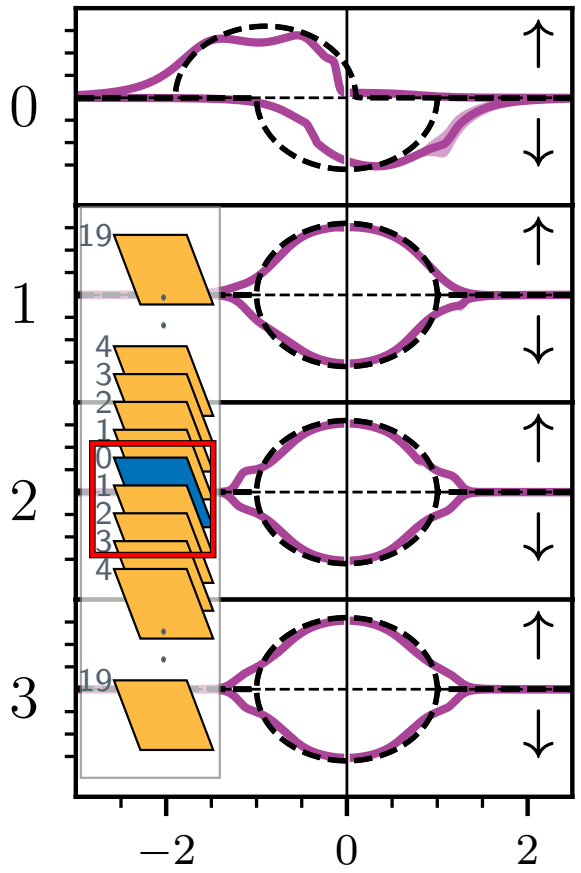
- CT-Hyb

Gull et al. RMP **83**, 349 (2011)

- long-ranged Coulomb interaction in MF

Charlebois et al. PRB **87**, 035137 (2013)

- M/HFM/M



Equilibrium and Dynamical properties of magnetic clusters

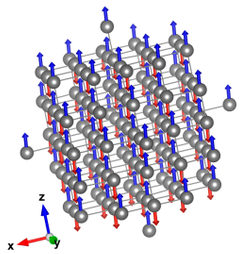
KING'S College LONDON

EPSRC Engineering and Physical Sciences Research Council

CANES CDT

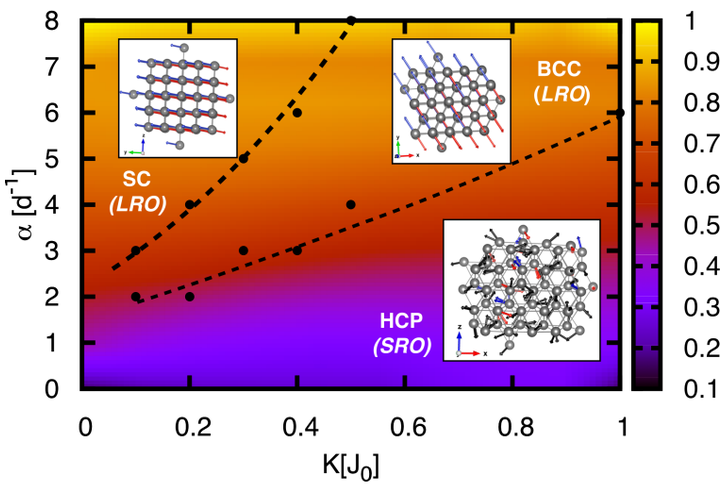
Extended Monte Carlo Simulations

We run extended Monte Carlo simulation with two dynamical variables spins (Heatbath Algo), positions (Metropolis) both at T=0 and finite T.



$$H(\mathbf{S}_i, \mathbf{S}_j, d_{ij}) = -\frac{1}{2}\sum_{i,j} J(d_{ij})\mathbf{S}_i \cdot \mathbf{S}_j + \frac{K}{2}\sum_{i,j}\left[\left(\frac{d^0}{d_{ij}}\right)^{12} - 2\left(\frac{d^0}{d_{ij}}\right)^{6}\right]$$

$$J(d_{ij}) = Je^{-\alpha\left(d_{ij}-d_{ij}^0\right)} \qquad J<0$$

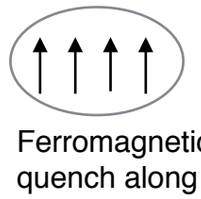


Spin Dynamics

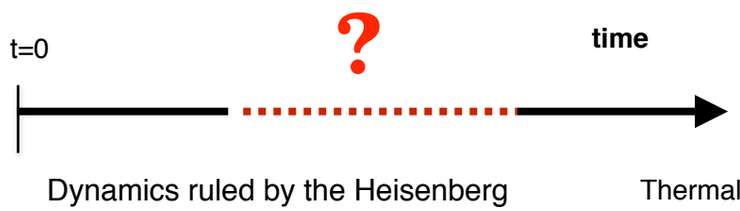
$$\frac{d\mathbf{S}_i}{dt} = \frac{1}{\hbar}\left[\mathbf{S}_i \times (-\mathbf{\Omega}_i + \mathbf{h}_i) - \gamma \mathbf{S}_i \times (\mathbf{S}_i \times (-\mathbf{\Omega}_i))\right]$$

$$\mathbf{\Omega}_i = -\sum_{j\neq i} J_{ij}\mathbf{S}_j$$

Stochastic Landau-Lifshitz-Gilbert equation



Ferromagnetic quench along z-axis

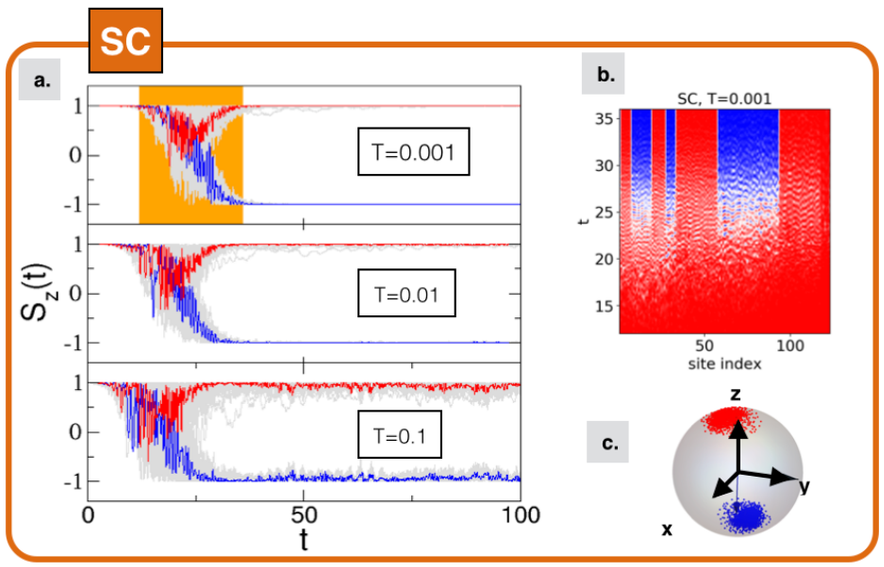


Dynamics ruled by the Heisenberg hamiltonian with **antiferromagnetic** interaction.

Thermal state(T)

How does the interplay between magnetic order and lattice vibrations affect the relaxation of the system?

Is there any non-trivial evidence of memory effects?



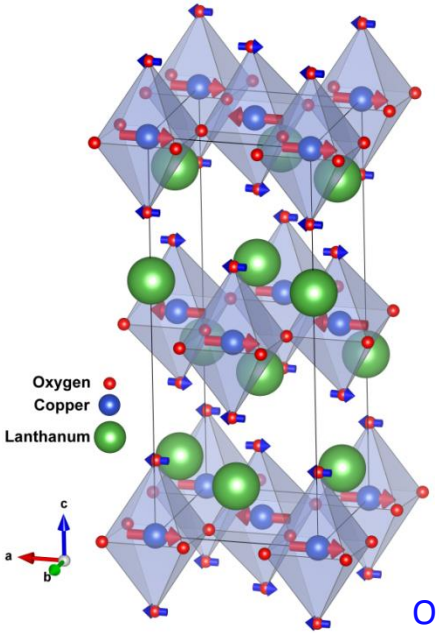
Carla Lupo

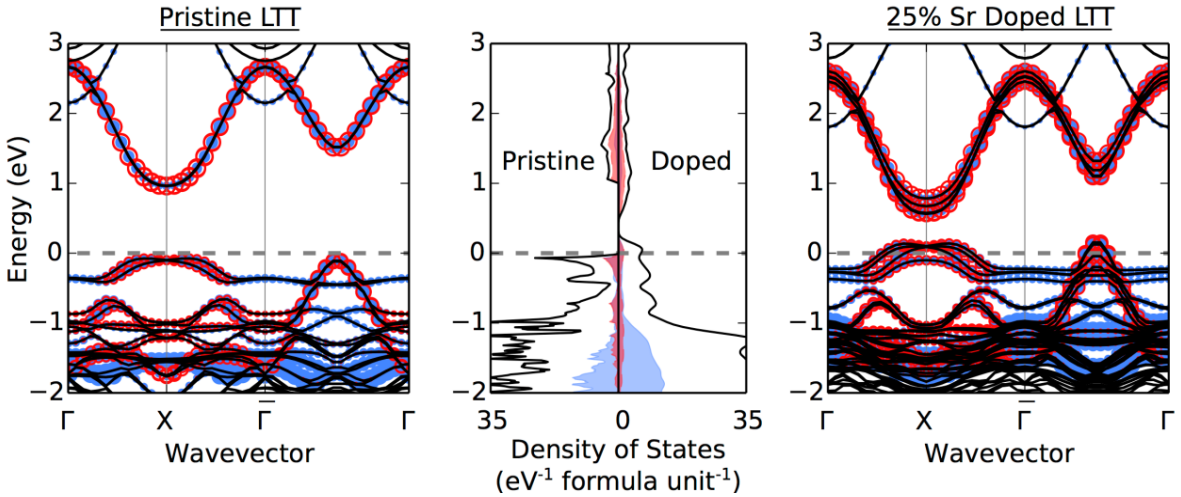
SUPERVISOR: Dr Cedric Weber

Accurate first-principles description of the antiferromagnetic state of La_2CuO_4

Christopher Lane[1], James Furness[2], Ioana Buda[1], Yubo Zhang[2],
Robert Markiewicz[1], Bernardo Barbiellini[3,1], Jianwei Sun[2], and Arun Bansil[1]

[1] Department of Physics, Northeastern University
[2] Department of Physics, Tulane University
[3] Department of Physics, Lappeeranta University of Technology





Our computations correctly predict the key experimentally observed features of the electronic structure and magnetism of LCO/LSCO without invoking any *free parameters*.

Corentin Bertrand (CEA/INAC)

Quantum Monte-Carlo for nanoelectronics

Real time and out-of-equilibrium

Anderson Impurity Model / Kondo physics

Corentin Bertrand

2nd year PhD student
CEA Grenoble / INAC

Under supervision of
Xavier Waintal
Christoph Groth

Quantum Monte-Carlo Algorithm for Correlated Out of Equilibrium Nanoelectronics

The fermionic Quantum Many-Body problem is the subject of many numerical works in the condensed matter community and beyond. However their hypothesis rarely overlap the requirements of nanoelectronics: calculating real-time/frequency quantities in out-of-equilibrium mesoscopic devices (*e.g.* current between leads), at low temperature. We developed a new Monte-Carlo algorithm suitable for nanoelectronics which compute perturbation series of Green's functions. Using the real-time Keldysh formalism, it is generic and grants easy access to experimental quantities such as the spectral function. We successfully benchmarked our method against NRG calculations on the Anderson Impurity Model.

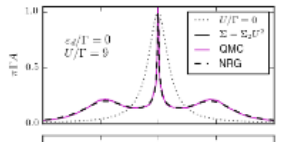
Goal: computing real-time many-body Green's functions in nanoelectronic devices

$$\hat{H} = \sum_{ij} H_{ij} c_i^\dagger c_j + U\theta(t) \sum_{ij} V_{ij} n_i n_j$$

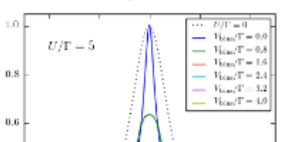
- Input: non-interacting Green's function g and interaction V

Results: application to the Anderson Impurity Model

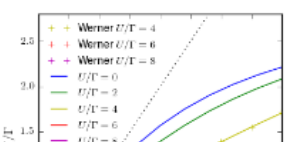
Kondo peak and Self-Energy:



Out-of-equilibrium DoS:



IV characteristics:



A study of electron correlation effects in SrVO3 : Dynamical mean-field theory with a quasi-continuous time QMC solver

E. Sheridan, C.* Rhodes*, E. Plekhanov*, C. Weber*
**King's College London, The Strand, WC2R 2LS London, UK*

THE THOMAS YOUNG CENTRE
EPSRC Engineering and Physical Sciences Research Council
KING'S College LONDON
CANES

We are developing a fully integrated ab-intio package with the aim at the equation of state for strongly correlated systems.

Our approach

- ☑ **Linear Scaling in β .**
- ☑ **Compact representations of $G(\tau)$.**
- ☑ **Quasi-continuous via extrapolation in a polynomial basis.**
- ☑ **Fully integrated into CASTEP.**
- ☑ **Interfaces to QC-BSS-QMC, CT-QMC, Hubbard I & IPT.**

Future Goals

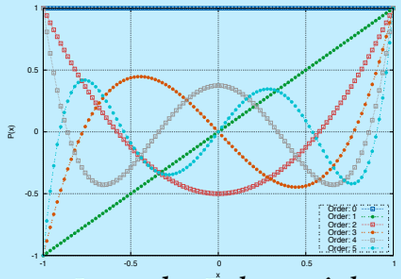
- ☐ **Investigation into f-systems and high pressures.**
- ☐ **Phonons and Equation of State.**
- ☐ **Cerium volume collapse.**

Case study: SrVO3

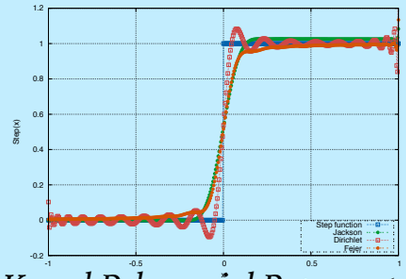
We are interested in the 3 t2g orbitals near the Fermi Level

$$H = H^0_{LDA} + \sum_m U_{mm} n_{m\uparrow} n_{m\downarrow} - \sum_{m\sigma} \mu n_{m\sigma} + \sum_{m<m'\sigma} U_{mm'} n_{m\sigma} n_{m'-\sigma} + \sum_{m<m'\sigma} (U_{mm'} - J_{mm'}) n_{m\sigma} n_{m'\sigma}$$

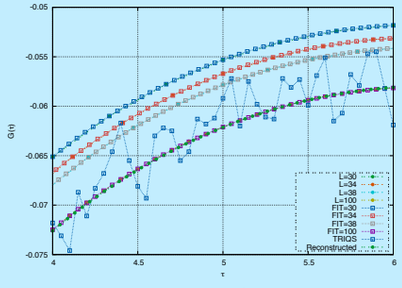
Our approach replicates the CT-QMC results at a fraction of the time



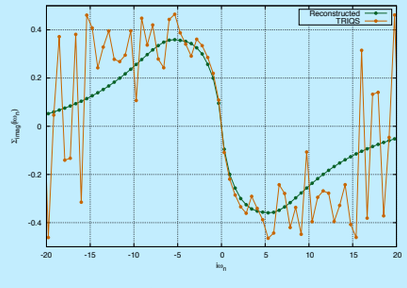
Legendre Polynomials



Kernel Polynomial Representation



Extrapolation



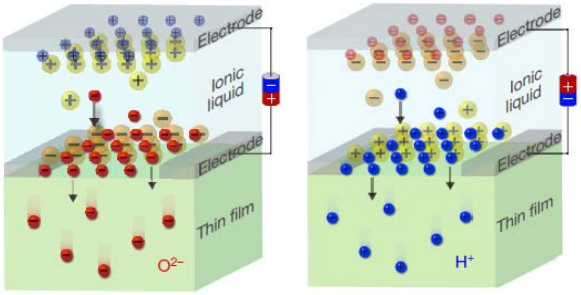
Self Energies

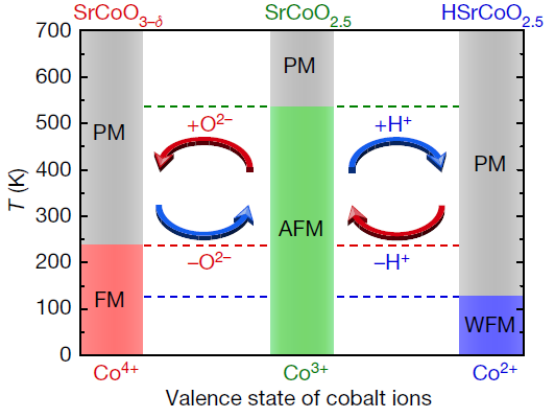
UNIVERSITÉ DE SHERBROOKE

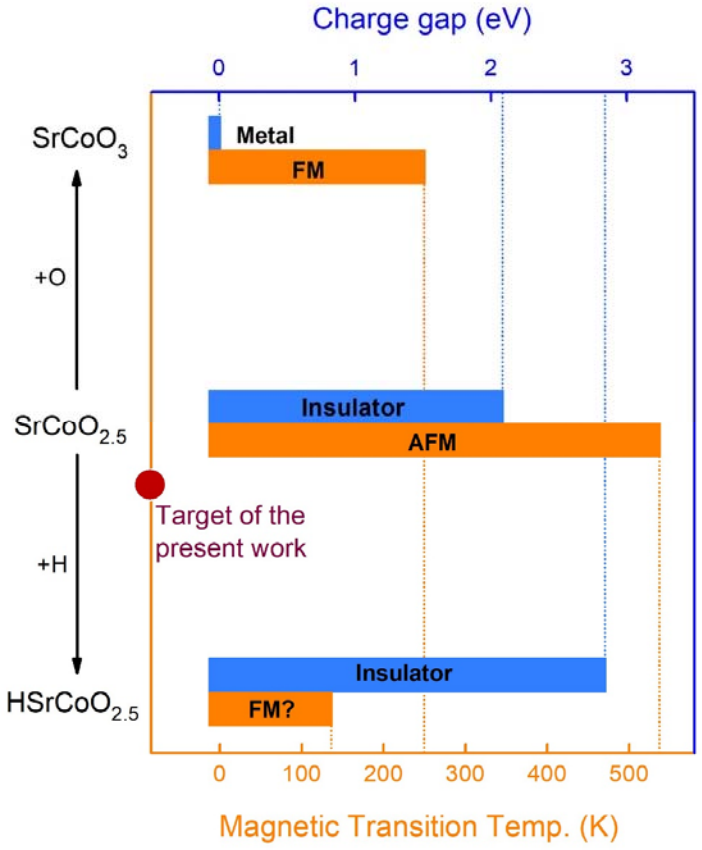
The role of interstitial hydrogen in $SrCoO_{2.5}$ antiferromagnetic insulator

Li Liang

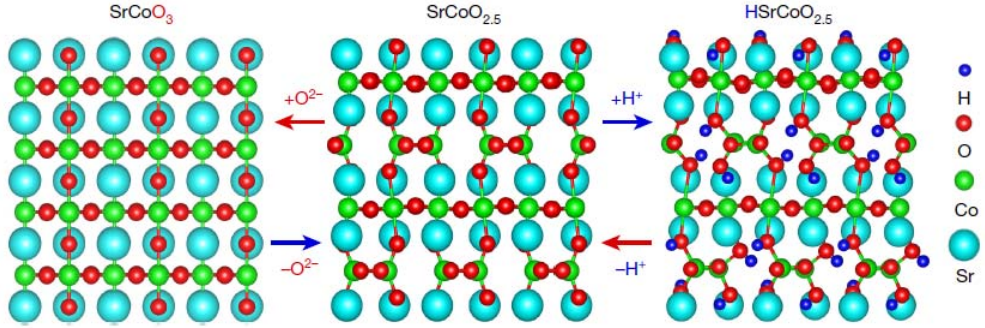
Department of Physics, Tsinghua University, China



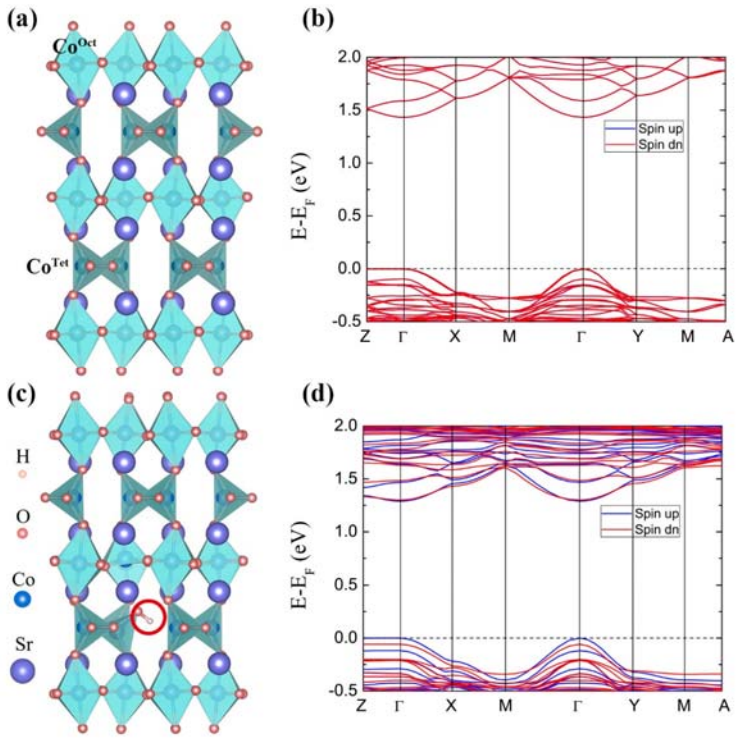




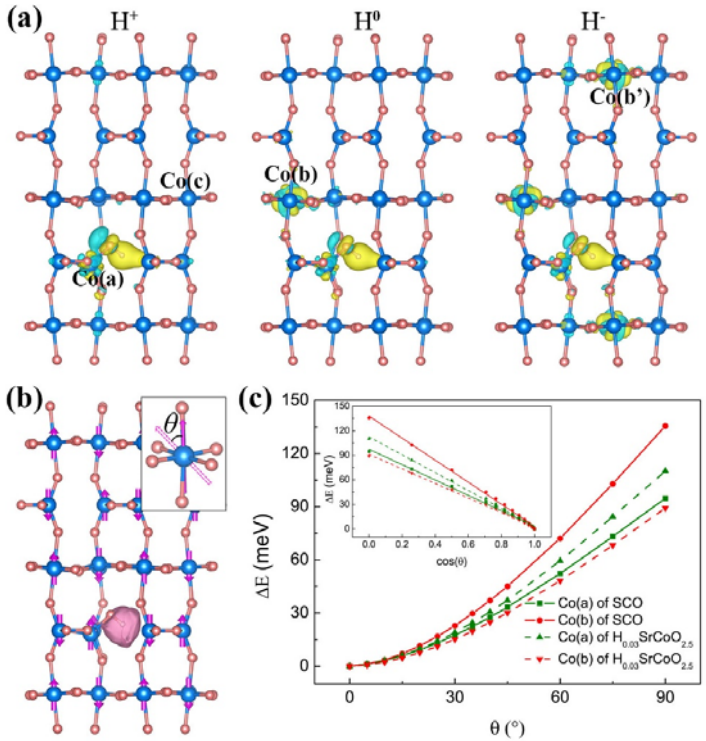
Reversible electric-field-controlled phase transformation



N. Lu, P. Yu, *et al*. Nature, 2017: 546, 124



Crystal structures of $SrCoO_{2.5}$ (a) before and (b) after H doping. Red circle marks the lowest-energy position of the interstitial H locating in the hollow channel. (c) and (d), the corresponding DFT+U band structures.



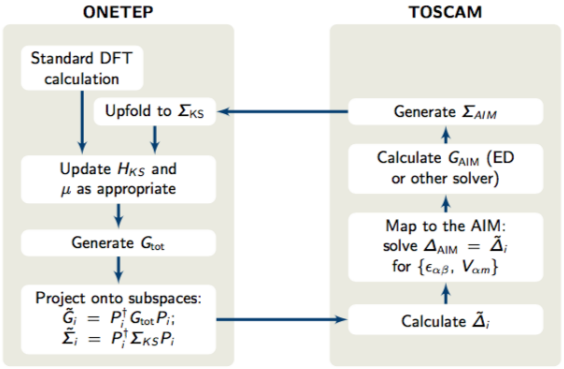
(a) Charge difference induced by an interstitial H in different charge states. (b) The electrostatic potential induced by the H+ ion. Also shown is the ground-state AFM configuration of the Co ions. (c) Change of total energy ΔE by rotating different Co sites before and after H doping. The inset shows the ΔE-cos(θ) fitting.

Thanks

Importance of Many Body Effects in The Kernel of Hemocyanin Ligand Binding

Mohamed Ali al-Badri [1], Edward Linscott[2] and Cédric Weber[1]

[1]) King's College London, Theory and Simulation of Condensed Matter (TSCM) The Strand, London WC2R 2LS, United Kingdom
mohamed.al-badri@kcl.ac.uk
[2]) Cavendish Laboratory, University of Cambridge, J. J. Thomson Avenue, Cambridge CB3 0HE, United Kingdom



We perform first-principle quantum mechanical studies of dioxygen ligand binding to the hemocyanin protein. Electronic correlation effects in the functional site of hemocyanin are investigated using a state-of-the-art approach, which treats accurately local many body effects beyond the density functional theory (DFT), where the treatment of localised copper $3d$ electrons are studied using DFT+U and Dynamical Mean Field Theory (DMFT) for the first time.

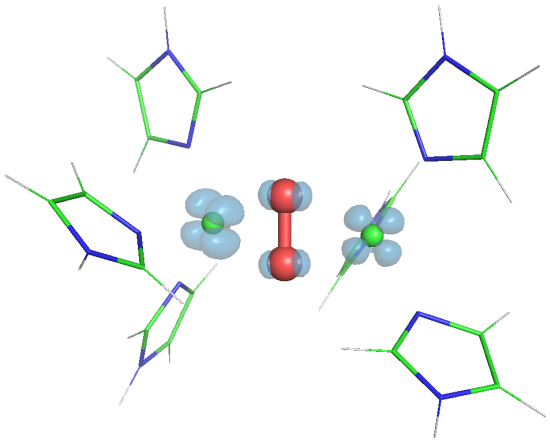
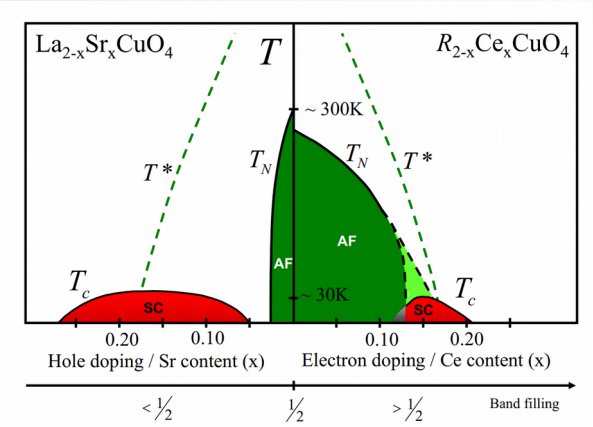
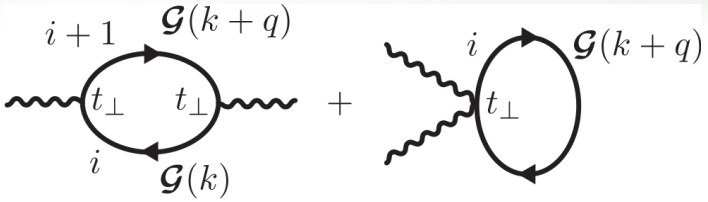


Figure 1: The side-on (μ-η^2:η^2) Cu_2O_2 'butterfly' core of Hemocyanin.

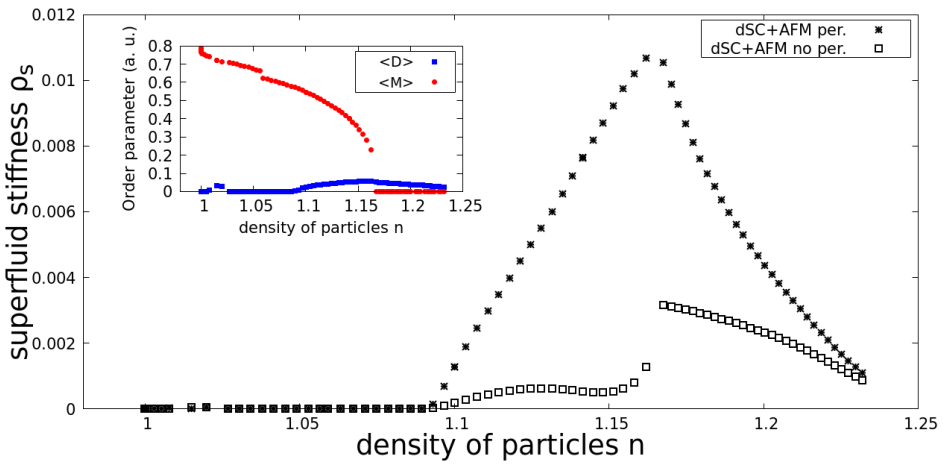
Phase competition effect on superfluid stiffness in CDMFT



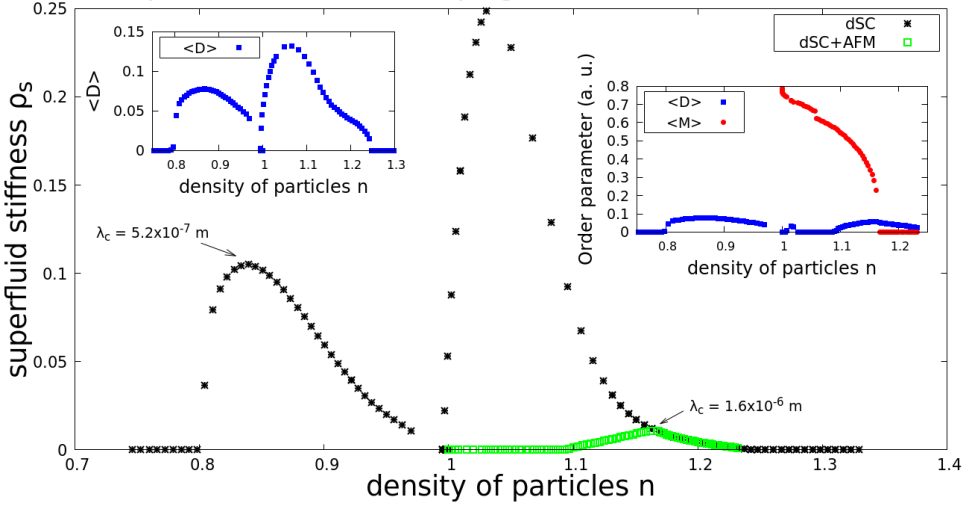


$$\hat{\mathcal{H}} = \sum_{\langle ij\rangle,\sigma} t_{ij}\left(\hat{c}^{\dagger}_{i,\sigma}\hat{c}_{j,\sigma} + \hat{c}^{\dagger}_{j,\sigma}\hat{c}_{i,\sigma}\right) + U\sum_{i}\hat{n}_{i,\uparrow}\hat{n}_{i,\downarrow} - \mu\sum_{i,\sigma}\hat{n}_{i\sigma}$$

Superfluid stiffness vs doping with AFM + dSC for U = 12t: periodization vs cluster trace



Superfluid stiffness vs doping with dSC + AFM for U = 12t



Armitage, N., RevModPhys.82.2421 (2010)

Name: Paresh Chandra Rout

Title: Predicting emergent phenomena across different epitaxial strain regions in Sr-doped double-perovskite multiferroic Bi_2FeCrO_6 thin-films

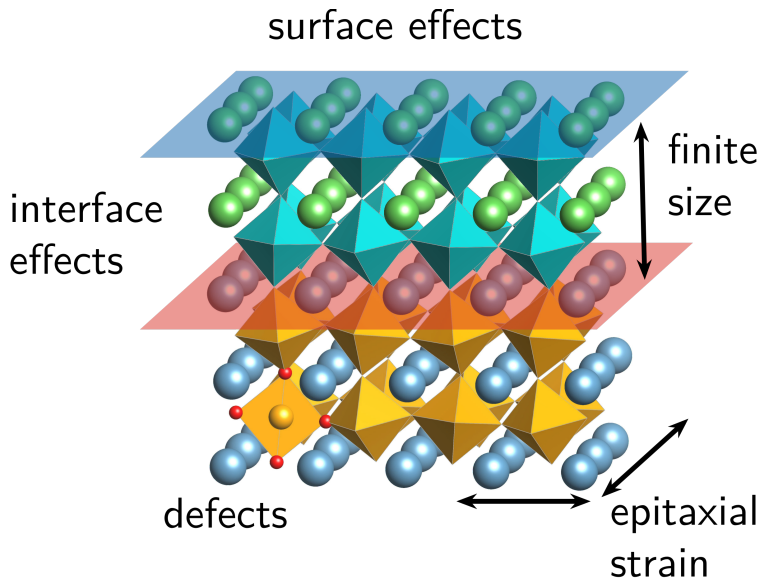
Abstract: We explore the interplay between epitaxial strain and A-site hole doping in a thin-film of Bi_2FeCrO_6 (BFCO) structure by using first-principles DFT calculations. By substituting Bi with Sr in, namely Bi2−x Srx FeCr6 (x = 1, 0.5) under epitaxial strain, we show the possibility of mitigating the existing issues like anti-site defects and low magnetism in the BFCO thin-films. While hole doping induces novel functionalities such as polar half-metal, metal-to-insulator transitions, polar-to-nonpolar structural transitions and orbital orderings, the epitaxial strain plays a role in stabilizing these phases. Our work provides a plausible route to encode novel functionalities in double-perovskite oxide thin-films.

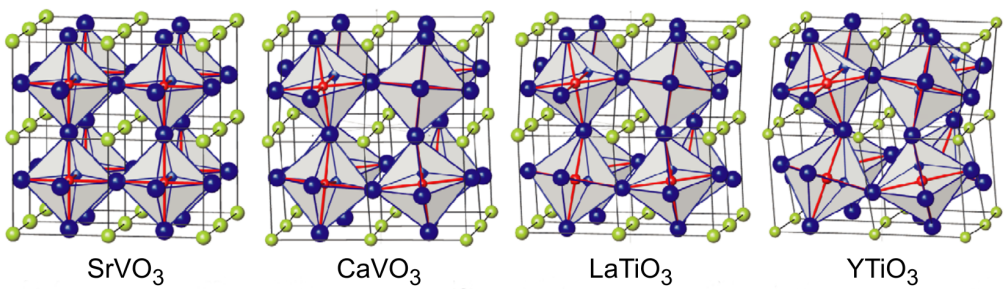
Metal-Insulator Transition in Oxide Heterostructures from DFT+DMFT

Sophie Beck & Claude Ederer, ETH Zürich, Switzerland

ETH zürich

- emerging phenomena at oxide interfaces
- "material-by-design" principle
- complex interaction between structural and electronic degrees of freedom





Pavarini *et al.*, New. J. Phys. 7, 188 (2005)

Materials:

- thin films and heterostructures of d^1, d^2 perovskites, Mott/band insulators, (correlated) metals

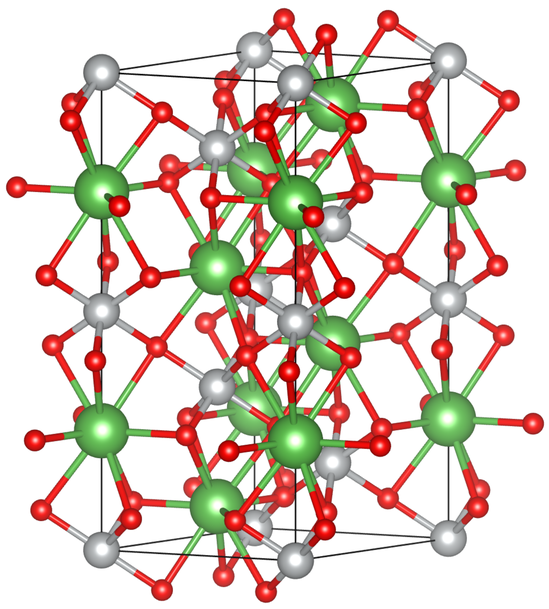
Development of computational methods for the characterization of novel strongly correlated materials

Uthpala Herath - West Virginia University, USA Email: ukh0001@mix.wvu.edu

International Summer School on Computational Quantum Materials
May 27th to June 8th
Sherbrooke, Québec

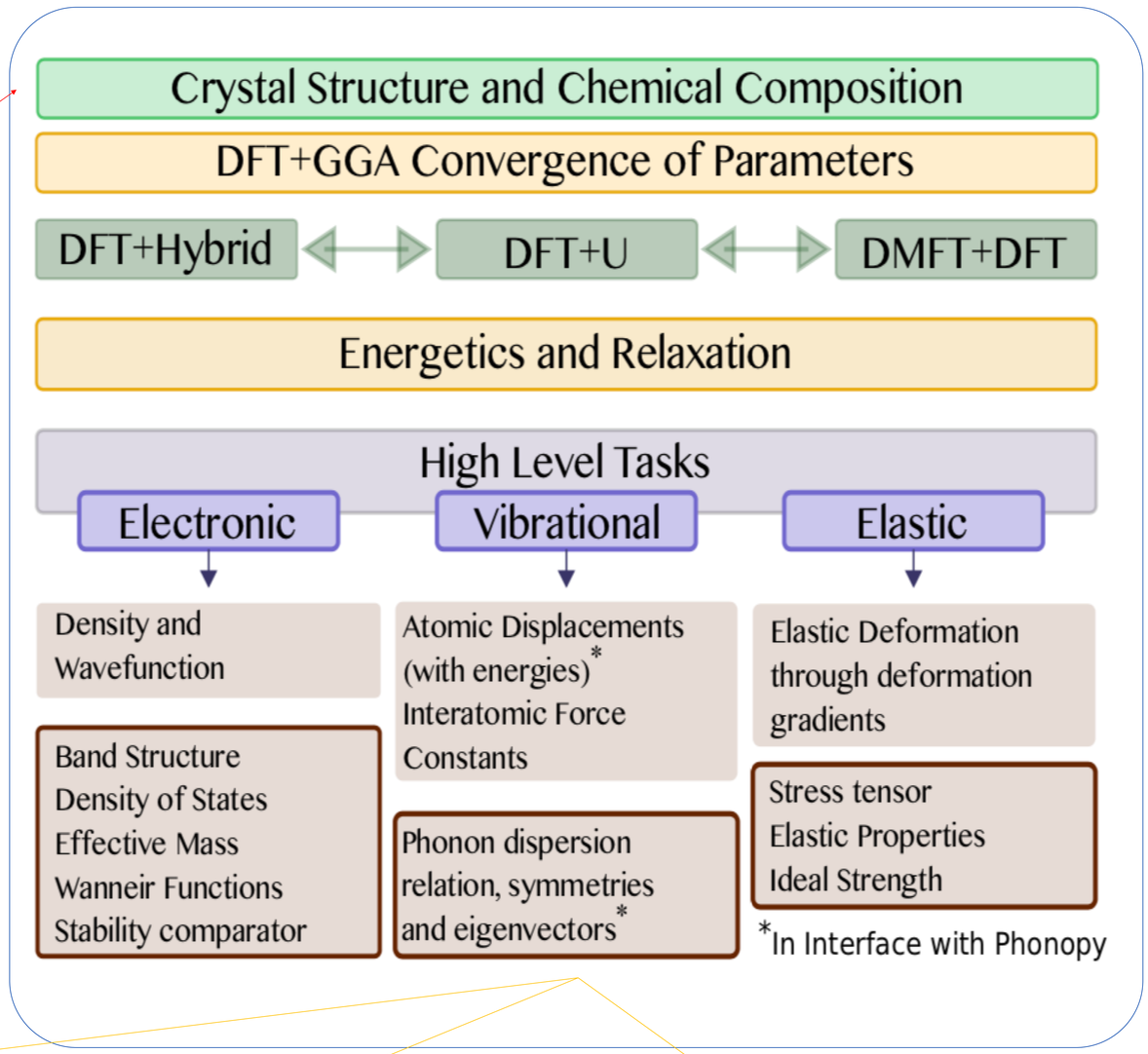
Project Goals

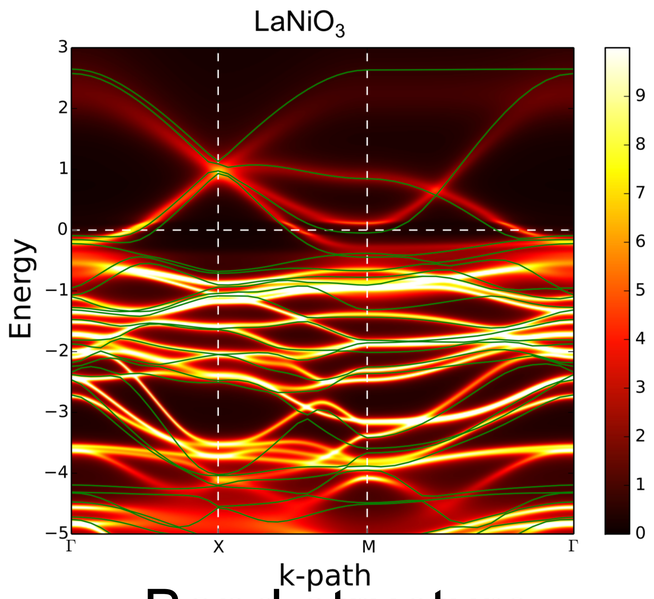
- To establish a user friendly software framework for investigating electronic, vibrational and elastic properties of strongly correlated materials using first-principles methods from DFT to DMFT.
- To investigate the evolution of strongly correlation for several complex materials such as Heusler alloys.



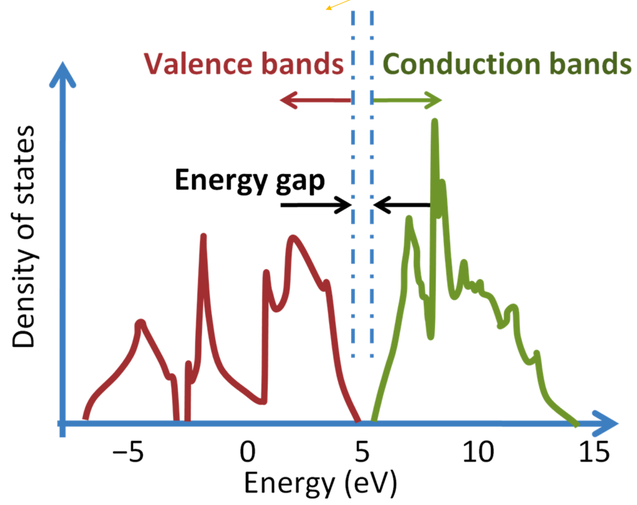
Input structure

GUI

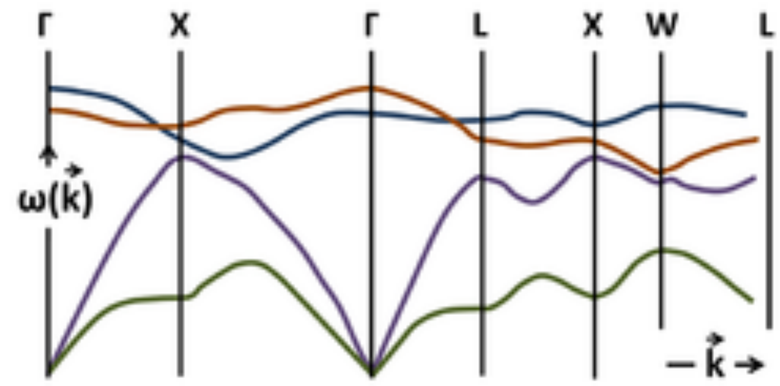




Band structure

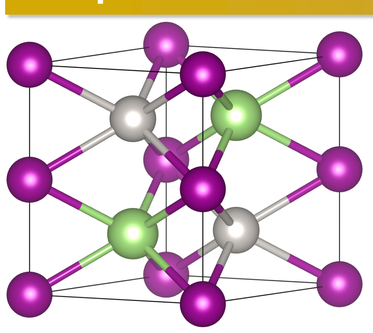


Density of States



Phonon dispersion

Proposed Materials

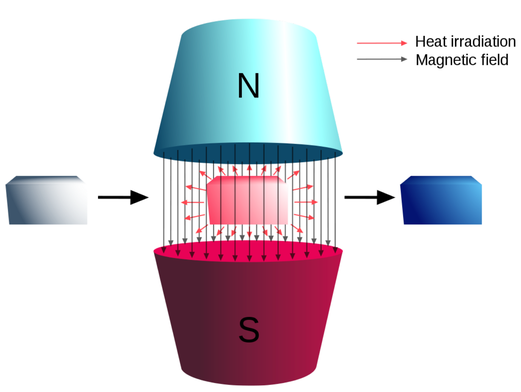


Heusler Alloy prototypes:
e.g.-

- CuMnSb
- Ni_2MnAl
- Co_2VGa
- MnFeGa
- MnPtGa

WHY?

- Interesting magnetic ordering
- Magnetic shape memory effect
- Giant magnetic caloric effect
  -> magnetic refrigeration



To be continued…

Development of computational methods for the characterization of novel strongly correlated materials

Uthpala Herath(1), Aldo H. Romero(1), Hyowon Park(2)
(1) West Virginia University , (2) University of Illinois at Chicago

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Sherbrooke, Québec

Project Goals

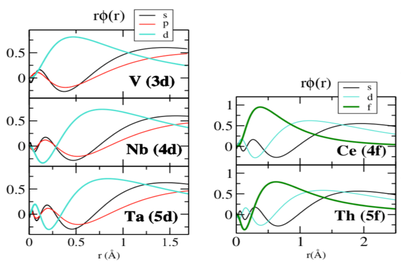
- To establish a software framework for investigating electronic, vibrational and elastic properties of stronlgy correlated materials using first-principles methods from DFT to DMFT.
- To develop a user-friendly and open-source DFT+DMFT code with various features based on effcient DFT implmentations.

Introduction

Motivation:

➢ **Strongly Correlated Materials**

- 3d,4f orbitals are localized.

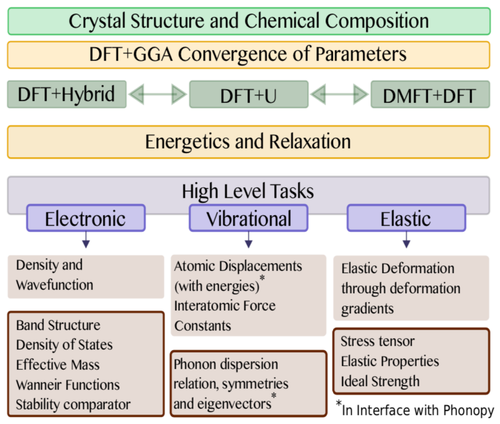


➢ **Density functional theory (DFT)**

- DFT has been a powerful first-principles method for weakly correlated materials.
- Currently available DFT codes has different interfaces for inputs, therefore it is difficult for users to take advantage of various features of different DFT codes.
- Application to the study of strongly correlated materials usually is not very accurate, therefore more advanced method beyond DFT is essential to treat the correlation problem.
- However, different choices of correlated orbitals, interaction parameters, and different levels of approximations to solve correlation problem have been the bottleneck of beyond DFT methods.

- Partial occupations of of d- and/or f- orbitals lead to strong electronic correlations.
- Novel phenomena of strongly correlated materials include magnetism, high-temperature superconductivity, colossal magnetoresistance, heavy fermion systems, metal to insulator transitions (Mott insulator), and thermo-magnetism.

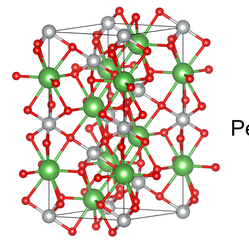
Overview:



Proposed Materials

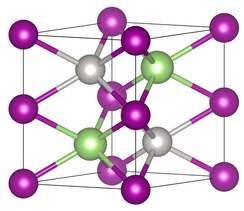
We are interested in:

- Materials with strong correlation effects to which both d- and f- orbitals can contribute ex) Gd, LaNiO3



Perovskite prototypes

- DFT+DMFT spectra can be directly compared to experimental photo-emission spectroscopy data of real systems



Heusler Alloy prototypes

Theory: Dynamical Mean Field Theory

➢ Within DFT, the correlation energy functional is crudely approximated.

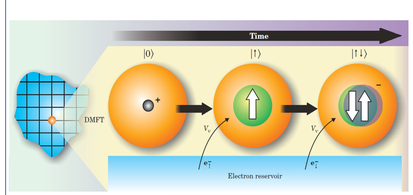
1) We do not know the exact form of the correlation energy functional.
2) The dynamical correlation effect is ignored since the DFT functional is based on a static charge density.

➢ Dynamical mean field theory (DMFT) : One defines a Free energy functional using a time-dependent and local Green's function *G*.

$$G_{i\sigma}(t-t') \equiv -\langle c_{i\sigma}(t) c_{i\sigma}^{\dagger}(t') \rangle$$

➢ Advantages of DMFT:

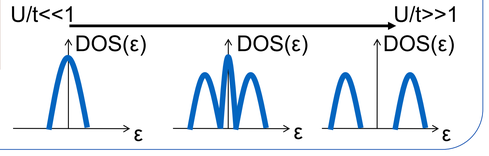
1) The lattice problem can be mapped onto a local Anderson impurity problem hybridized to a self-consistently determined bath.
2) The impurity problem can be numerically solved in a non-perturbative way using quantum Monte Carlo and capture both itinerant and localized nature of electrons.
3) The DMFT calculation scales as O(N) where N is the number of the correlated atoms while DFT scales as $O(N^3)$.



The self-consistency condition

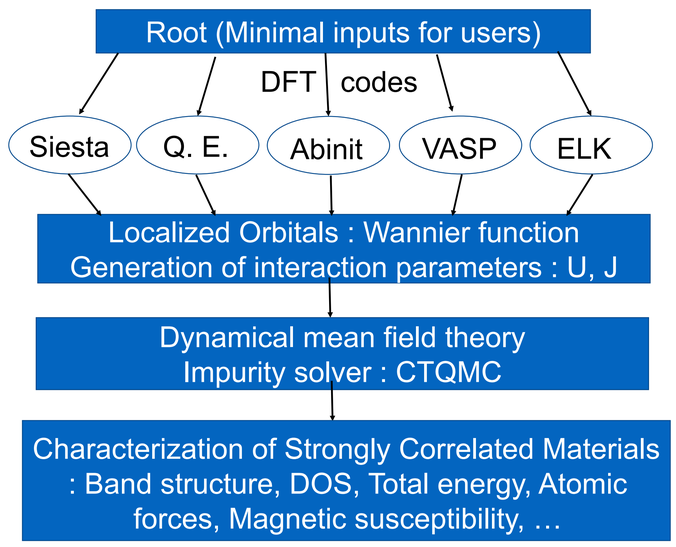
$$G[\Delta(\omega)] = \sum_{k} \{\omega - \Sigma[\Delta(\omega)] - t_k\}^{-1},$$

Hybridization: $\Delta(\omega) = \sum_{\nu} \frac{|V_\nu|^2}{\omega - \varepsilon_\nu^{bath}}$,

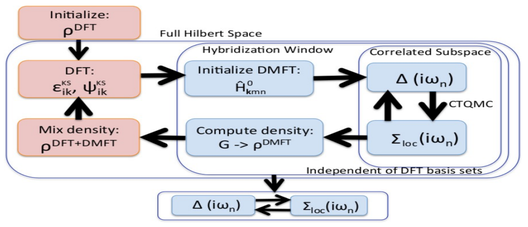


Methodology

➢ Outline of new code



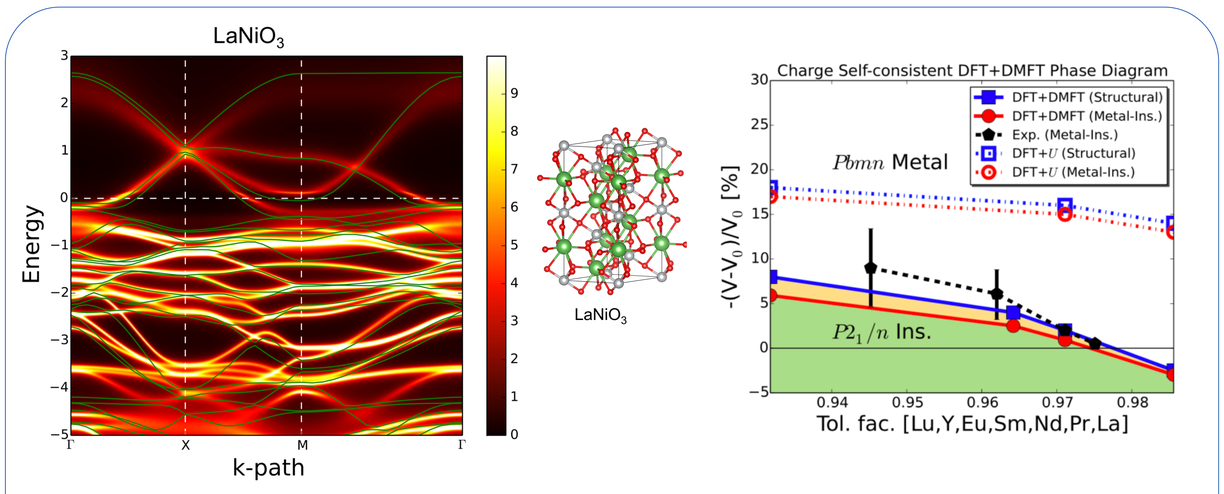
➢ Schematic flow diagram of the full charge-self-consistent DFT+DMFT



➢ Features of our DFT+DMFT code

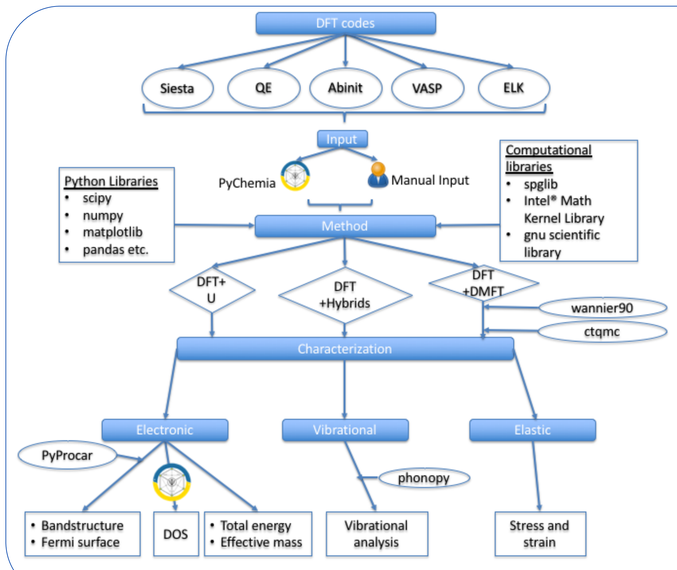
1) Various free-license DFT codes are available for DFT+DMFT simulations and same correlated basis sets (Maximally localized Wannier function) are used to obtain DMFT solutions to minimize the ambiguity of different DFT codes and to perform fair comparisons.
2) The DMFT part of the code scales linearly with the number of correlated atoms.
3) Interaction parameters U and J are obtained using the linear-response constrained DFT method.
4) Band structure, total energy, atomic force calculations are currently being implemented.
5) Other post-processing codes are also interfaced including Wannier90, phonopy,…

Proof of concept



DFT+DMFT bandstructure of $LaNiO_3$ compared to DFT bands (green) (left) and Metal-insulator and structural phase diagram computed using charge self-consistent DFT+DMFT as a function of volume and the series of rare-earth ions (right).

The interface




```
*******  Software Suite for the Characterization of Strongly Correlated Materials *******

Version: 1.0
--------------------------------------------------------------------------------

Select DFT code:
(1) VASP
(2) Siesta
(3) Abinit

Your choice:1

VASP selected.

Input method:
(1) PyChemia
(2) Manual

Your choice:1

Initializing PyChemia...
Done.
```

The structural diagram of the interface (left) and the current state of the program (top)

- The VASP+DMFT interface has been implemented.
- The interface of DMFT with Siesta, QE, Abinit and ELK is currently being implemented.
- A GUI version of the program will be implemented in the future.

Conclusions

- DFT is not suitable for studying electronic structure and energetics of strongly correlated materials.
- DFT+DMFT has been a powerful method but existing implementations are based on licensed DFT codes such as Wien2K.
- We implement a user-friendly and public DFT+DMFT code based on various free-licensed DFT programs by adopting the Wannier function as correlated orbitals.
- Our implementation can be linearly scalable (O(N)) for large-scale correlated systems by interfacing DMFT to efficient DFT codes such as Siesta.

Future work

- Implementation of the interatomic forces [5,6] within DFT+DMFT and extend the functionality to calculate phonons and stress of strongly correlated materials.
- Two-particle susceptibility calculations including the optical conductivity and the magnetic susceptibility.
- Fermi surface calculations.

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Acknowledgements

This work was supported by the NSF OAC-1740111 and DOE DE-SC0016176 projects

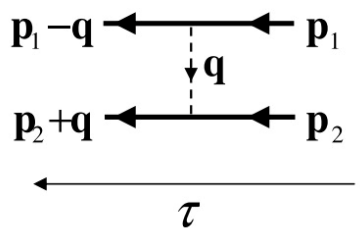
UNIVERSITY OF WATERLOO

Wen Jin

Diagrammatic Monte Carlo technique for frustrated spin system

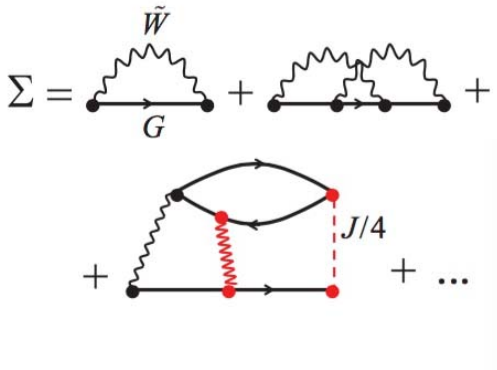
Simulation of diagrams

Rather than evaluating integrals over internal variables for each diagram, one samples their momenta, time and expansion orders stochastically (Markov-chain).



K. Van Houcke et al., Physics Procedia 6, 95-105 (2010).

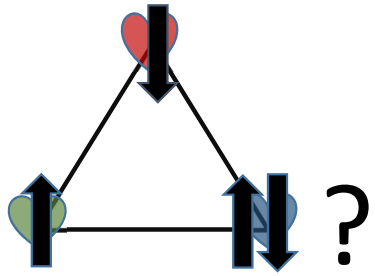
Feynman diagram



S. A. Kulagin et al., Phys. Rev. B 87, 024407 (2013).

Magnetic frustration

- Large degeneracy
- Exotic magnetic state: quantum spin liquid
- Very rich behavior



Ab initio study of cross-interface electron-phonon couplings in FeSe thin films on $SrTiO_3$ and $BaTiO_3$

Yan Wang,[1,2] A. Linscheid,[3] T. Berlijn,[4] and S. Johnston[2]

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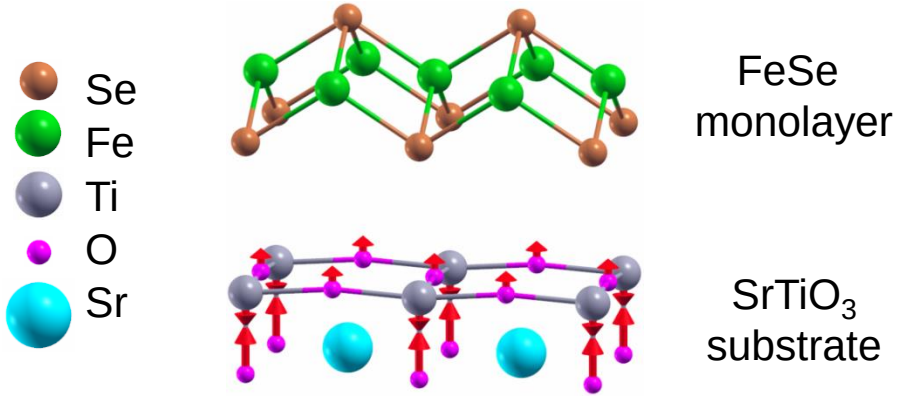
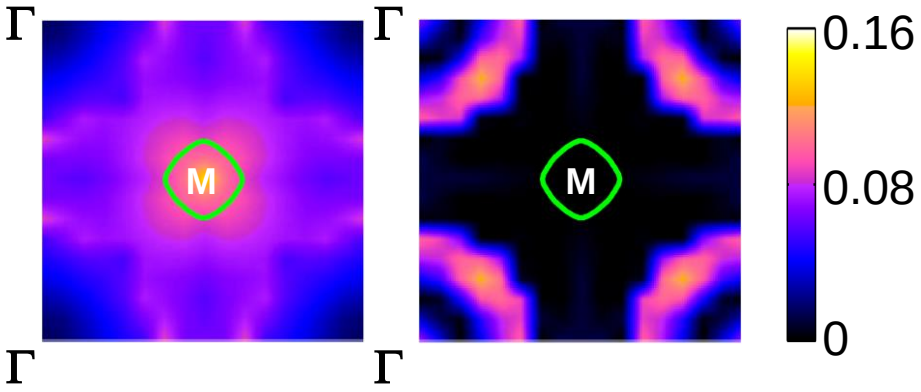
2 Department of Physics and Astronomy, University of Tennessee, Knoxville, Tennessee 37996, USA

3 Department of Physics, University of Florida, Gainesville, Florida 32611, USA

4 Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA

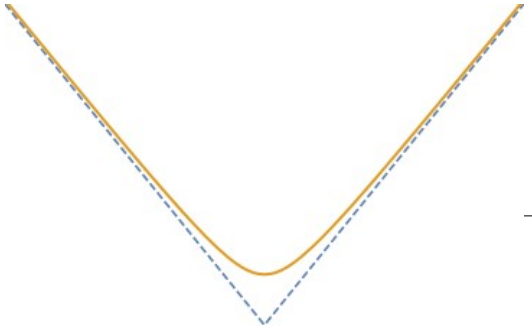


Red arrows: atomic displacements for the oxygen polar mode mode ($\Omega \sim 100$ meV) at $\mathbf{q} = (0,0)$.

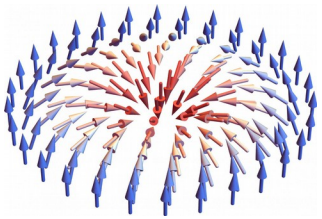


Coupling function $|g(\mathbf{k},\mathbf{q})|^2$ in the first Brillouin zone as a function of $\mathbf{k}$. Left: $\mathbf{q} = (0,0)$. Right: $\mathbf{q} = (0,\frac{\pi}{64})$ and $400 \times |g(\mathbf{k},\mathbf{q})|^2$.

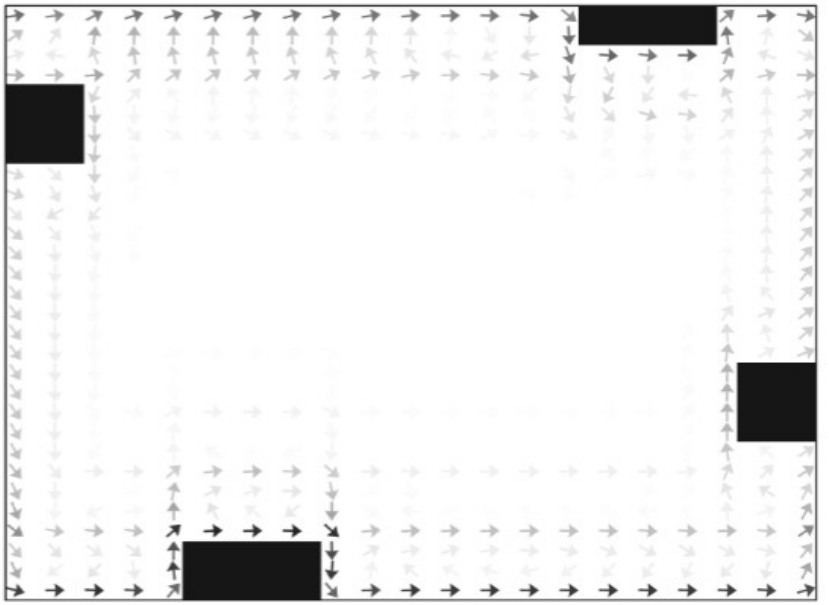
- Monolayer FeSe thin film on STO or BTO substrates has superconducting $T_c \sim 60 - 70$ K.
- *Replica energy bands* seen in ARPES spectra indicate a strong forward-focused electron-phonon coupling $g(\mathbf{k},\mathbf{q})$ peaked at small $|\mathbf{q}|$.
- We find from *ab initio* calculation that for the oxygen polar mode with mode energy $\Omega \sim 100$ meV, $g(\mathbf{k}, |\mathbf{q}| > \frac{\pi}{64}) \approx 0$, consistent with a forward-focused electron-phonon coupling.



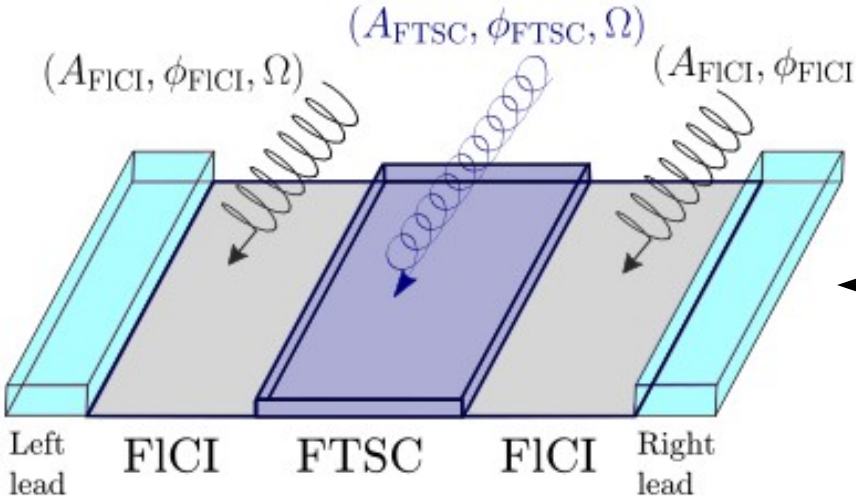
Gapped superconductor



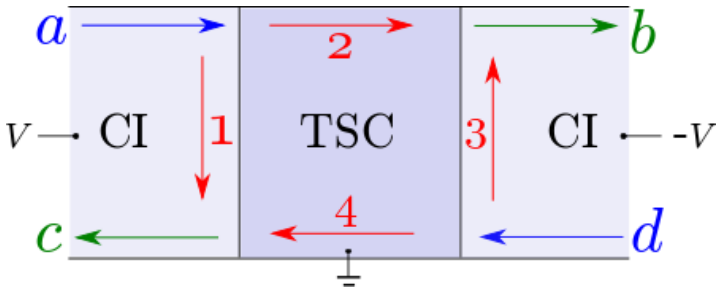
Chern number $\neq 0$



Robust edge excitation



Transport signatures of photoinduced topological superconductor heterostructure ?



$$\sigma = \frac{1}{2}\frac{e^2}{h}$$

Half-quantized longitudinal conductance

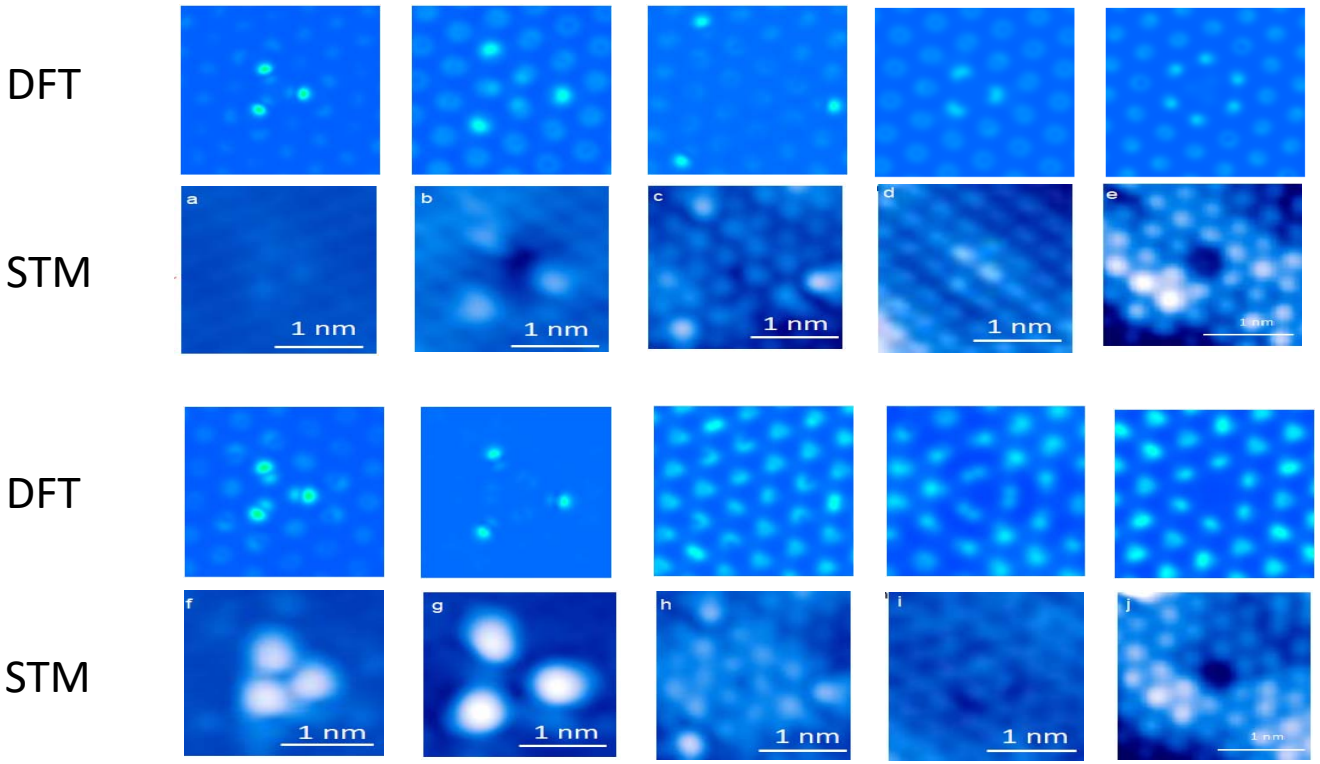
$$\gamma = \gamma^\dagger$$

Self-Hermitian Majorana

Identification of intrinsic surface defects in a thin $PtSe_2$ film from first-principles

Yichul Choi, Fazel Baniasadi, Husong Zheng, Chenggang Tao, and Kyungwha Park

Department of Physics, Virginia Tech



VIRGINIA TECH

Theoretical Prediction of Oxygen-functionalized Mixed MXene as Topological Insulator

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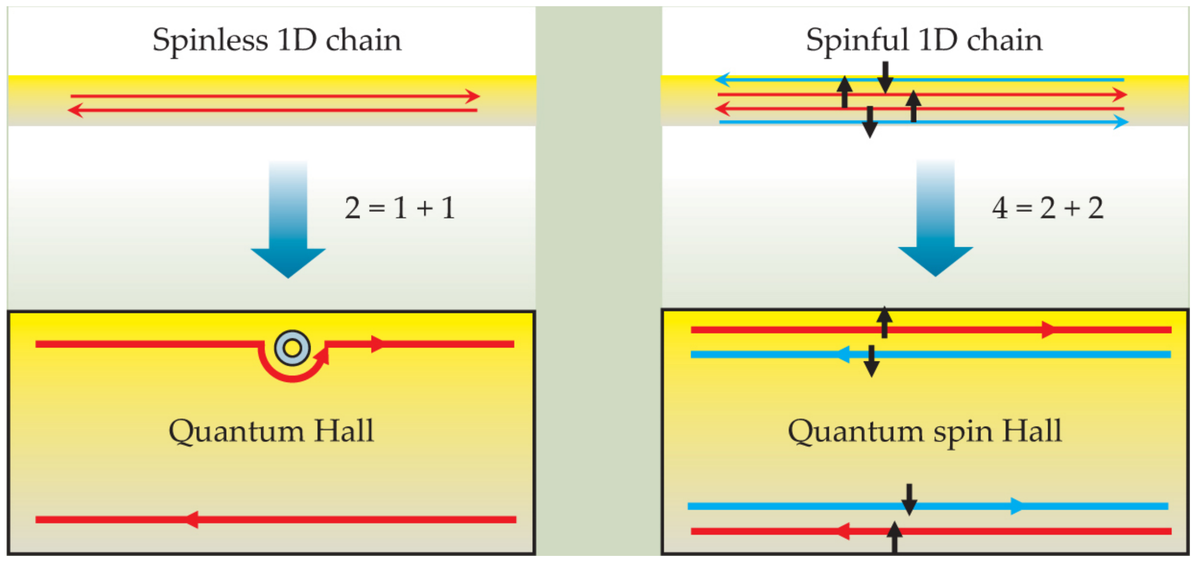
Department of Mechanical Engineering, Carnegie Mellon University
Email: *azeeshan@cmu.edu, +venkvis@cmu.edu

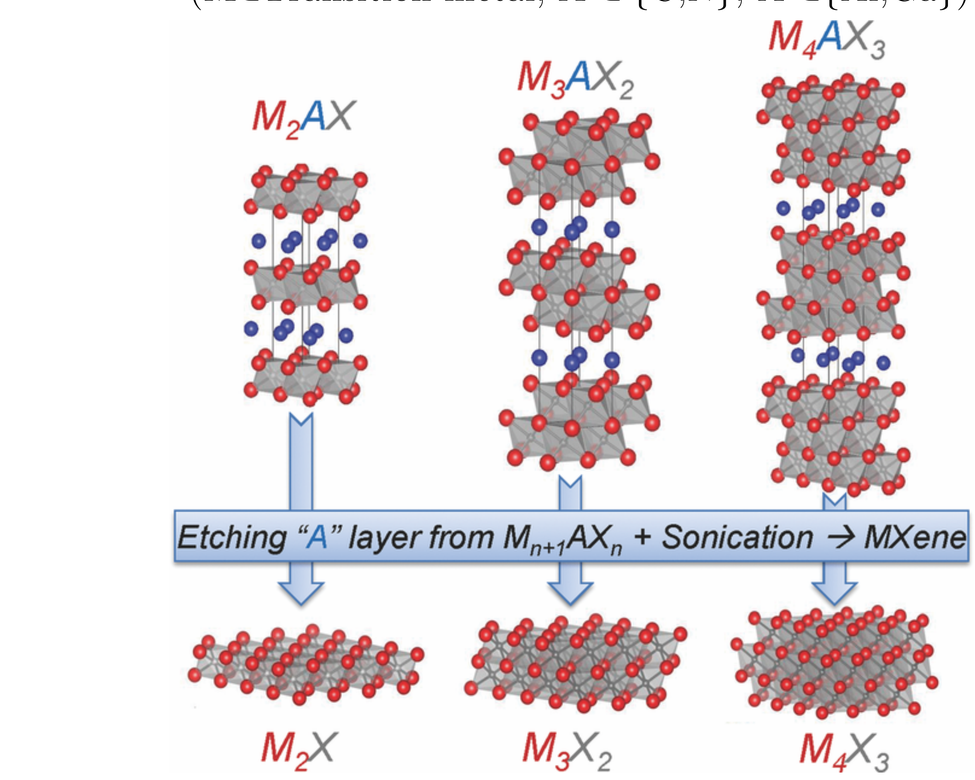
INTRODUCTION

Quantum Spin Hall Effect[1]

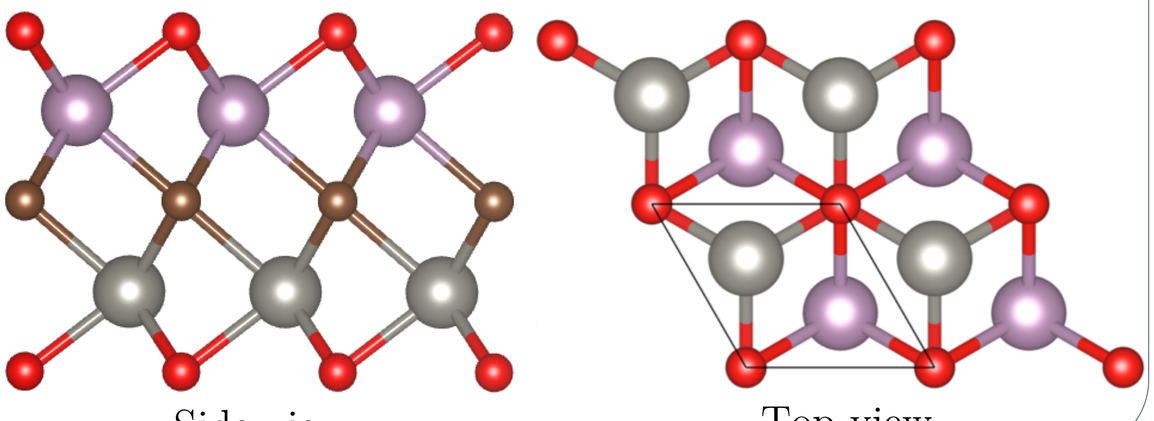


- 2D gapped phases characterized by a $\mathbb{Z}_2$ invariant which distinguishes a topological from a trivial insulator
- Bulk energy gap but gapless edge states protected by time reversal symmetry
- First proposed using the Kane-Mele model: two copies of the Haldane model for up and down spin
- Zero charge-Hall conductance but finite spin-Hall conductance
- Z2pack computes topological invariant based on evolution of hybrid Wannier functions, equivalent to the computation of the Wilson loop

MXenes: Layered MAX phases exfoliated into 2D single/multilayers (M∈Transition metal, X ∈ {C,N}, A ∈{Al,Ga})[2]

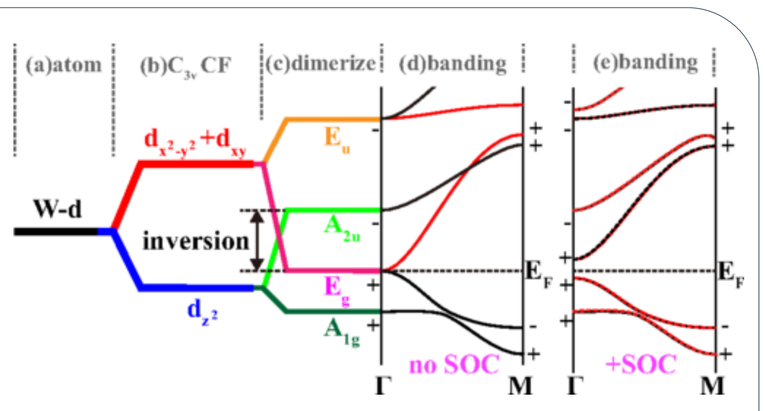


Structure of Oxygen-functionalized MoWCO2: A layer of C atoms (brown) is surrounded by a top layer of W atoms (pink) and a bottom layer of Mo atoms (gray). The red atoms are oxygens as functional group attached to M_1M_2Xene

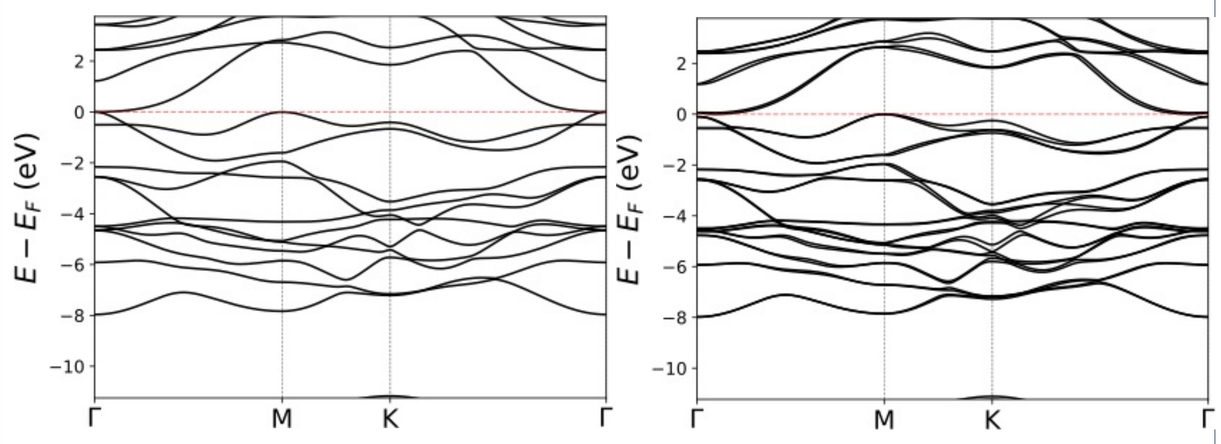


Side view Top view

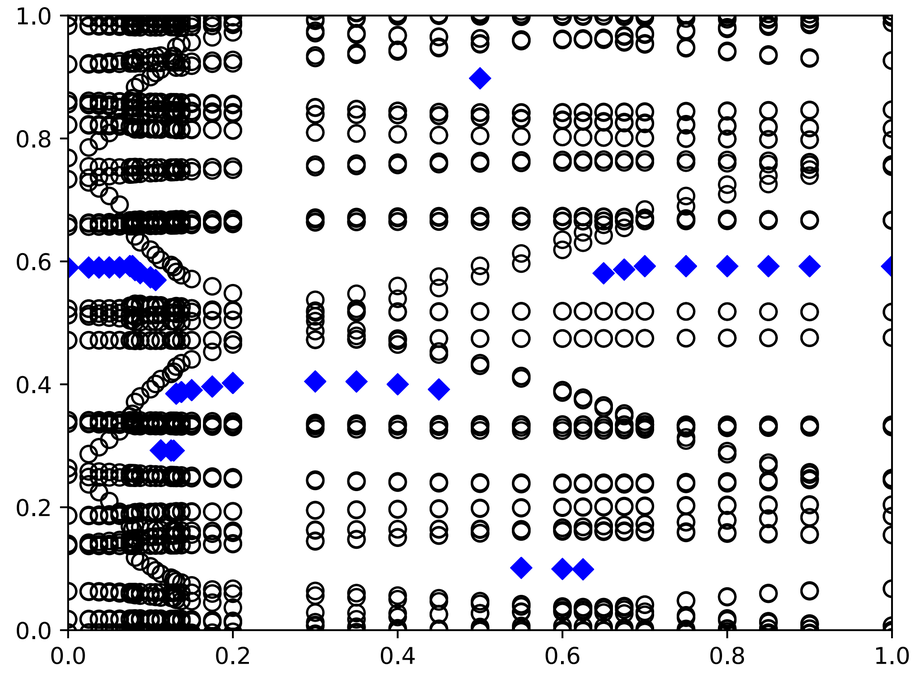
Band inversion among Tungsten d orbitals in W_2CO_2 (Ref. 3)



RESULTS



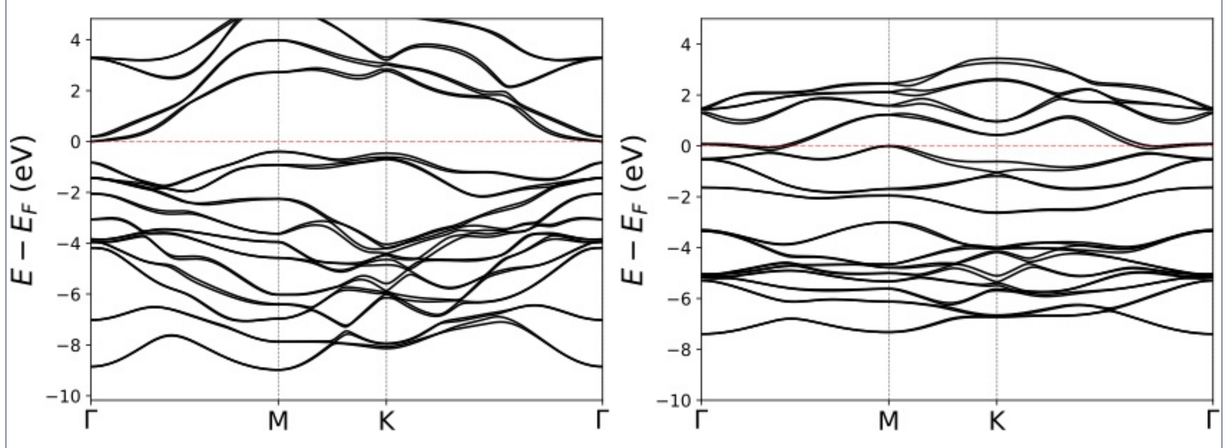
Band structure without SOC Band structure with SOC



Movement of the Wannier Charge Center

Effect of strain

-10% strain +10% strain



Phase Transition from Topological to Trivial Insulator

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4. Weng, Hongming, et al., Phys. Rev. B 92, 075436 (2015).

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