UNIVERSITÀ DI PAVIA

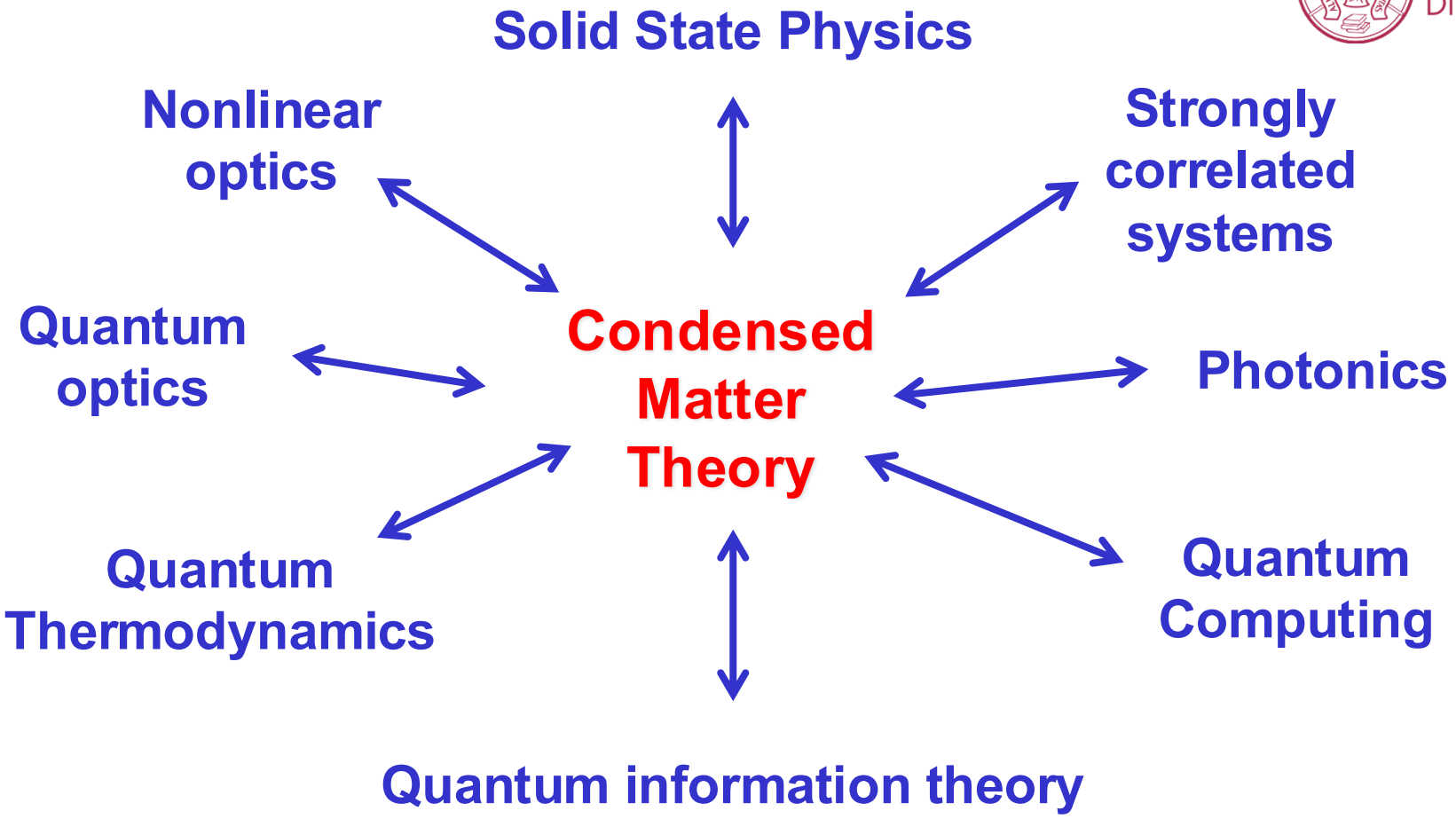
Fisica Teorica della Materia
Condensed Matter Theory

Dipartimento di Fisica «Alessandro Volta»

Istituto Nazionale di Fisica Nucleare

Consiglio Nazionale delle Ricerche

Congresso del Dipartimento di Fisica «A. Volta» & INFN – 17/02/2026


Solid State Physics
Nonlinear optics
Strongly correlated systems
Quantum optics
Condensed Matter Theory
Photonics
Quantum Thermodynamics
Quantum Computing
Quantum information theory

Research Lines & Coordinators

UNIVERSITÀ DI PAVIA

Advanced Quantum Mechanics & Quantum Info

Chiara Macchiavello

Lorenzo Maccone

Massimiliano Sacchi (CNR)

Giacomo Guarnieri

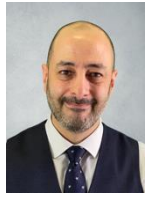
First principles condensed matter theory

Matteo Cococcioni

Quantum Photonics and Nanostructures

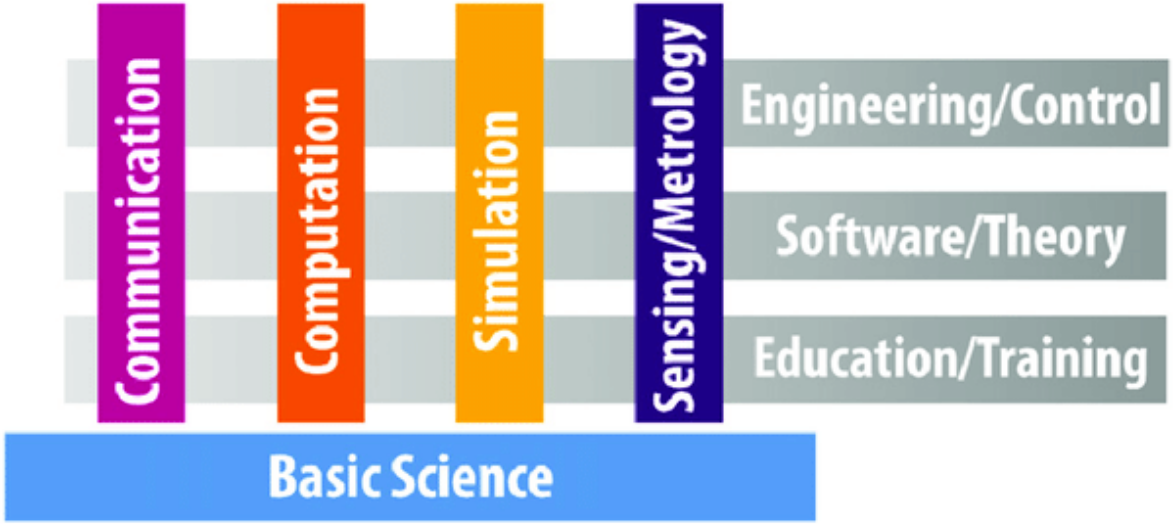
Lucio Andreani

Dario Gerace



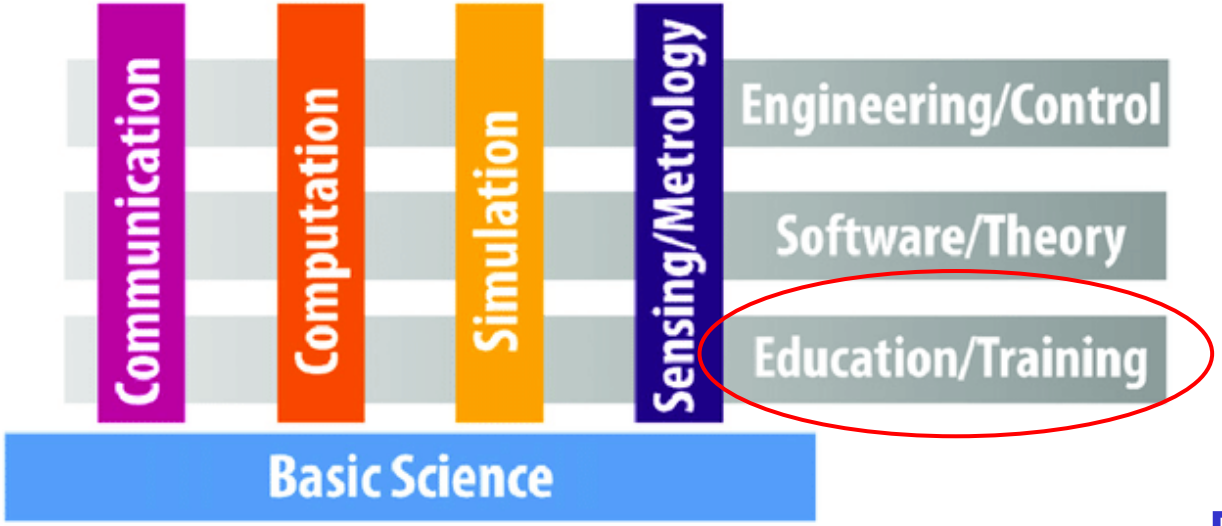
Marco Liscidini

All the related applications in Quantum Technologies



The quantum technologies roadmap: a European community view, New J. Phys. **20**, 080201 (2018)

All the related applications in Quantum Technologies



The quantum technologies roadmap: a European community view, New J. Phys. **20**, 080201 (2018)

LM curricula:

Fisica della Materia

Fisica delle Tecnologie Quantistiche

Lucio Andreani

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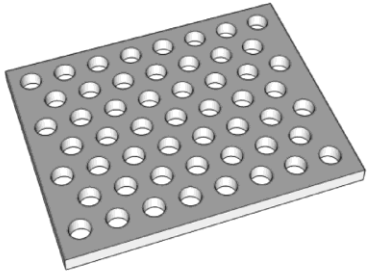
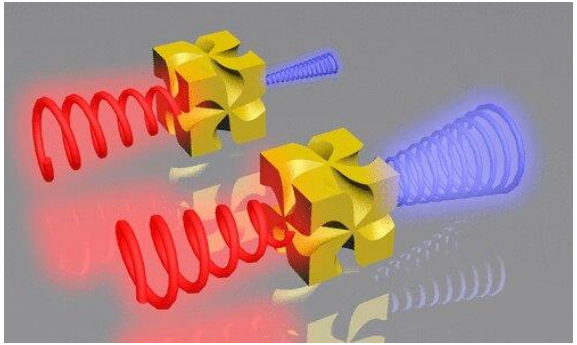
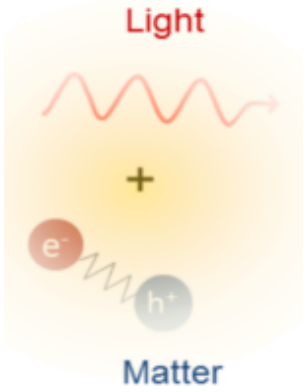
Photonic crystal slabs and metasurfaces



Chiral and topological photonics



Light-matter interaction, exciton and polaritons
(= half wave, half matter: mixed modes of the electromagnetic field and of a material excitation)



Expt and applications: quantum, silicon photonics, optoelectronics

& development of computational methods: optimization, inverse design…

Recent highlights

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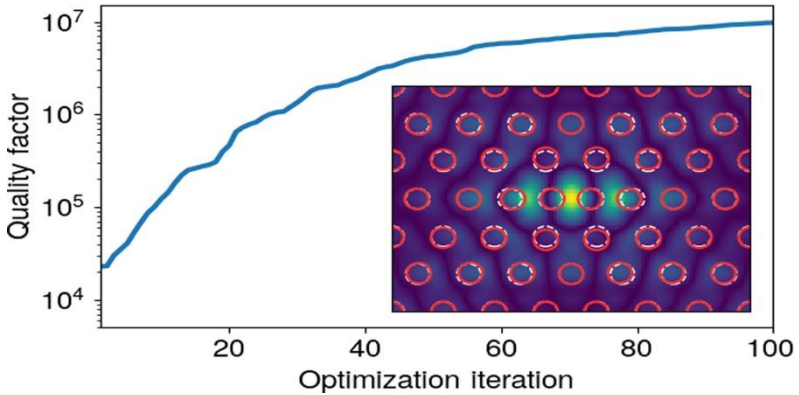
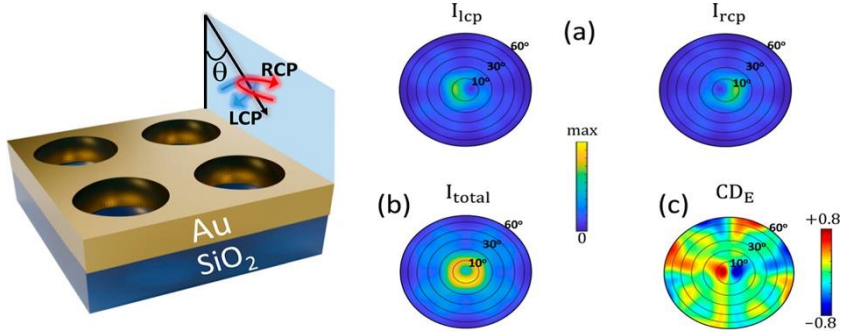
Legume: A guided-mode expansion method for photonic crystal slabs for inverse design and light-matter interaction



Poster no 11 (day 1)

Boosting Chirality with Bound States in the Continuum in Plasmonic Metasurfaces



Posters no 64 & 78 (day 2)

with various colleagues: D. Gerace, S. Zanotti, H. Ali, G. Pellegrini, F. Marabelli, F. Floris…

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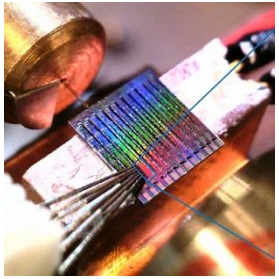
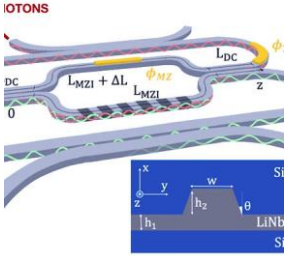
Marco Liscidini

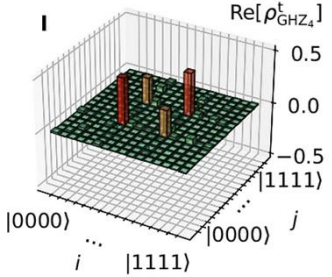
NQSTI
National Quantum Science and Technology Institute



Classical and quantum nonlinear photonics

Light-matter interaction integrated photonic systems





Generation and characterization of quantum states

liscidini.com

Quantum fluids of light

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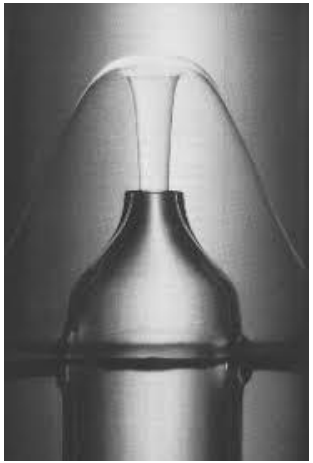
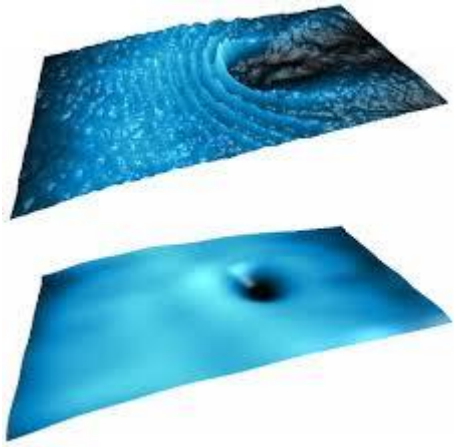
- **Emulating the physics of quantum fluids with optical systems**

classical fluid



superfluid He



superfluid light

- **new physics arising from driven-dissipative nature of photonic systems**

Quantum fluids of light, Rev. Mod. Phys. **85**, 299 (2013)

Condensation from a photonic crystal BIC

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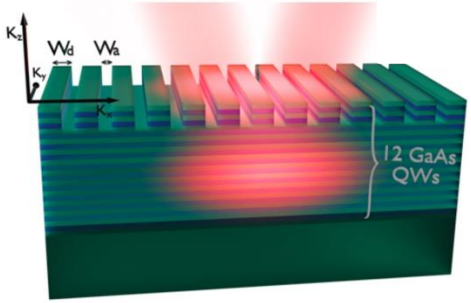
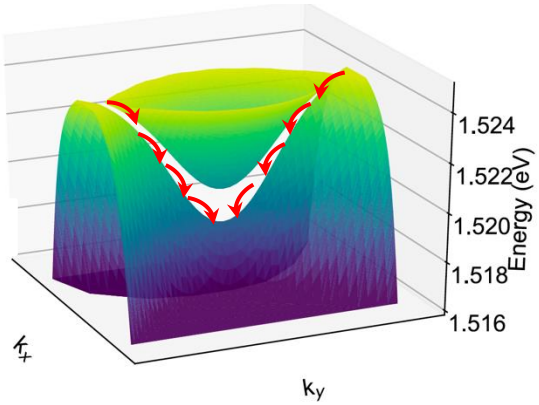
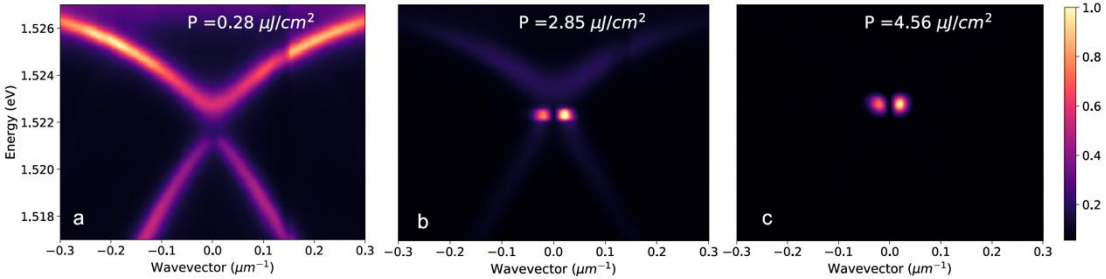
Symmetry-protected BICs at Γ are supported by 1D gratings



2D lower polariton branches



< threshold **@ threshold** **> threshold**



Ardizzone et al., Nature **605**, 447 (2022)

Nigro & Gerace, PRB **108**, 085305 (2023)

Riminucci et al., PRL **131**, 246901 (2023)

Collaboartion with CNR-Nanotec

Recent highlights

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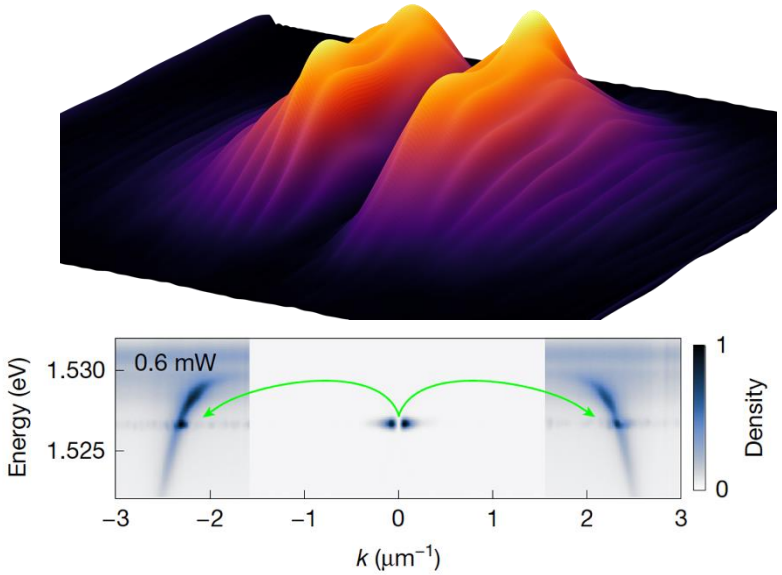
D. Nigro, D. Trypogeorgos, A. Gianfrate, D. Sanvitto, I. Carusotto, D. Gerace, *Supersolidity of Polariton Condensates in Photonic Crystal Waveguides*, Phys. Rev. Lett. **134**, 056002 (2025)



D. Trypogeorgos et al., *Emergent supersolidity in Photonic Crystal Polariton Condensates*, Nature **639**, 337 (2025)

Collaboartion with CNR-Nanotec

Quantum nonlinear interferometers

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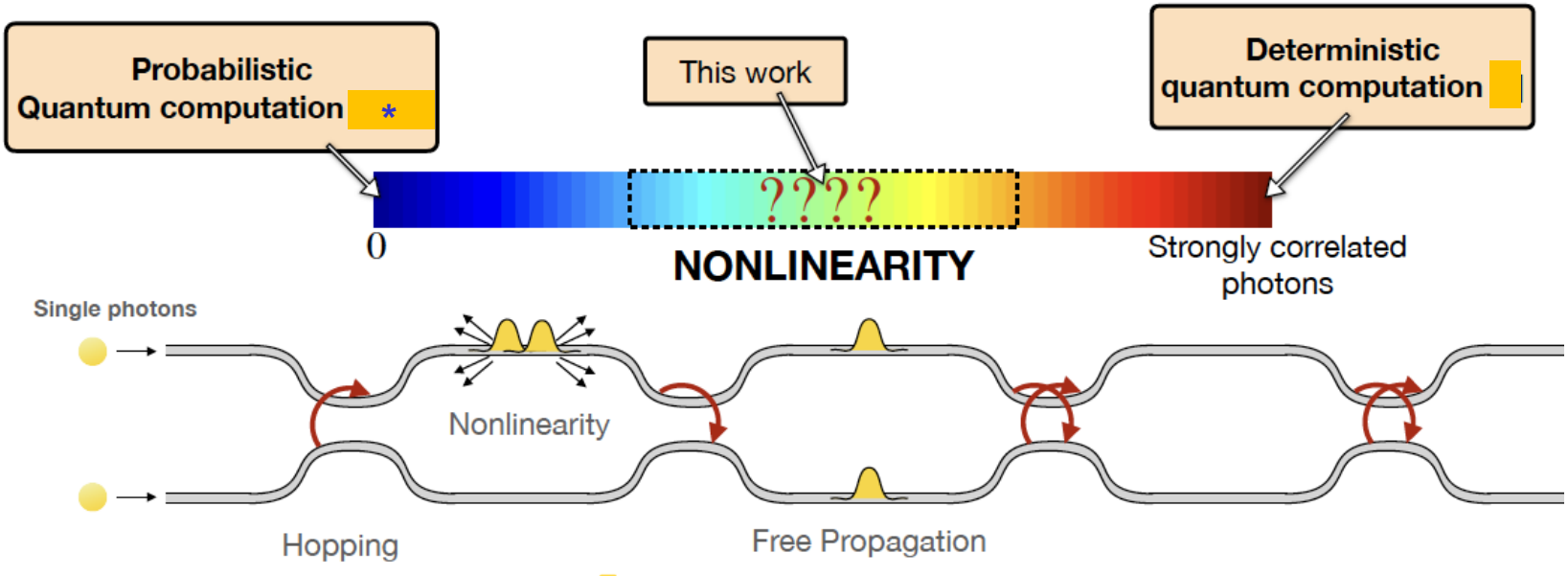

Current students involved: Davide Rinaldi (PhD)
Antonio Martucci (Master)
Matilde Miccoli (Master)

* KLM (Knill-Laflamme-Milburn) paradigm

Recent highlights

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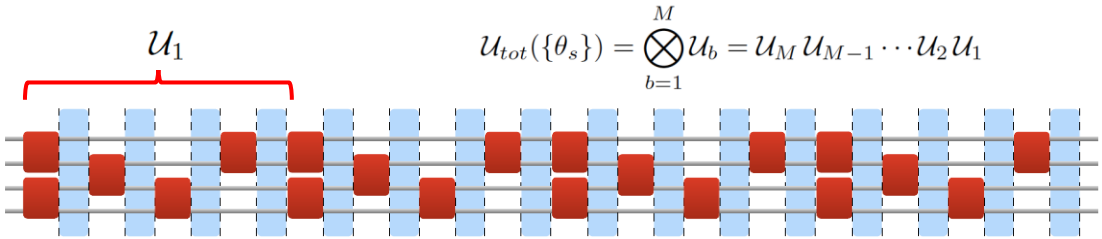
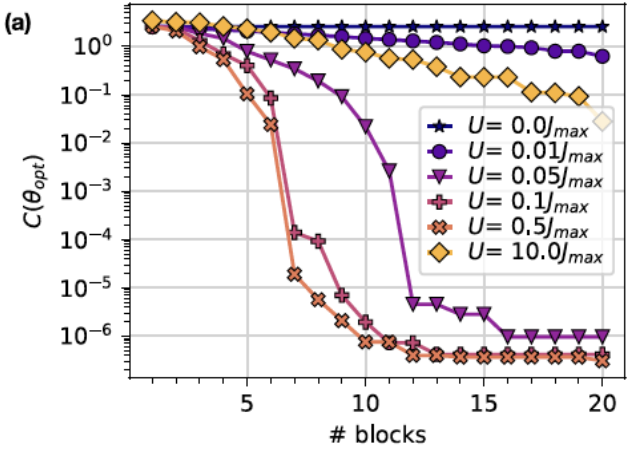
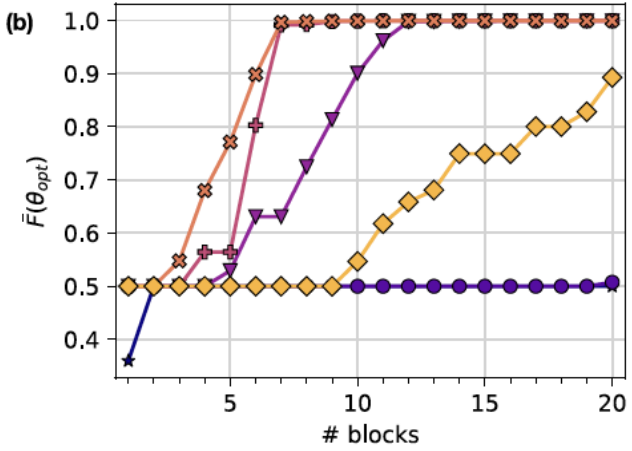


cost function → $C(\{\theta_s\}) = \sum_{i,j\in S} |\mathcal{U}_{tot}(\{\theta_s\})_{i,j} - \mathcal{T}_{i,j}|^2$

gate fidelity → $\bar{F}(\{\theta_s^{opt}\}) = \frac{1}{|S|}\sum_{i\in S} |\langle i|\mathcal{U}_{tot}^{\dagger}(\{\theta_s^{opt}\})\mathcal{T}|i\rangle|^2$





Scala, Nigro, Gerace,
"*Deterministic entangling gates with nonlinear quantum photonic interferometers*"
Communications Physics **7**, 118 (2024)

Quantum computers as a digital quantum simulators

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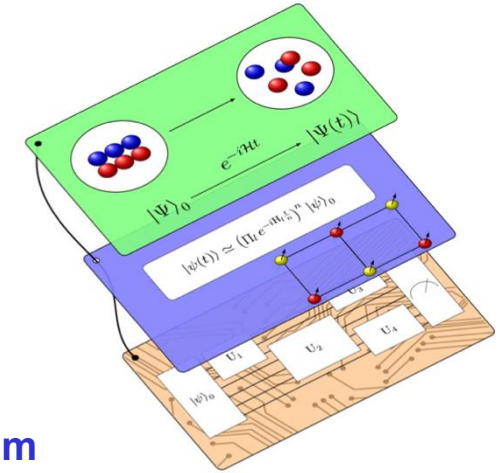
Most physical models can be expressed as sum of local terms

$$\hat{\mathcal{H}} = \sum_k^L \hat{\mathcal{H}}_k$$

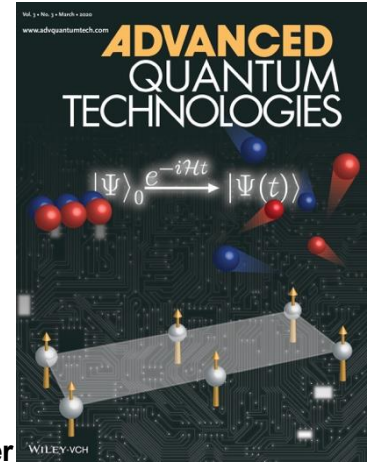


QC as a programmable device that uses quantum mechanics to simulate any such model efficiently

→ New frontier for CM theory

F. Tacchino, A. Chiesa, S. Carretta, D. Gerace,
review on *Quantum Computers as universal quantum simulators*
Adv. Quant. Tech. **3**, 1900052 (2020)

Front Cover



Quantum simulations & Quantum Machine Learning

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- **Adiabatic quantum state preparation on quantum hardware**
- **Digital quantum simulation of Lattice Gauge Theories**
- **Digital quantum simulation of Hubbard models on a lattice**
- **Resource-efficient quantum algorithm for linear systems of equations**

See Poster n. 46, A103

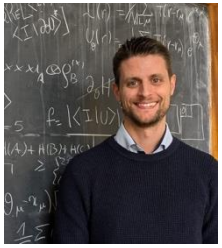
Cugini, Nigro, Bruno, Gerace, Phys. Rev. Research **7**, L012074 (2025)

Cugini, Guarnieri, Motta, Gerace, arXiv preprint arXiv:2505.13717 (to appear 2026)

Ghisoni, Scala, Bajoni, Gerace, arXiv preprint arXiv:2409.08929 (to appear in PRA, 2026)

Current students involved: Davide Cugini, Francesco Ghisoni (PhD)

Alice Montemezzani (Master)



GIACOMO GUARNIERI

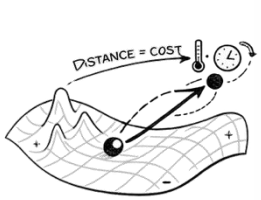
With many collaborators @UNIPV, e.g. Dario Gerace, Marco Liscidini, Chiara Macchiavello, Lorenzo Maccone, Massimiliano Sacchi, Davide Rinaldi, Davide Cugini, Gaia Candreva, Emanuele Tumbiolo, Luca Razzoli, Giovanni Chesi

UNIVERSITÀ DI PAVIA

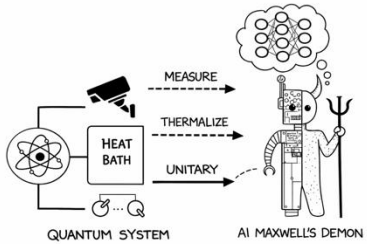
MAIN RESEARCH LINES

❖ Quantum Thermodynamics of Precision

Ultimate limits and optimal control protocols that connect information, measurements and feedback to dissipation and fluctuations; stochastic trajectory analysis of work, heat and entropy production.



QUANTUM THERMODYNAMIC GEOMETRY



QUANTUM SYSTEM AI MAXWELL'S DEMON

❖ Quantum Maxwell's demon with finite resources

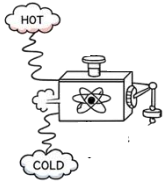
Fundamental bridge between Thermodynamics and Information Theory, including the role of measurements, of quantum coherence and engagement and of finite resources.

❖ Quantum thermal machines, refrigerators and thermometers

Models and strategies to estimate the efficiency of quantum thermal machines and thermodynamic parameters such as temperature.

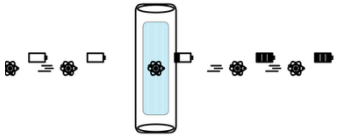
❖ Collision models and quantum batteries

Microscopic and stroboscopic descriptions of open quantum systems, applied to optimal energy storage and extraction in the paradigm of quantum batteries.



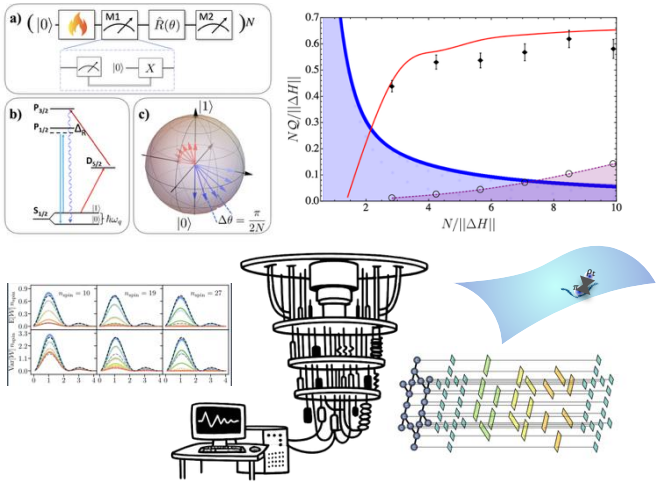
QUANTUM HEAT ENGINE / REFRIGERATOR

QUANTUM THERMOMETER


QUANTUM BATTERY

RECENT HIGLIGHTS

THE IMPACT OF QUANTUM SIGNATURES IN QUANTUM THERMODYNAMICS



H. Miller, G.G. et al, **PRL** 125, 160602

H. Miller, …, G.G. **PRL**126, 210603 ; **PRE** 103, 052138

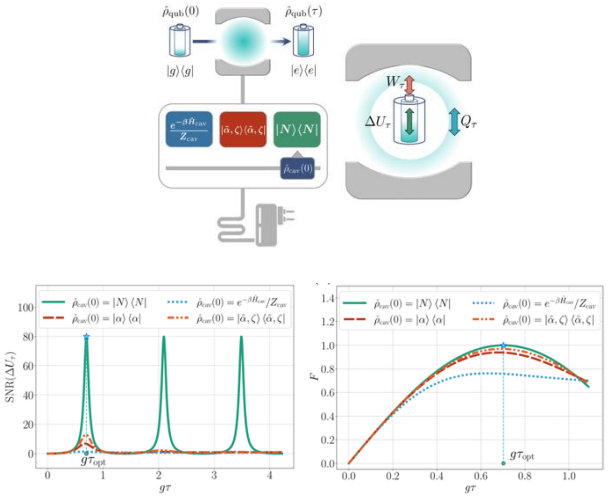
G.G. , J. Eisert, H. Miller , **PRL** 133, 070405

O. Onishchenko & G. G., et al. **Nat. Comm**. 15 (1), 6974

M. Motta, …, G.G. , **PRL** 135, 180601

POSTER 45 (day 1)

GENUINE QUANTUM ADVANTAGES IN QUANTUM BATTERY CHARGING



D. Rinaldi, R. Filip, D. Gerace, G.G. **PRA** 112, 012205

D. Rinaldi, R. Filip, D. Gerace, G.G. **arXiv** 2601.12183

POSTER 94 (day 2)

UNIVERSITÀ DI PAVIA

Quantum information theory

Research areas:

Quantum computation

Quantum machine learning

Quantum communication

Quantum metrology

Fundamental concepts

Quantum thermodynamics

Team:

Chiara Macchiavello, Lorenzo Maccone, Massimiliano Sacchi

Giovanni Chesi, Giacomo Guarnieri, Davide Poderini

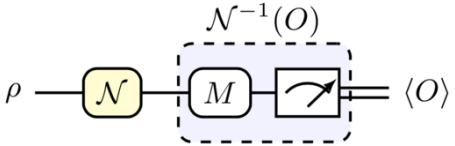
Simone Roncallo, Angela Rosy Morgillo, Emanuele Tumbiolo

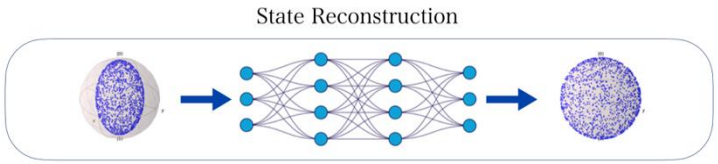
Quantum computation

- **Quantum algorithms**: q JPEG (downsampling via QFT & discard high frequency qubits), resampling algorithms for multidimensional signals

See Poster 65

- **Noise mitigation**: noise deconvolution (analytic), state reconstruction by ML



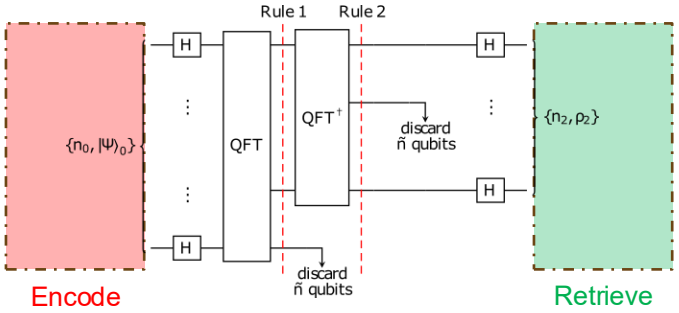


Encode

512 x 512 pixels
18 qubits

Retrieve

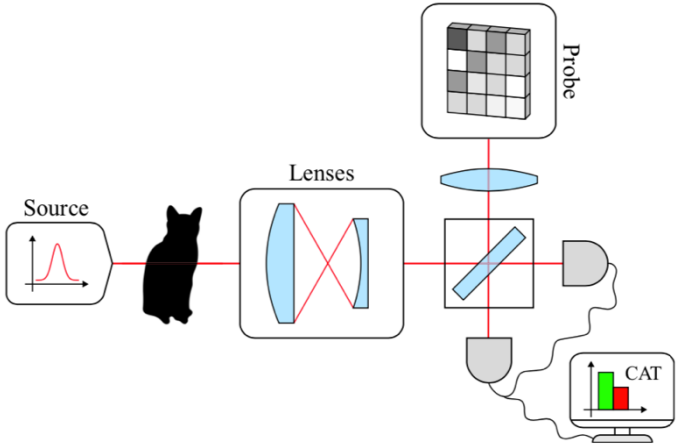
64 x 64 pixels
12 qubits



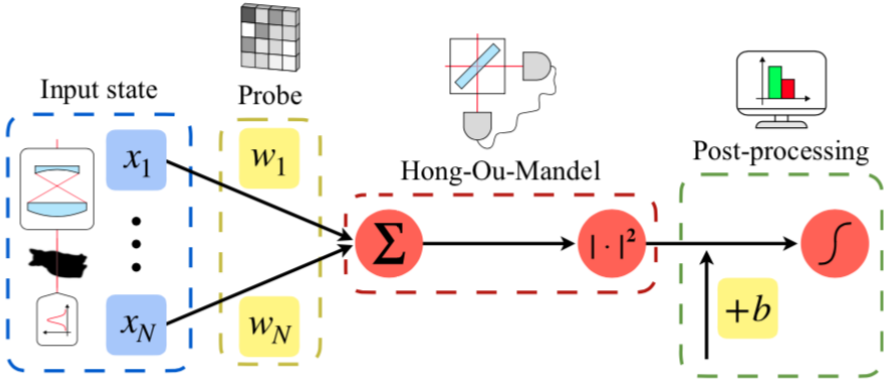
with L. Maccone, R. Morgillo, S. Roncallo, E. Tumbiolo

Quantum machine learning

- **Quantum optical classifier with superexponential speedup (classification without image reconstruction via Hong-Ou-Mandel effect)**



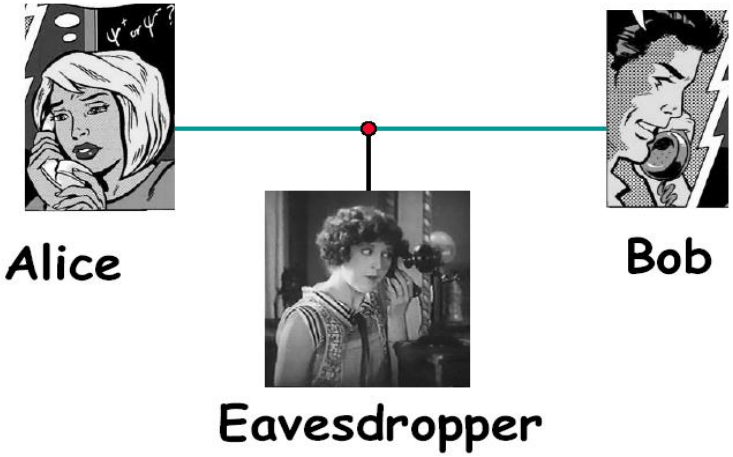
- **Quantum optical protocol for a shallow network, keeping superexp. advantage**



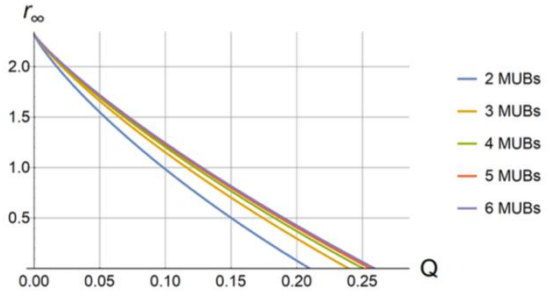
See Poster 65

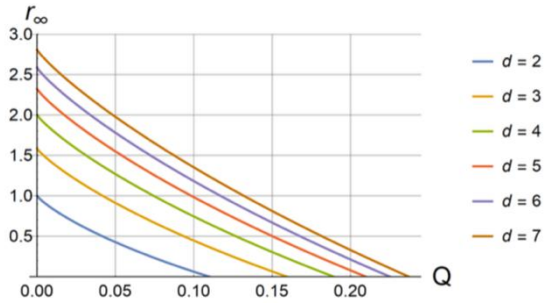
with Maccone, Morgillo, Roncallo, Tumbiolo

Quantum communication



- **Quantum cryptography:** study the performance (security) of QKD protocols
- Proof of advantage for increasing dimension and number of bases, realistic scenarios with imperfections





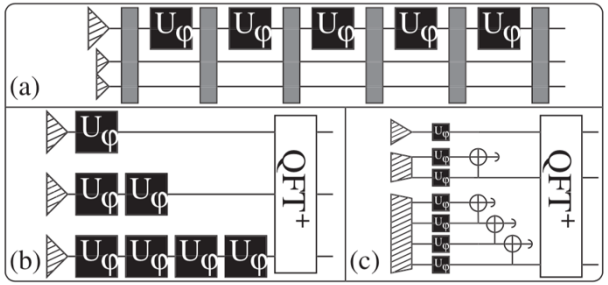
See Poster 92

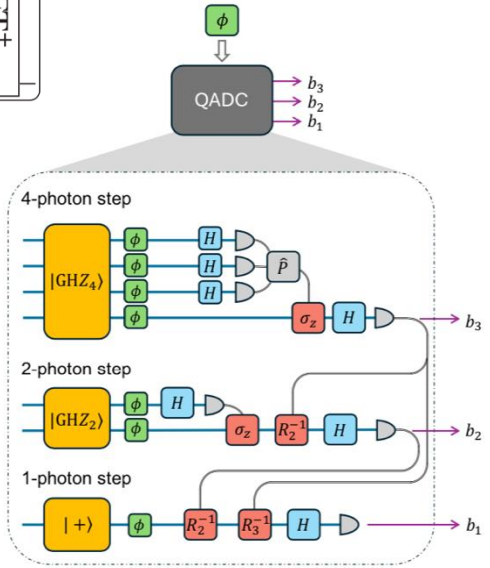
with G. Chesi

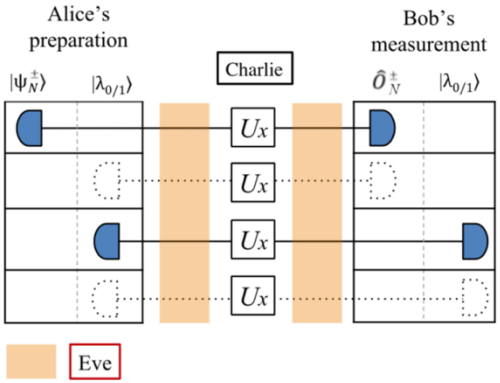
Quantum metrology

Optimal estimation strategies:

- **Digital quantum estimation**
- **Analog-to-digital converter (QADC)**
- **Protocols for multiphase estimation**
- **Cryptographic quantum metrology**

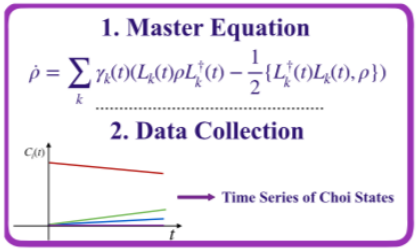


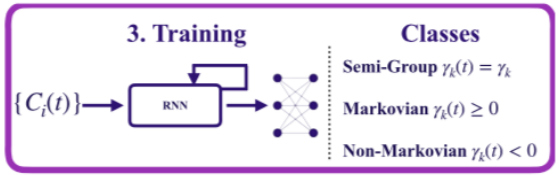


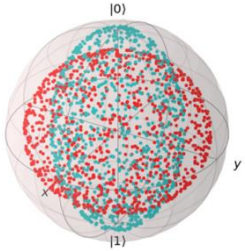


with Chesi, Maccone, Roncallo

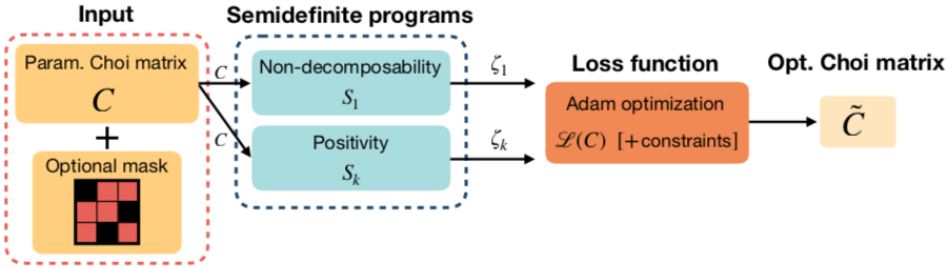
Open quantum systems and quantum operations







- Noise classification
- Detection of non-Markovian properties
- Learning properties of quantum channels (time-varying channels)
- Channel discrimination (resource features for optimal performance: entanglement/non stabiliserness…)
- Chasing non-decomposable positive maps (applications to entanglement detection)

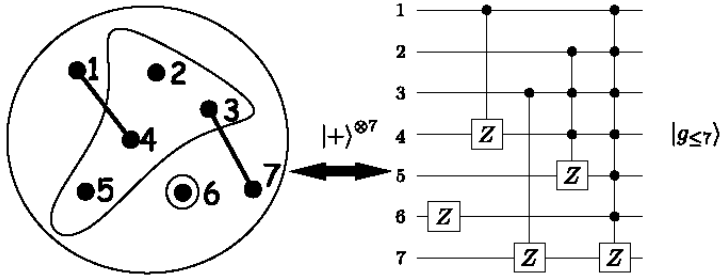


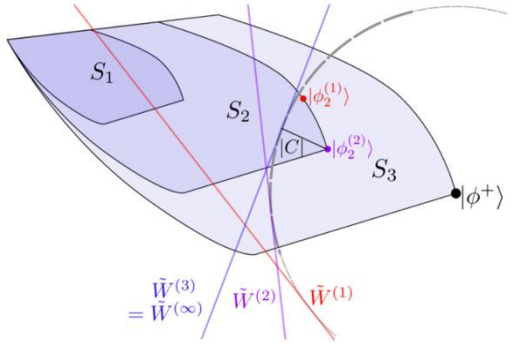
See Poster 66

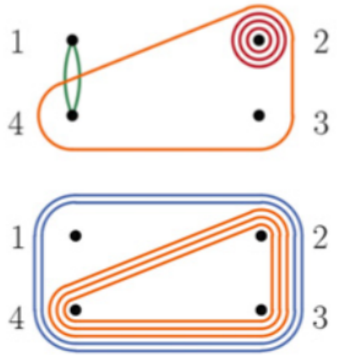
with R. Morgillo, D. Poderini, M. Sacchi

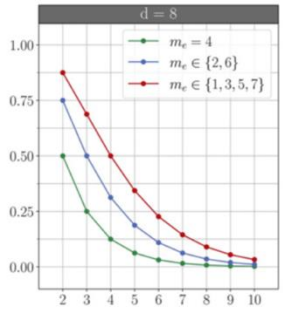
Entanglement properties of quantum states

- Entanglement detection methods
- Multipartite systems: Hypergraph states
- Schmidt number witnesses in arbitrary dimension





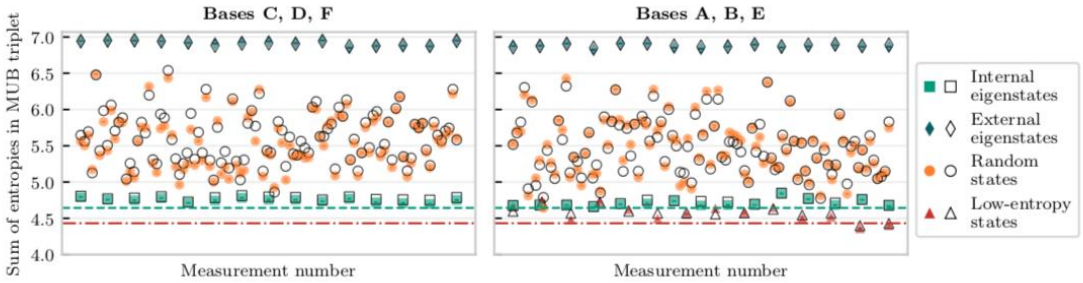




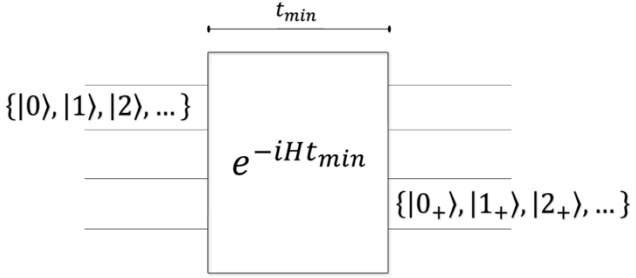
with G. Chesi, D. Poderini

Uncertainty relations and quantum speed limits

- **Entropic uncertainty relations**: for complementary properties optimality can depend on the explicit choice of bases



- **Q speed limits** (ultimate bound for the time required to transform states): for change of basis they depend on the explicit form in d>2

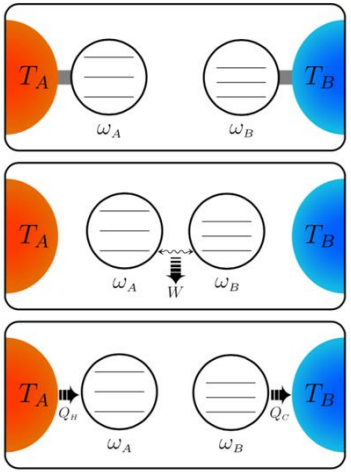


with Maccone, Chesi, Poderini

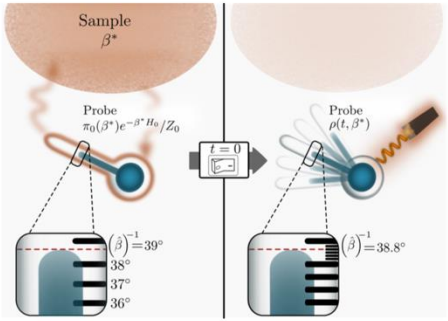
Quantum thermodynamics

Study laws and concepts of thermodynamics including quantum effects and using quantum information tools

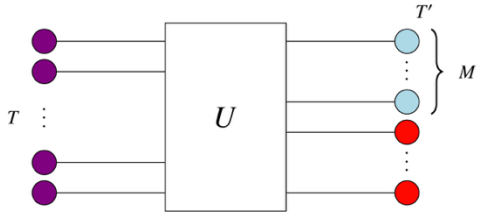
- Quantum thermal machines



- Quantum thermometry: external unitary driving as a resource to improve temperature precision

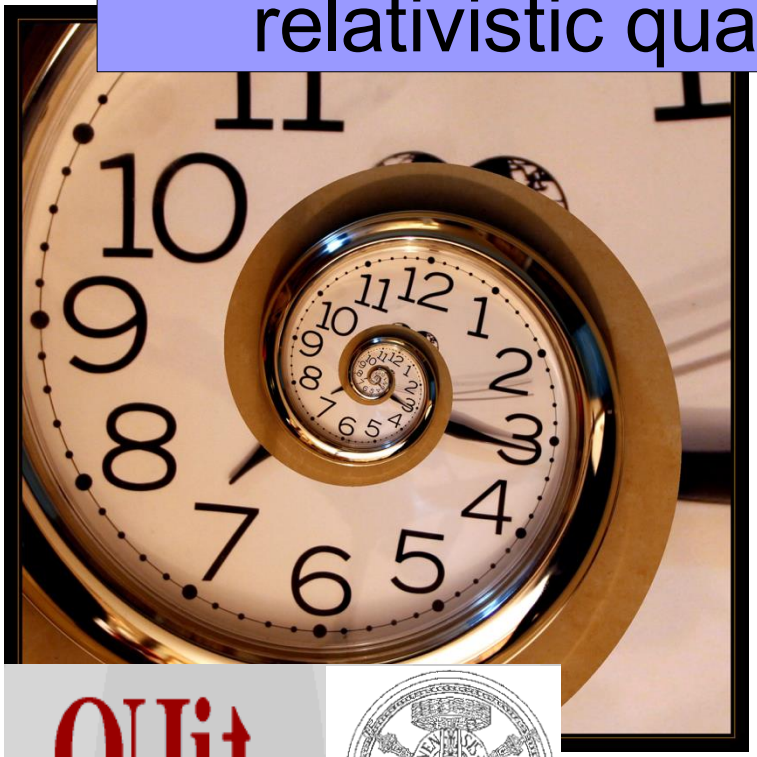


- Dynamical cooling



with Chesi, Guarnieri, Maccone, Sacchi, Tumbiolo

Geometric Event-Based QM:
relativistic quantum spacetime



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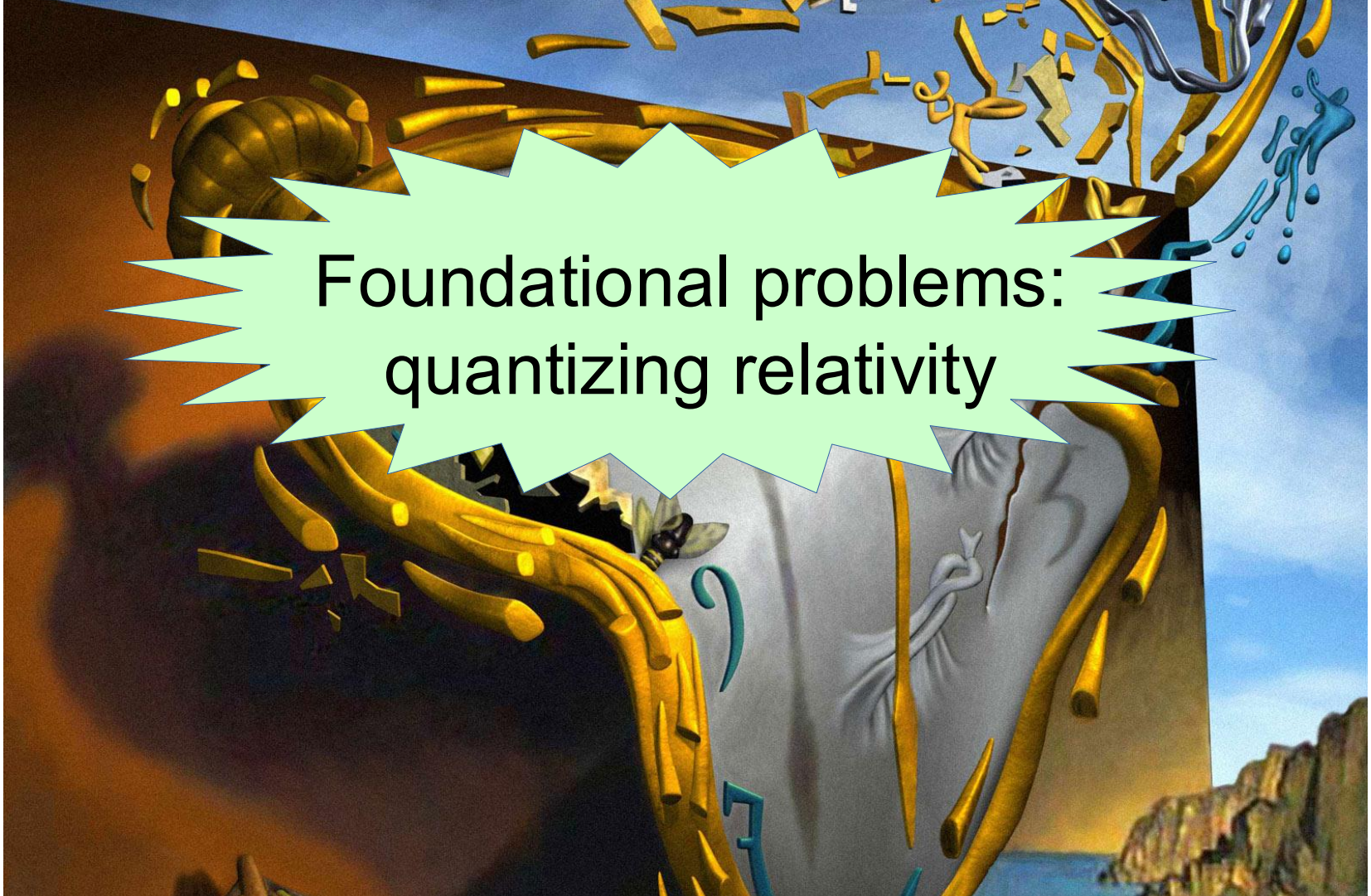
Seth Lloyd
MIT

Vittorio Giovannetti
Scuola Normale Superiore, Pisa

FQXi Foundation,
"The physics of what happens"

QUIT quantum information theory group
www.qubit.it


Foundational problems:
quantizing relativity

What is the problem?

What is the problem?

- QM ⟶ quantum systems
- GR ⟶ events
-

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- QM → quantum systems

  Inifinitely extended in time
  (finite or infinite in space)

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  Finite in space *and* time

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Our two main theories talk
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Which is the most fundamental concept?

What is the problem?

- QM → quantum systems

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  Finite in space *and* time

Our two main theories talk
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Which is the most fundamental concept?

Two approaches:

- General relativistic theory of QM

Systems are more fundamental: GR is made of quantum fields

- Quantum theory of GR

Events are more fundamental:

-

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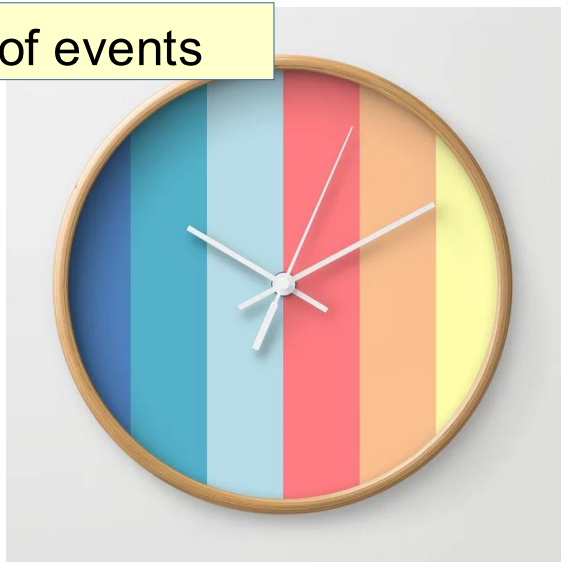
Quantum system=succession of events



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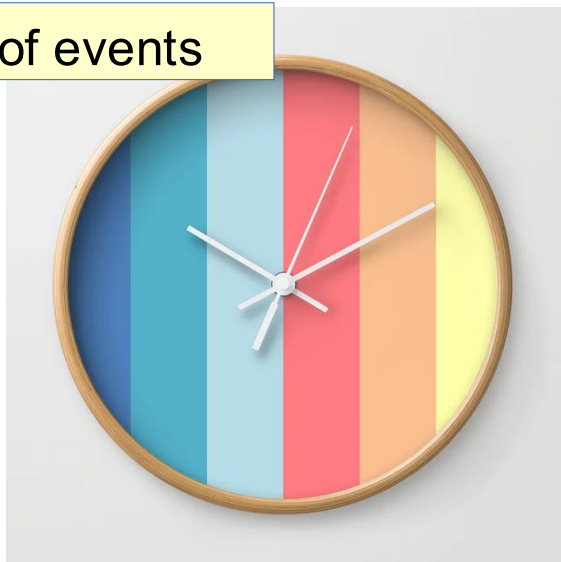

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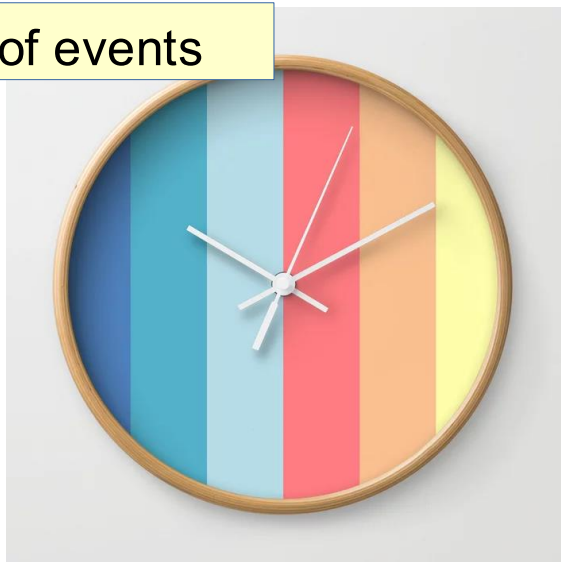

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Explore the alternative!!

- Start with SPECIAL relativity

- Let’s deal with GR in the future (much in the future!)

- QM uses **time conditioned quantities**
-

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- $|\psi(t)\rangle$ States (Schroedinger picture)

  $X(t)$ Observables (Heis. picture)

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⇓

CANNOT be relativistically covariant

(covariance="formulas look the same in all reference frames")

Wait?!? What about QFT?

- QFT uses a couple of tricks to recover covariance:

1) use observables in the Heisenberg picture with covariant spacetime dependence, e.g. $a^\dagger e^{-ix^\mu p_\mu}$

2) Use a state that is invariant for Lorentz transforms, e.g the vacuum $|0\rangle$

Our approach: Geometric Event-Based QM

GEB

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GEB

- **quantum events → fundamental**
-

Our approach: Geometric Event-Based QM

GEB

- **quantum events → fundamental**
- quantum systems → derived: a **quantum state for a succession of events** in q spacetime

A quantum event has a **position** in spacetime, but also an **energy-momentum**

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(without energy nothing can happen, without momentum, nothing can be localized)

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why?!? ↘

Poincare' algebra:

$$\begin{aligned} [M^{\mu\nu}, P^\rho] &= -i(\eta^{\mu\rho}P^\nu - \eta^{\nu\rho}P^\mu), \\ [M^{\mu\nu}, M^{\rho\sigma}] &= i(\eta^{\nu\rho}M^{\mu\sigma} - \eta^{\mu\rho}M^{\nu\sigma} \\ &\quad -\eta^{\mu\sigma}M^{\rho\nu} + \eta^{\nu\sigma}M^{\rho\mu}) \end{aligned}$$

A universe with a single event

$$|\Phi\rangle = \int d^1x\ \Phi(\overline{x})\ |\overline{x}\rangle = \int d^1p\ \tilde{\Phi}(\overline{p})\ |\overline{p}\rangle$$

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Not all GEB states are physical!

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Physical states are the ones that satisfy some constraints (e.g. PW WdW).

A universe with a single event

$$|\Phi\rangle = \int d^1x\ \Phi(\overline{x})\ |\overline{x}\rangle = \int d^1p\ \tilde{\Phi}(\overline{p})\ |\overline{p}\rangle$$

Amplitudes (wavefunctions)

$$\Phi(\overline{x}) := \langle \overline{x}|\Phi\rangle\ ,\ \ \tilde{\Phi}(\overline{p}) := \langle \overline{p}|\Phi\rangle = \int \frac{d^1x}{4\pi^2} e^{i\overline{x}\cdot\underline{p}}\ \Phi(\overline{x})$$

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Born rule in QM is **CONDITIONED**

$$p(\vec{x}|\psi,t) = |\langle \vec{x}_S|\psi_S(t)\rangle|^2 = |\langle \vec{x}_H(t)|\psi_H\rangle|^2$$

Probability that the particle is at position $\vec{x}$ *given* that the time is t!!!

QM

Born rule: $P(\overline{x}|\Phi) = |\Phi(\overline{x})|^2 = |\langle \overline{x}|\Phi\rangle|^2$

UNCONDITIONED probability that the event is in spacetime position $\overline{x}$

QM probabilities are NOT covariant
GEB probabilities ARE covariant

Born rule in QM is **CONDITIONED**

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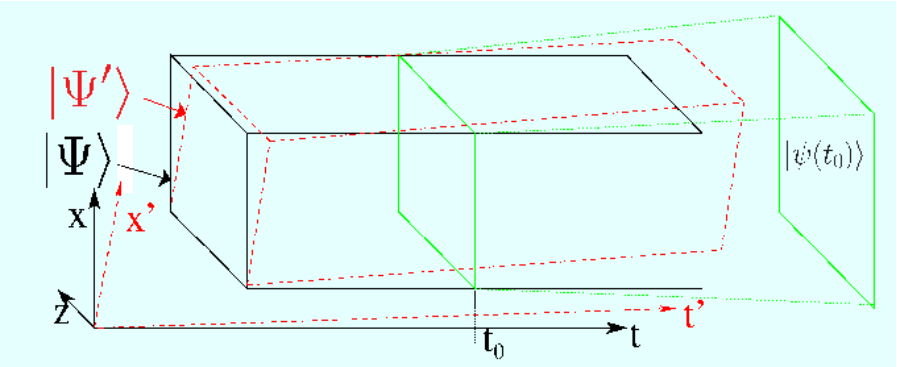
Probability that the particle is at position $\vec{x}$ *given* that the time is t!!! QM

LORENTZ TRANSFORMS IN GEB

Just a **unitary transformation on the GEB state** (Wigner's prescription on how to describe symmetries of a theory)

$$|\Phi'\rangle = U_\Lambda |\Phi\rangle$$



Multiple events: tensor products!

(if fixed number of events n)

$$|\Phi^{[n]}\rangle = \sum \int d^4x_1 \cdots d^4x_n \, \Phi^{[n]}(\overline{x}_1, \sigma_1; \cdots; \overline{x}_n, \sigma_n) \, |\overline{x}_1, \sigma_1; \cdots; \overline{x}_n, \sigma_n\rangle$$

EACH EVENT WITH ITS OWN TIME!!!!

(cfr Dirac's multiparticle-multitime)

$$P^{[n]}(\overline{x}_1, \sigma_1; \cdots; \overline{x}_n, \sigma_n) = \left|\Phi^{[n]}(\overline{x}_1, \sigma_1; \cdots; \overline{x}_n, \sigma_n)\right|^2$$

Joint probability for the n events to happen in spt positions $x_1 \ldots x_n$

Fock space

$$= \frac{1}{\sqrt{n!}} \sum_{\sigma_1,\cdots,\sigma_n} \int d^4x_1 \cdots d^4x_n \, \Phi^{[n]}(\overline{x}_1,\sigma_1;\cdots;\overline{x}_n,\sigma_n) \; a^\dagger_{\overline{x}_1,\sigma_1} \cdots a^\dagger_{\overline{x}_n,\sigma_n} |0\rangle_4$$

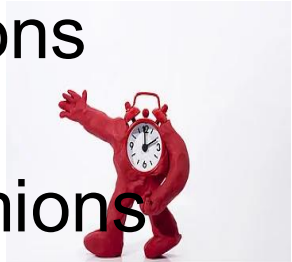
Commutators:

$$\text{Bose: } \left[a_{\overline{x},\sigma}, a^\dagger_{\overline{x}',\sigma'}\right] = \delta_{\sigma,\sigma'}\delta^{(4)}(\overline{x}-\overline{x}'), \; \left[a_{\overline{x},\sigma}, a_{\overline{x}',\sigma'}\right] = 0,$$

$$\text{Fermi: } \left\{a_{\overline{x},\sigma}, a^\dagger_{\overline{x}',\sigma'}\right\} = \delta_{\sigma,\sigma'}\delta^{(4)}(\overline{x}-\overline{x}'), \; \left\{a_{\overline{x},\sigma}, a_{\overline{x}',\sigma'}\right\} = 0$$

Bosonic events ⟶ Bosons

Fermionic events ⟶ Fermions



The dynamics

The dynamics

Use **constraints** (as in the quantum time P&W, WdW, etc.)!

The dynamics

Use **constraints**

Klein-Gordon eq. constraint in Fock sp:

$$K^{(\mathrm{Fock})}_{\mathrm{KG}+} := \int d^4p \ \left[\Theta(p^0)\ \overline{p}\cdot\underline{p} - m^2\right]^2 \ a^\dagger_{\overline{p}} a_{\overline{p}}$$

Similarly for the Dirac eq. constraint.

No claim that QFT is incorrect.

GEB is an **alternative** in the sense “a different way to obtain the same results”

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WHY?

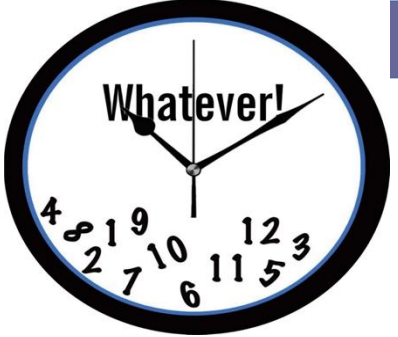
No claim that QFT is incorrect.

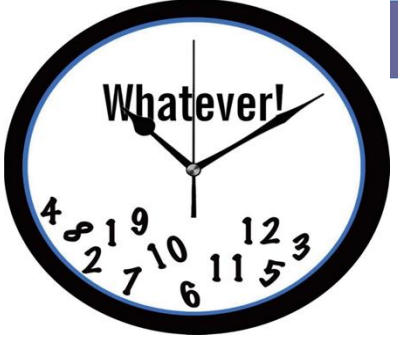
GEB is an **alternative** in the sense “a different way to obtain the same results”

WHY?

To get a better ontology?
To go further than QFT can go?

Conclusions





Conclusions

- GEB: new approach to relativistic QM

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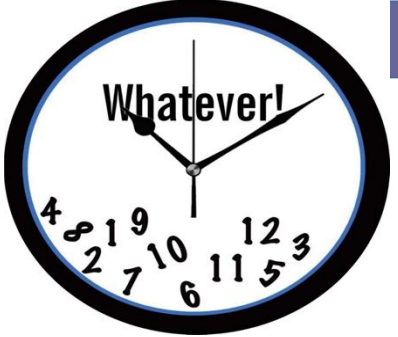
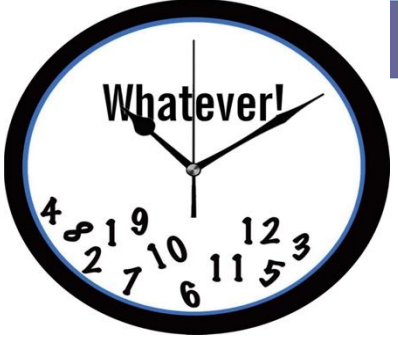
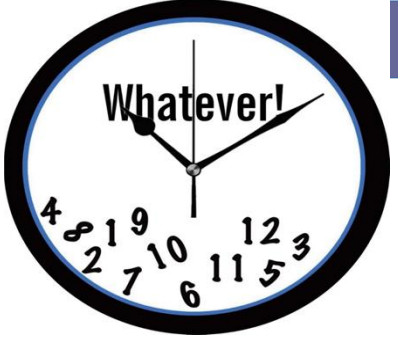


- GEB: new approach to relativistic QM
- quantum events

Conclusions



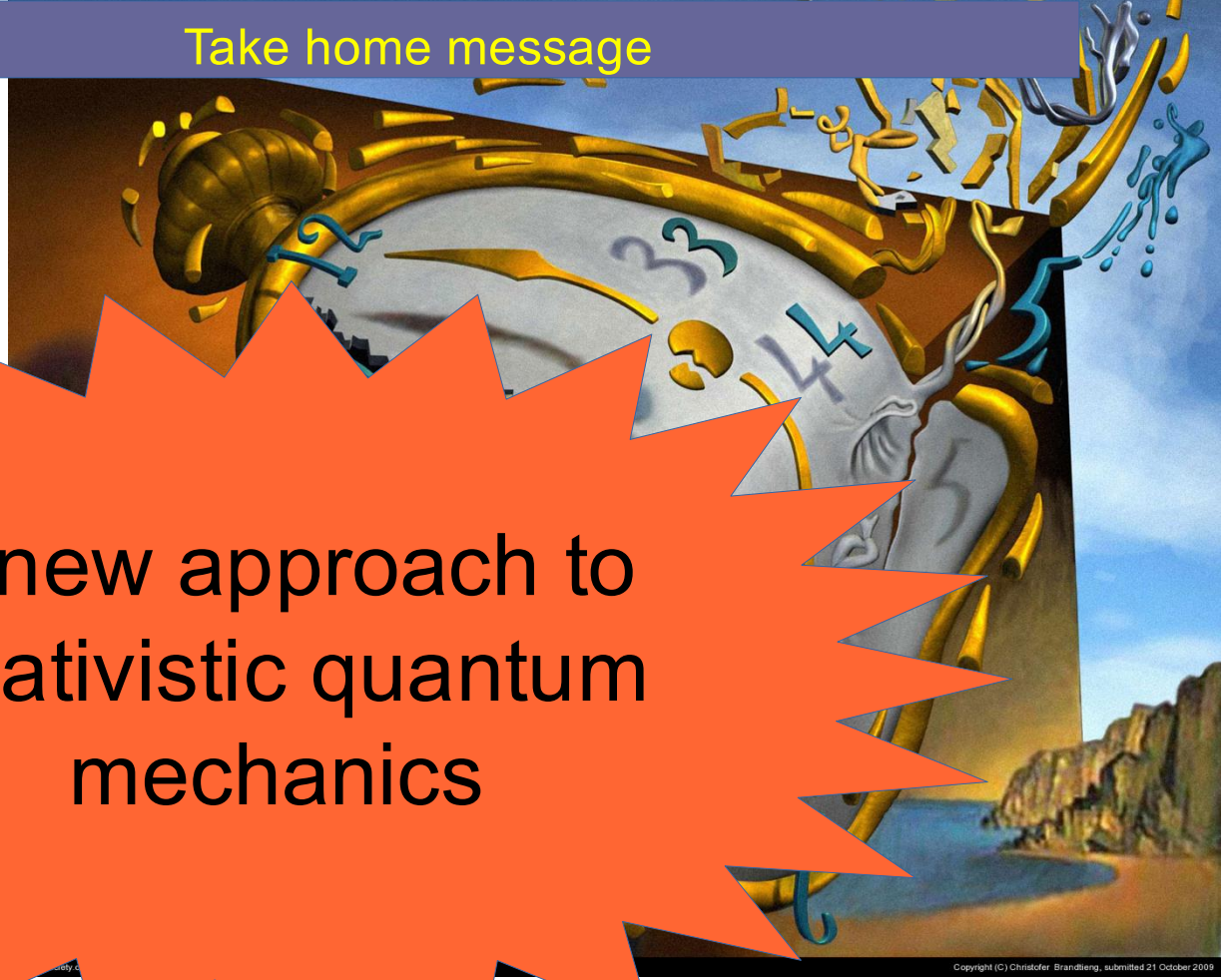
- GEB: new approach to relativistic QM
- quantum events
- observables, Hilbert space, Fock space, Bosonic and Fermionic events



Conclusions

- GEB: new approach to relativistic QM
- quantum events
- observables, Hilbert space, Fock space, Bosonic and Fermionic events
- QFT from GEB: KG and Dirac

Take home message



A new approach to relativistic quantum mechanics

Lorenzo Maccone
maccone@unipv.it

NJP 25, 023027

Modelling of materials from first-principles

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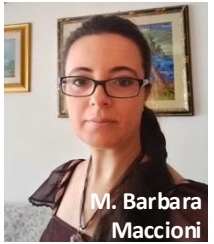
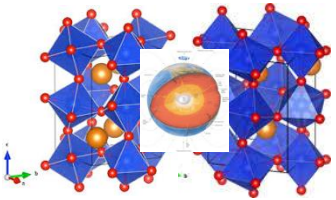
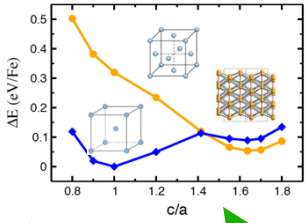
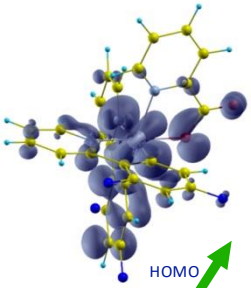
current members

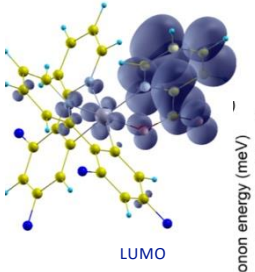
former members

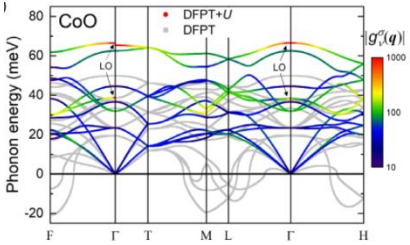


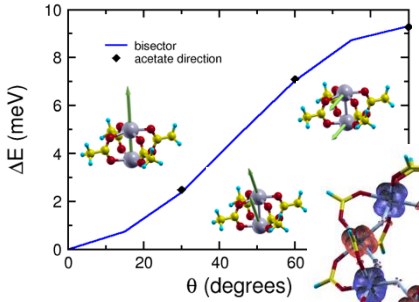


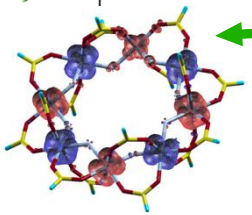


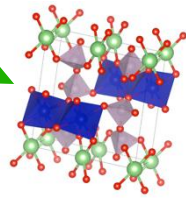


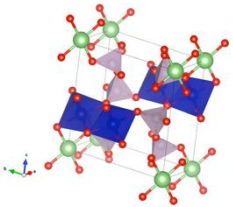


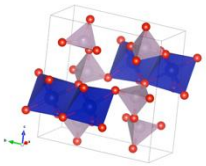












Modelling of materials from first-principles

UNIVERSITÀ DI PAVIA

Objective: to comprehend and predict the physical properties of systems from the solution of the electronic problem

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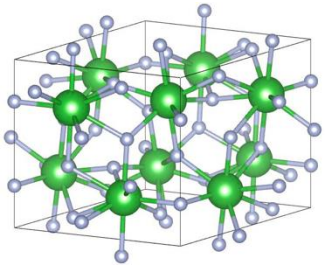

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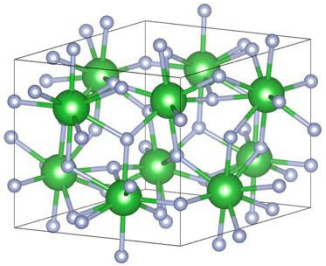

HPC Leonardo @ CINECA

$$\hat{H}\Psi = E\Psi$$

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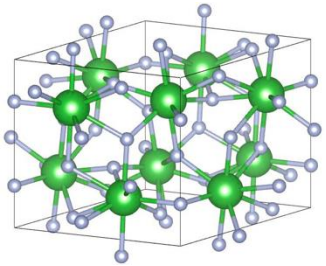

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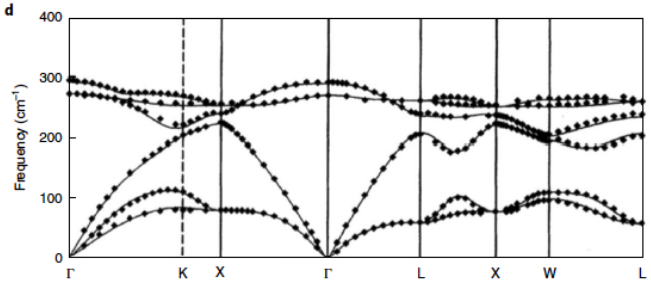

Properties

Modelling of materials from first-principles

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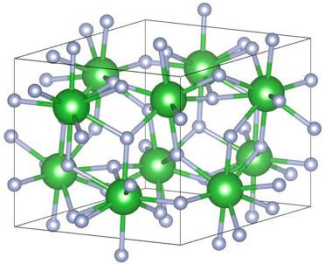

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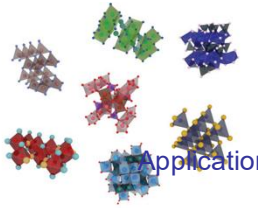
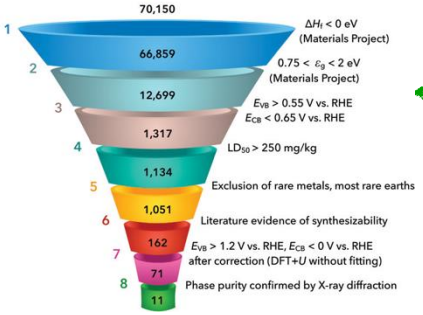
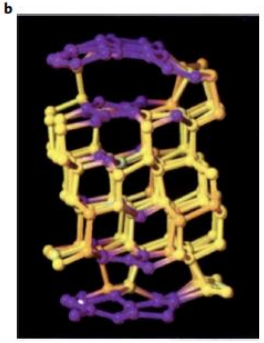
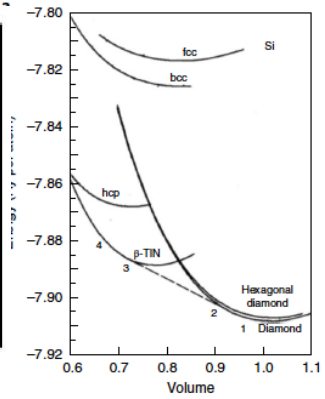


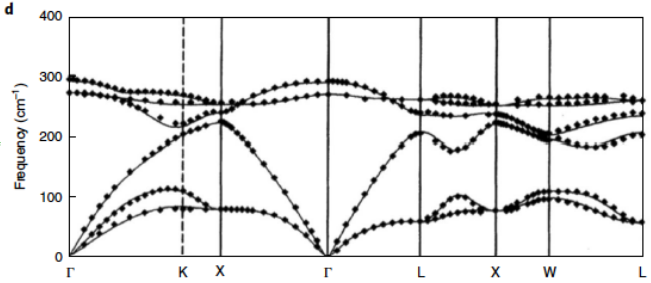
Applications







Behavior



Properties

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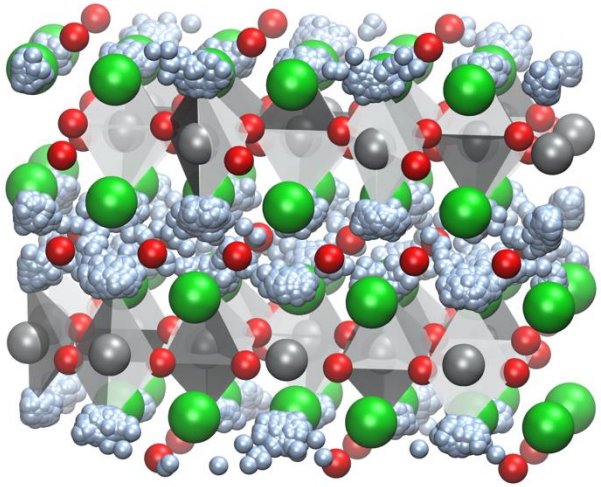
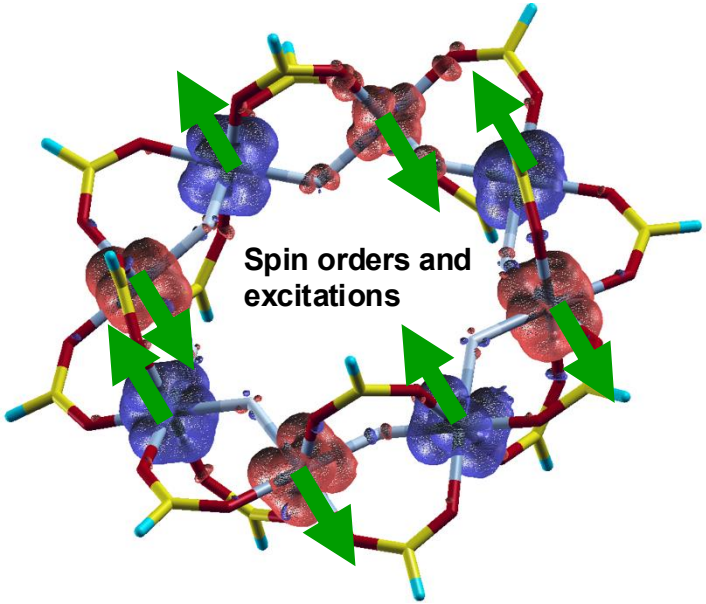
Main projects under development

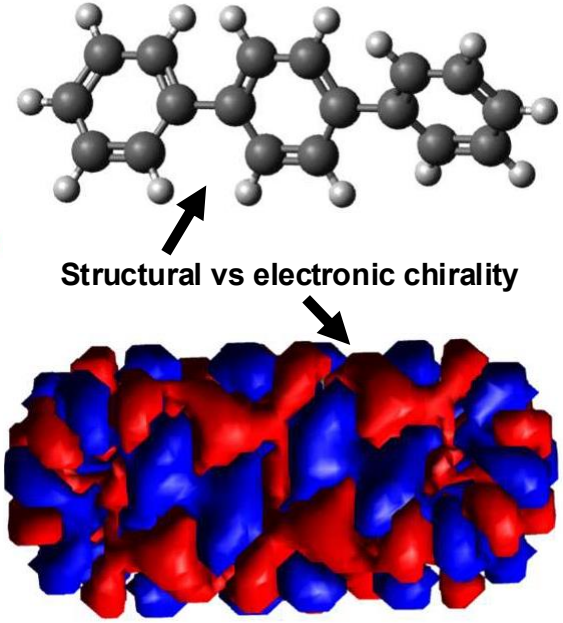


Phase stability and ion diffusion

Fluoride-ion batteries



Molecular magnets



Spin-polarisation in chiral systems

Modelling of materials from first-principles

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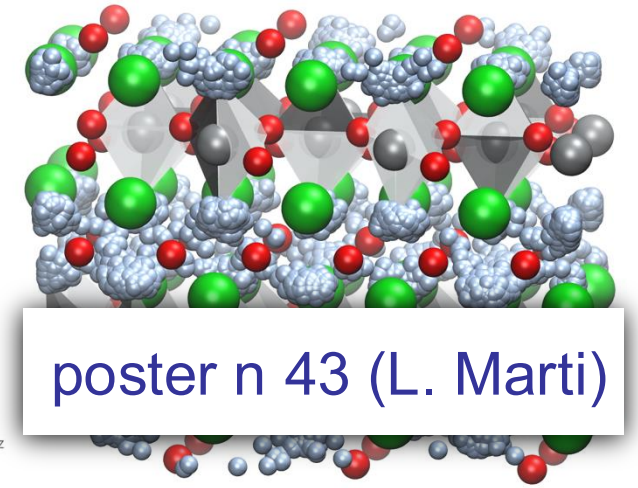
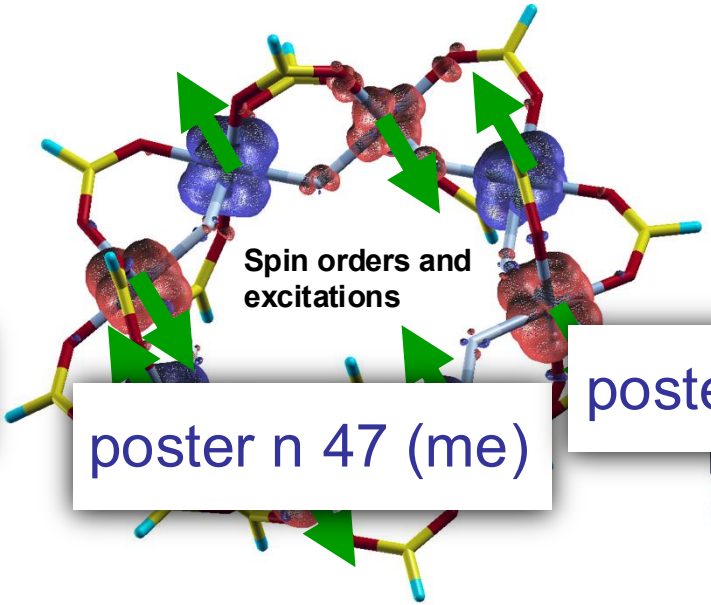


poster n 43 (L. Marti)

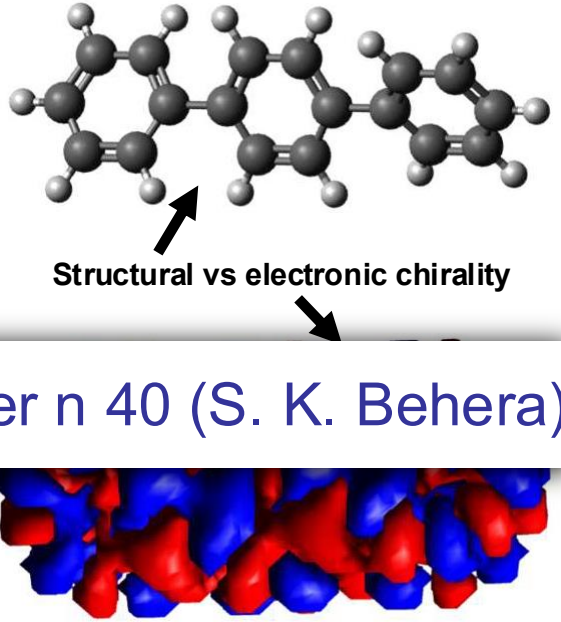
Phase stability and ion diffusion

Fluoride-ion batteries



poster n 47 (me)

Molecular magnets

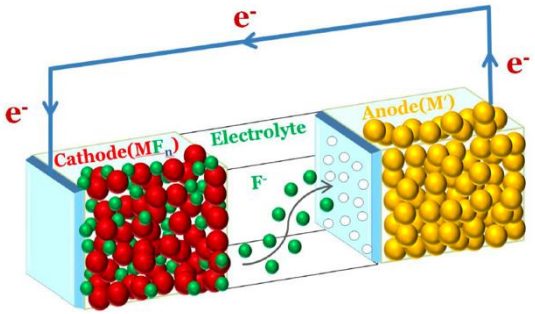


poster n 40 (S. K. Behera)

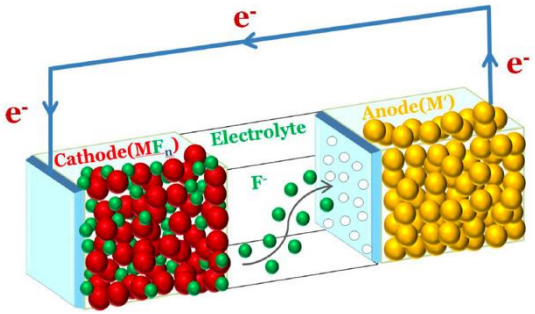
Spin-polarisation in chiral systems

Fluoride-ion batteries

(In collaboration with P. Galinetto, M. C. Mozzati, C. Tealdi)



Fluoride-ion batteries



(In collaboration with P. Galinetto, M. C. Mozzati, C. Tealdi)

Research needed on all components

- Electrochemical stability
- Intercalation energetics (voltage)
- Diffusivity of charge carriers
- Phase recognition

Fluoride-ion batteries

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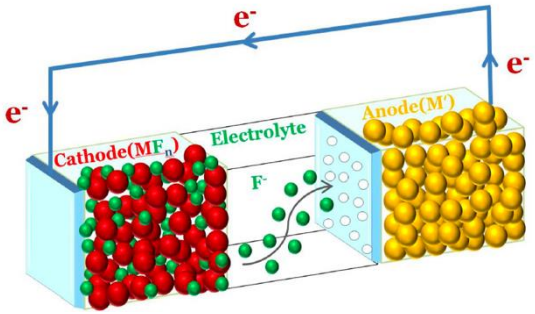

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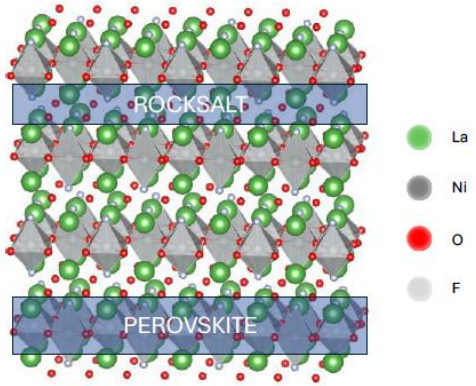
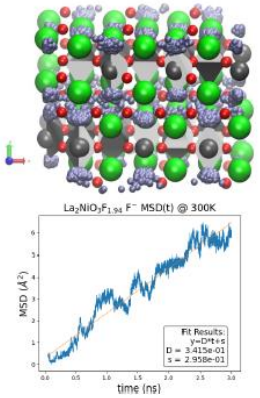
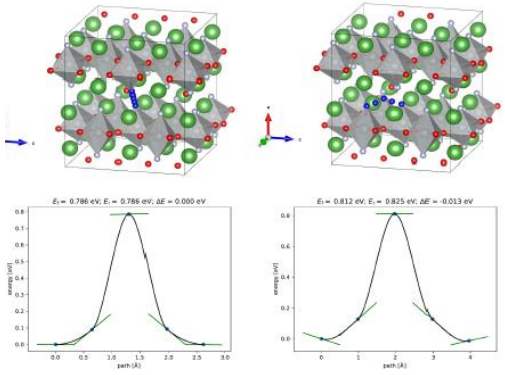




Diffusion of F from molecular dynamics



Potential energy barriers along diffusion paths

Fluoride-ion batteries

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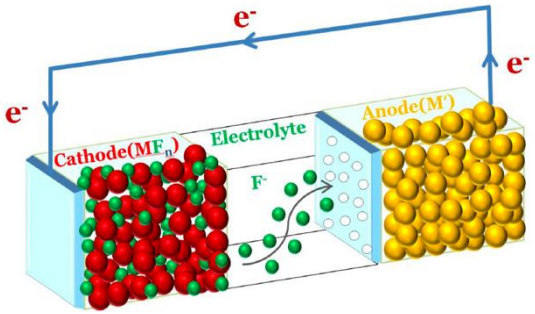
(In collaboration with P. Galinetto, M. C. Mozzati, C. Tealdi)



Elettrolita

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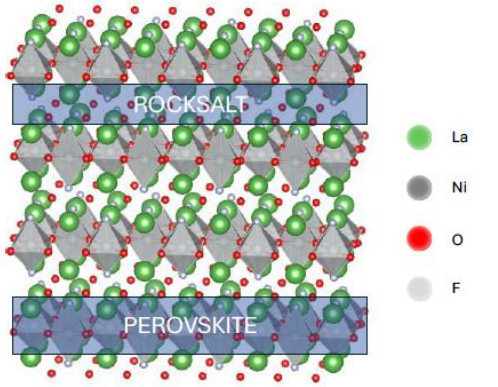
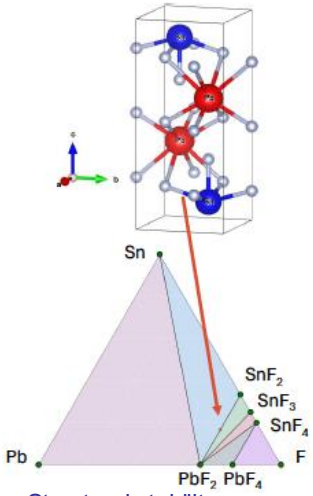
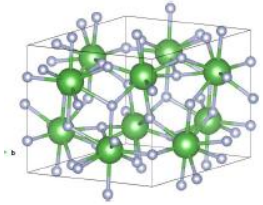


$PbSnF_4$



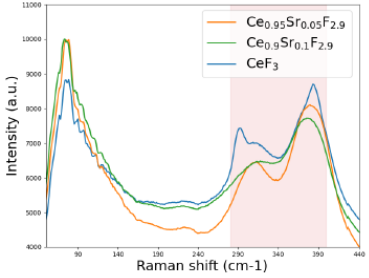
Structural stability

CeF_3

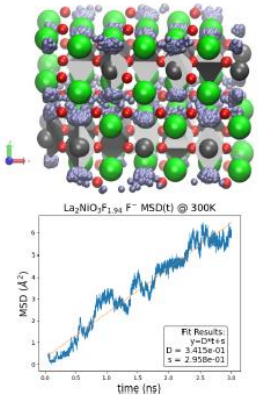


Irrep	Frequency (cm^{-1})		
E_g	76.8	A_{1g}	232.3
E_g	112.4	E_g	295.4
A_{1g}	121.2	A_{1g}	299.9
E_g	144.7	E_g	304.9
E_g	159.0	E_g	315.7
E_g	200.3	E_g	367.0
A_{1g}	210.5	E_g	373.2
E_g	220.0	A_{1g}	393.0
		E_g	443.3

$\Gamma_{Raman} = 5A_{1g} + 12E_g$



Raman spectroscopy (exp and calc) for phase recognition and characterisation



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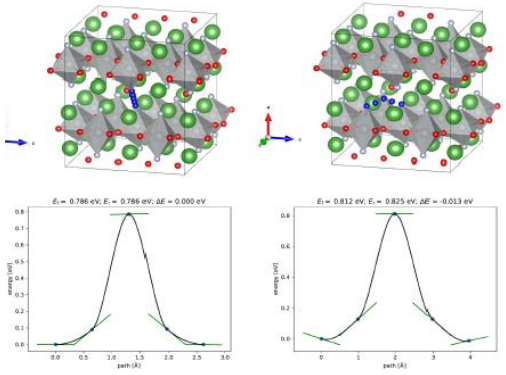
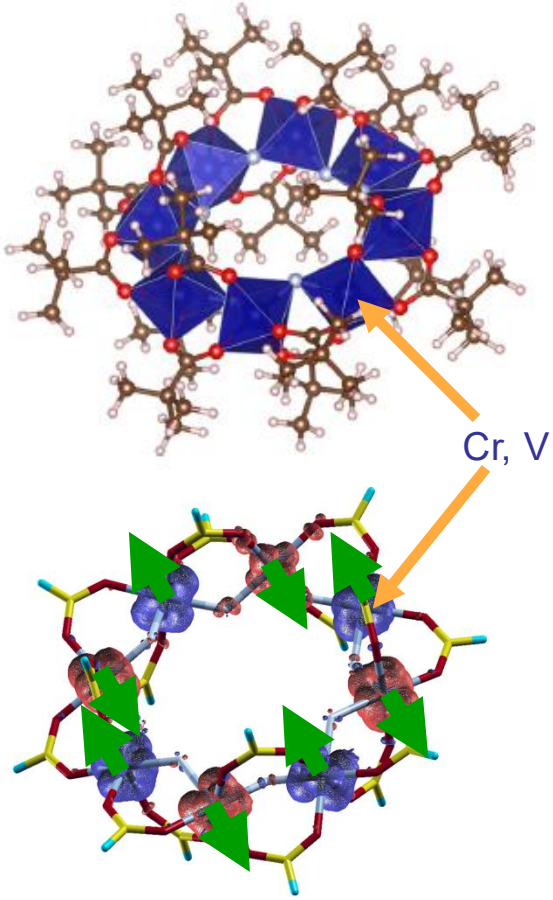
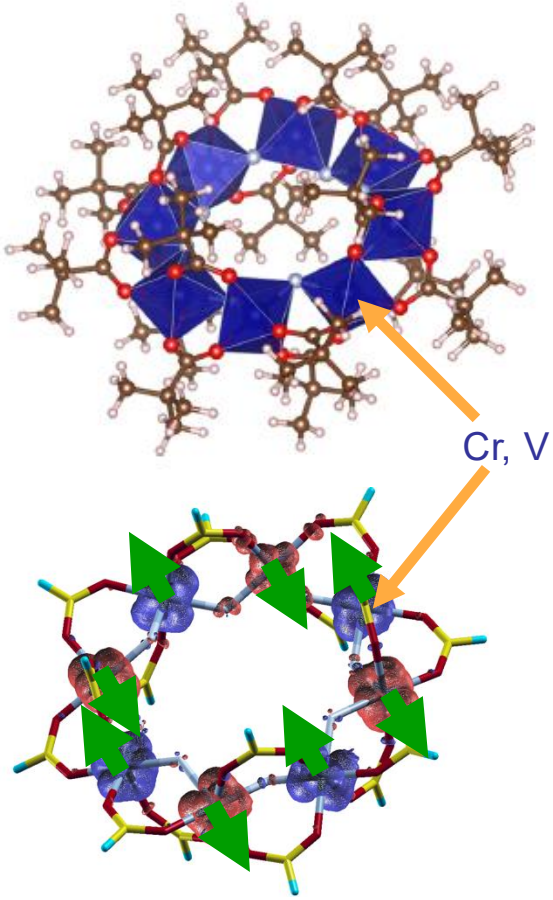


Potential energy barriers along diffusion paths

Molecular magnets



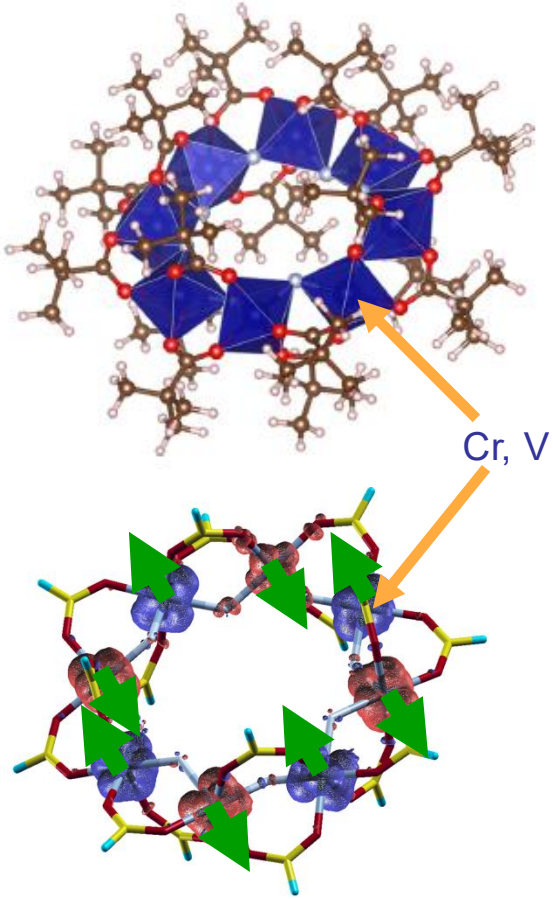
Molecular magnets



Magnetic orders and spin excitations in Cr_8 and V_8 from the exact diagonalization of model spin Hamiltonians:

$$\hat{H}_{spin} = \hat{H}_{ex} + \hat{H}_{bq} + \hat{H}_{dm}$$

Molecular magnets



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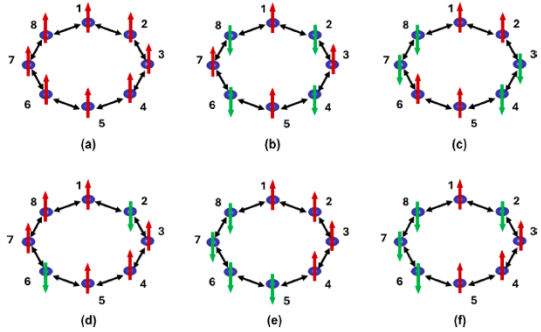
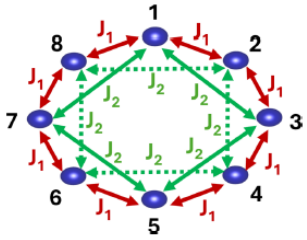
$$\hat{H}_{spin} = \hat{H}_{ex} + \hat{H}_{bq} + \hat{H}_{dm}$$

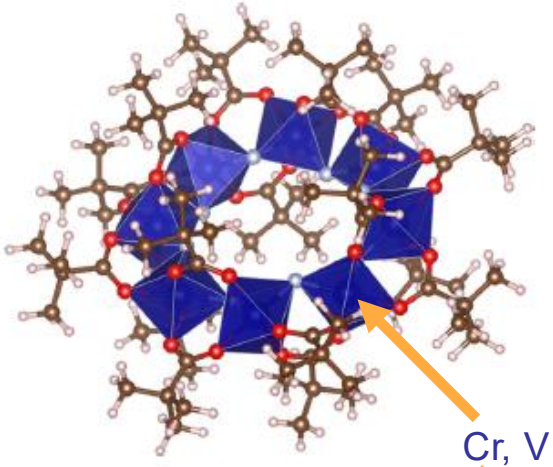
Computational strategy: $E^{\alpha}_{DFT} = \langle \Psi_\alpha | \hat{H}_{spin} | \Psi_\alpha \rangle$



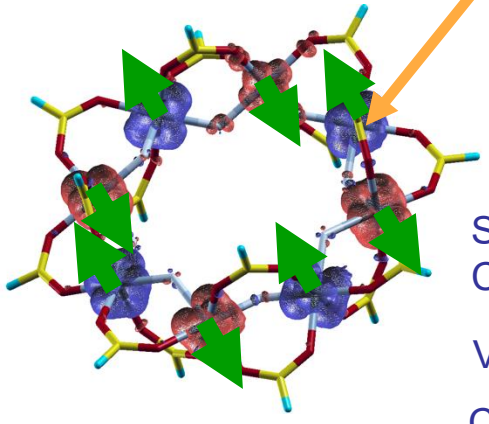


$\hat{H}_{spin}$

Molecular magnets



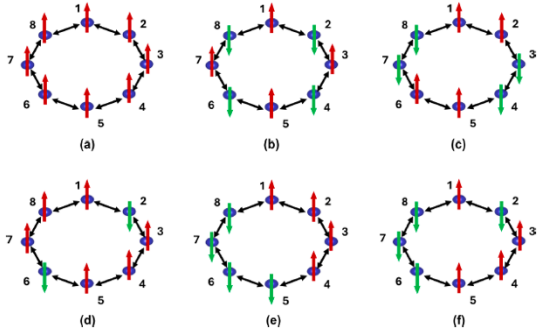
Cr, V

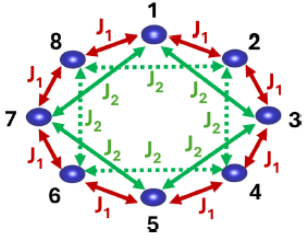


Magnetic orders and spin excitations in Cr_8 and V_8 from the exact diagonalization of model spin Hamiltonians:

$$\hat{H}_{spin} = \hat{H}_{ex} + \hat{H}_{bq} + \hat{H}_{dm}$$

Computational strategy: $E^{\alpha}_{DFT} = \langle \Psi_\alpha | \hat{H}_{spin} | \Psi_\alpha \rangle$





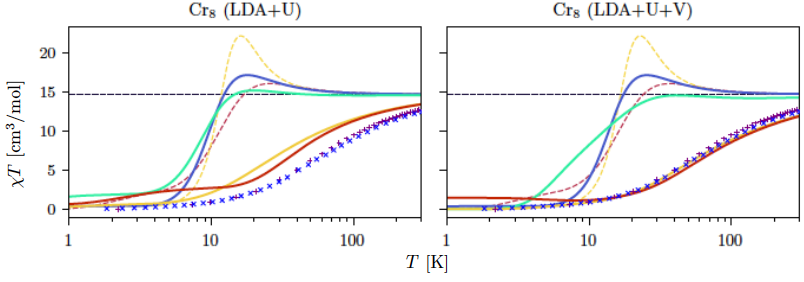
$\hat{H}_{spin}$

Significant differences between Cr_8 and V_8:

V_8 ferromagnetic

Cr_8 antiferromagnetic

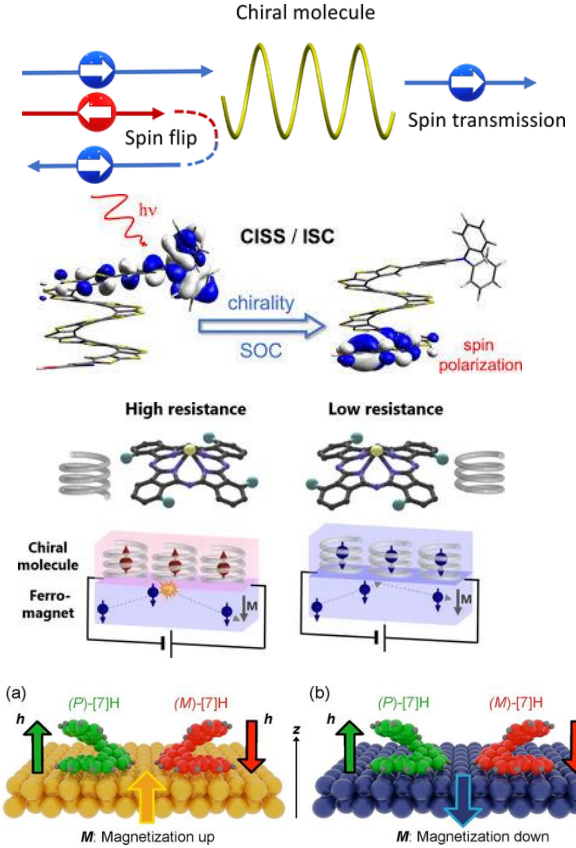
$$\chi_{zz} = \mu_0 \beta \left[\langle \hat{m}_z^2 \rangle - \langle \hat{m}_z \rangle^2 \right]$$



Spin and chirality

Chirality-induced spin selectivity (CISS): can we explain it?

CISS phenomenology



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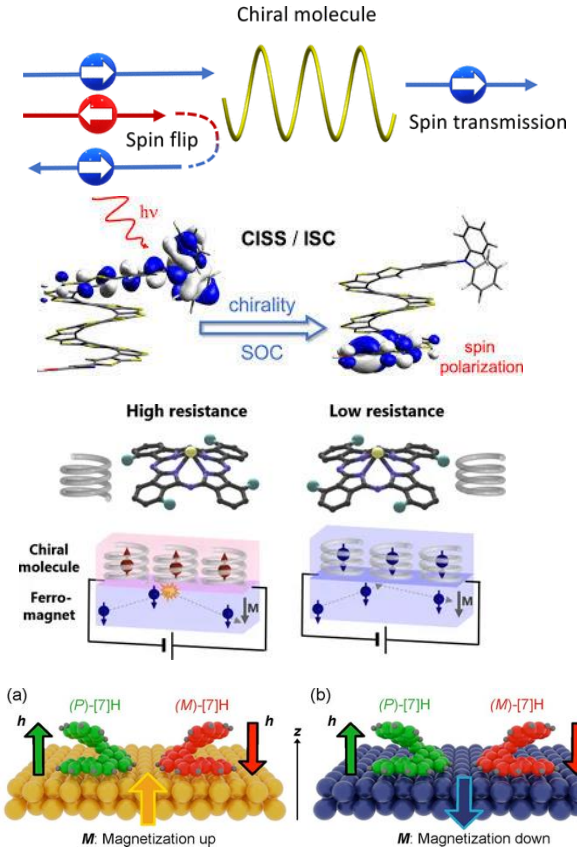

A new descriptor: electron chirality $\chi(\mathbf{r}) = \sum_{\mu\nu} \psi^*_\mu(\mathbf{r}) \gamma^5_{\mu\nu} \psi_\nu(\mathbf{r})$

Where: $\gamma^5 = i\gamma^0\gamma^1\gamma^2\gamma^3 \approx \sigma \cdot \mathbf{p}$ (massless particles or WRL)

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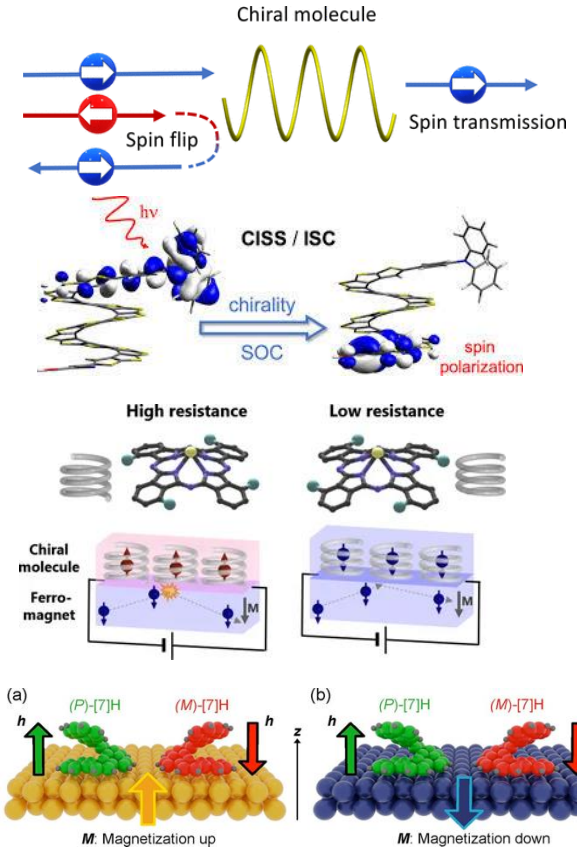

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DFT su eq. di Dirac:

DIRAC 24

Molecules of tunable chirality: ethane, trichloroethane and triphenil

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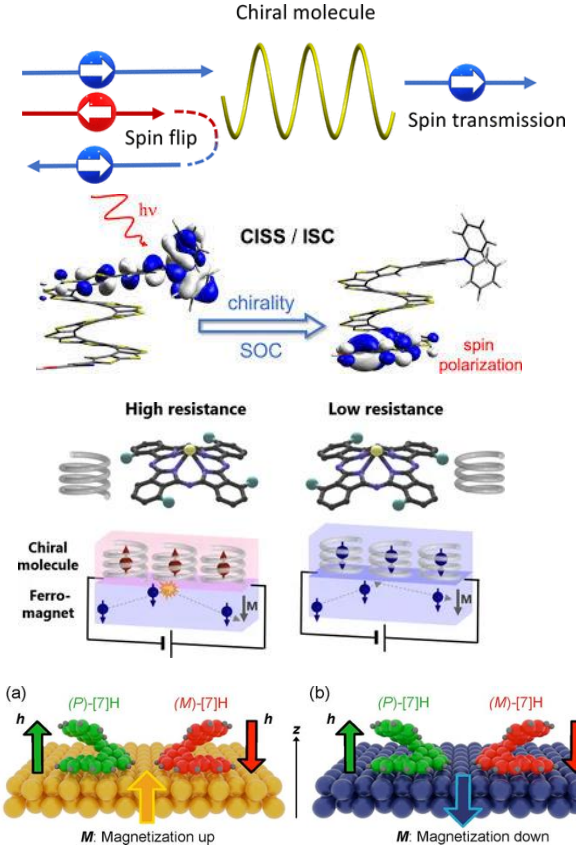

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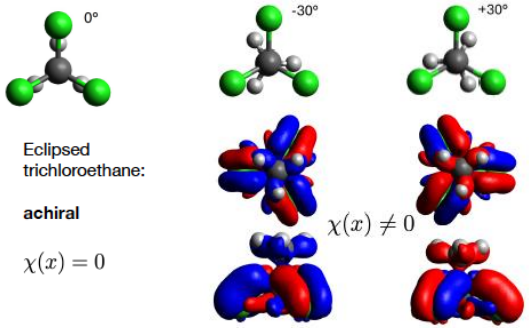
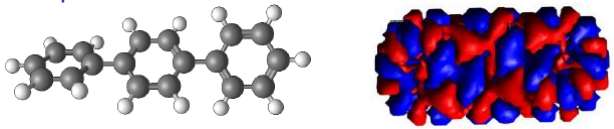


chiral triphenil



Spin and chirality

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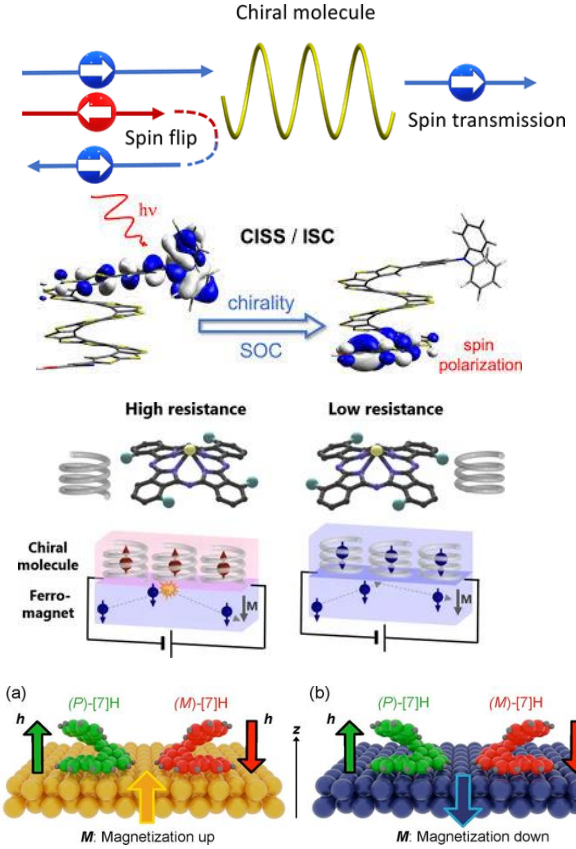

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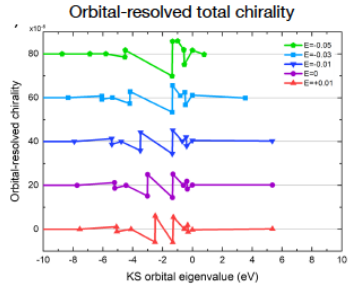

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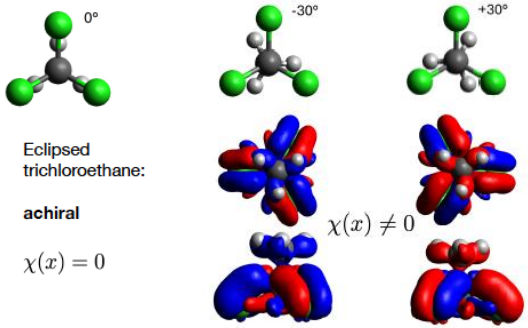
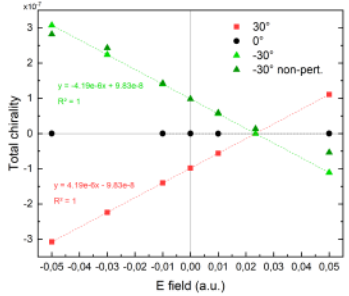


Response to electric fields



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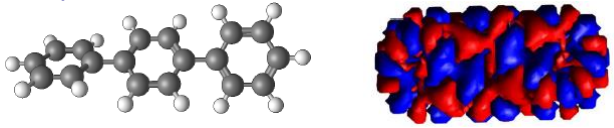

Modelling the modelling engine

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Main computational tool: density functional theory (DFT):

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Excited states

Superconductivity

Out-of-equilibrium conditions

Topological materials

Non-collinear magnetism and
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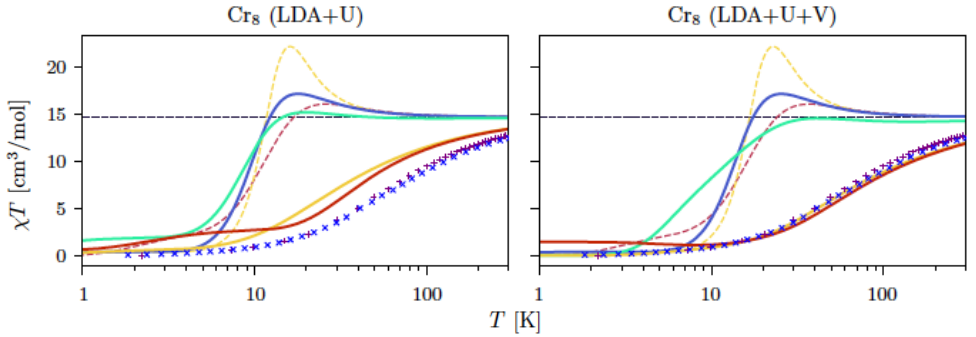

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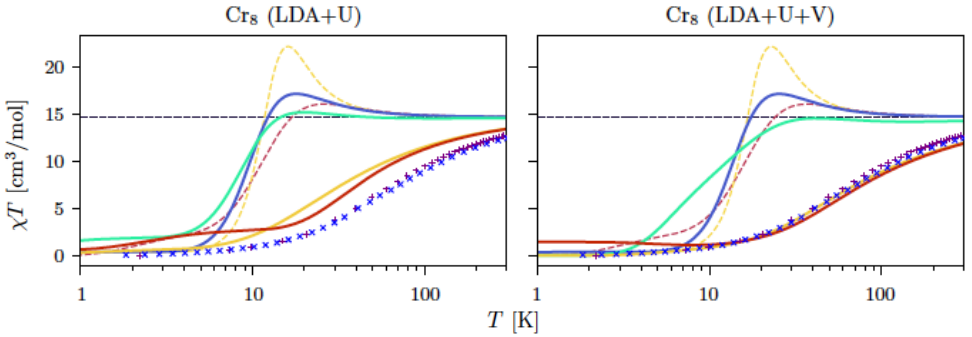

Much theoretical work still needed

Gauge fields formalism

Dependence on (spin) currents

Non-hermitian terms

Etc…