Ways to collaborate between theory group and experimental research, based on current expertise in theoretical physics and physical systems

Theory group for condensed matter physics and statistical physics

Roles that **researchers from theory group** can take in collaboration with experimental colleagues

- Electronic, magnetic and lattice **phase transitions**, physical **properties in proximity to instabilities**
- Insights into **electronic** and magnetic **structure**, bulk and interfaces, system **excitations**, through *ab-initio calculations*, and various analytical and numerical **modeling**
- Influence on electron-phonon and electron-electron interactions on system properties (scatterings, dispersions, spectra)
- **Modeling** whole electronic **devices**
- Various insight into the **roots of particular experimental properties**, including electronic and thermal properties
- Giving the **wider context/mechanism to new experimental findings**
- **Project proposals** and **paper preparation and writing**
- ... and many, many more.

Theorists:
“Too many?”,
or “too few?”,
or “just fine”?

How it goes:

Physics experiment and theory are very, very distinct activities, although we remember having commons roots, and have some memories of the branching points!

it starts slow, and lasts long ..
lot of patience from both sides

Possible/best methods:

- Just **hang around**, and **listen regularly** and carefully **about** what the other side is doing.
- **Do your regular job**, theoretical and experimental jobs, **to best quality possible**. This fills person with confidence, it feels in collaboration, and produces will and optimism to crack any problems. Have your "my only, pure research project" all the time at your side.
- **Tell about your recent findings** before or after publications, **in most friendly way**. Enlighten your prospective collaborators.
- **No premature optimism**, but **the things will precipitate eventually**, if **inclination** exists from both sides.
- **Set time apart** to **discuss small/medium things** when an opportunity shows.
- **Read highly influential papers** to see those which present **wide range of expertise.**
- **Show your work process**, expose your thinking, to get appreciated.
- Ensure to apply for some **small common projects**, or a share of a bigger one, to provide **some financing** for the joint activity.
- Mere "salad dressing" has limited capability to "sparkle joy".
- …

Plan your project/ activity/ papers where your other-side collaborators may take a slot, or not.

Recognize people that share the optimism for continuous collaboration, though one-job-at-the-time.

OSB: Transport properties

Subject: Thermal transport properties of semiconductors, phonon scattering mechanisms, electron-phonon interaction
Method: Combination of analytical and phenomenological modeling
Joint publications with experimentalists:

- Communications Physics 2, 123 (2019): *Tailoring thermal conduction in anatase* TiO_2
- J. Phys. Chem. C 119, 3918 (2015): *The Role of Transport Agents in* MoS_2 *Single Crystals*
- J. Phys. Chem. Lett. 5, 2488 (2014): *Ultra Low Thermal Conductivity in organic - inorganic hybrid perovskite* $CH_3NH_3PbI_3$
- Phys. Rev. B 78, 104204 (2008): *Anisotropic magnetic, electrical and thermal transport properties of Y-Al-Ni-Co decagonal approximant*

Spinoff theoretical work:

- Phys. Rev. B 102, 241111(R) (2020): *Exact solution of electronic transport in semiconductors dominated by scattering on polaronic impurities*

Emphasis on resonant scattering due to nondispersive internal degrees of freedom:

a) polaronic impurities
b) rotational degrees of freedom

OSB: ARPES experiments and theory

Subject: ARPES spectra characterized by strong polaronic effects
Method: Diagrammatic approach to electron and phonon quasi-particle properties
Joint publications with experimentalists:

- Nat. Commun. 7, 10386 (2016): *Polaronic metal state at the* $LaAlO_3/SrTiO_3$ *interface*
- Phys. Rev. Lett. 110, 196403 (2013): *Tunable Polaronic Conduction in Anatase* TiO_2

Spinoff theoretical works:

- Phys. Rev. B 102, 121108(R) (2020): *Manifestations of the electron-phonon interaction range in angle-resolved photoemission spectra*
- Phys. Rev. B 106, 075207 (2022): *Importance of coupling strength in shaping electron energy loss and phonon spectra of phonon-plasmon systems*

Identification of phonon sidebands as fingerprints of electron-phonon coupling

OSB: Cuprates

Subject: Transport and optical properties
Method: Phenomenological modeling
Joint publication with experimentalists:

- Phys. Rev. B (2023): *Characterization of two electronic subsystems in cuprates*
- *through optical conductivity*
- *Transport properties and doping evolution of the Fermi surface in cuprates*

Emphasis on two electronic subsystems: FL + localized holes

Other themes that may get relevant for local experimental community

IB,2015-2019
Subject: Hysteresis phase transition
Method: Functional renormalization group, differential equation analysis
Publication: * Phys. Rev. B 97, 094204 (2018)
** Journal of Statistical Mechanics: Theory and Experiment 2019 (10), 103301*
** Phys. Rev. E 102, 062154 (2019)*
**Phys. Rev. B 91, 214201 (2015)*

Developing understanding of the hysteresis phase transition and its glassy dynamics

Analytical features of the disorder driven phase transitions in fermionic systems

IB 2018,2019
Subject: Universality in fermionic systems with disorder
Method: Functional renormalization group, perturbative methods, differential equation analysis
Publication: * Physical Review Letters 121, 166402 (2018)
* Journal of Statistical Mechanics: Theory and Experiment 2019 (3), 033215

Constructing observables out of renormalization group quantities

IB2022
Subject: Probabilistic interpretation of the renormalization group
Method: Functional renormalization group, Monte Carlo methods, large deviations
Publication: Physical Review Letters 129 (21), 210602 (2002)

Pop1988, ET

Method: Calculation of various transport **coefficients** using **standard (Boltzmann) transport theory** and the tight-binding model and **peculiar energy gaps** suggested earlier, and compared with experimental results

Publication: Joint paper with exp. group Solid State Commun. (1988): M. Petravić, E. Tutiš, A. Hamzić, L. Forro, *Hall effect measurements in* $La_{2-x}Ba_xCu_4$

A side job for a theoretical guy!

Sip2008,ET

Subject: Superconductivity in electronically phase-separated charge-density-wave system

Method: Concepts and modelling in the (CDW) systems with partial/frustrated electronic phase separation. Interpretation, writing.

Publication with L. Forro exp. group : Nat. Mat. (2008) *From Mott state to superconductivity in* 1T-TaS_2,

Then, very much related to most dear theoretical interests!

...

Mar2020, ET

Stunning conductivity anisotropy in layered CDW system

Th. Methods: Ab-initio calculations inspired by nearly commensurate CDW phase measured experimentally

Publication: npj 2D Mat. & Appl. (2020) *Preferential out-of-plane conduction and quasi-one-dimensional electronic states in layered* 1T-TaS_2

It is stunning and I believed that I knew the system!

Pop2023

Subject: Many physical properties of a layered metallic-magnetic system

Th. Methods: DFT and various theoretical modeling

Publication with exp group submitted Phys. Rev. B.(2023): *Electronic transport and magnetism in the alternating stack of metallic and highly frustrated magnetic layers in* $Co_{1/3}NbS_2$

Elaborate study, after getting known the system! @IFS driven!

init by Forro!

ET1991

Subject: The emergence of phason and amplitudon modes from ordinary phonons. **Dynamic structure factor** S(k,ω) in Peierls systems, calculated and experimentally measured by neutron diffraction..
Method: Monte Carlo + Molecular dynamics numerical simulations of strongly non-linear crystal lattice system.
Publication: **Exp.** (exp: J.P.Pouget group, Paris) **and theor. papers appearing together** in
Phys. Rev. B (1991): *Dynamic structure factor of a one-dimensional Peierls system,*

Pointed to study an unsolved theoretical problem!
(any way you choose!)

OLEDs2001++, ET

Subject: Elaborate **experimental investigation and theoretical modelingof processes in of organic multilayers**
Method: Modeling polaron hopping transport, injection, recombination. Electrostatic modeling of rough electrodes.
Numerical solution to a large sparse matrix problems
Joint publications with experimentalists:

- J. Appl. Phys. 89 (**2001**) Numerical model for organic light-emitting diodes,
- J. Appl. Phys 93 (**2003**) Internal electric field and charge distribution in multilayer organic light-emitting diodes,
- J. Appl. Phys. 95 (**2004)** Splitting of the recombination zone in organic light emitting diodes by dye doping.
- Adv. Fun. Mat. 15 (**2005**) Doping-induced charge trapping in organic light-emitting devices,
- Phys. Rev. B. (**2004**) Injection and strong current channeling in organic disordered media,
- J. Appl. Phys. (**2006**): Investigation of the charge transport through disordered organic molecular
- Phys.Rev.B. (**2009**) Diffusion of triplet excitons in an operational organic light-emitting diode.

Modeling the complex experimental system.
From grounds up!

YUB2023

Subject: Electronic structure of metallic-magnetic systems.
Layered metallic system intercalated by Ni magnetic ions
Methods: DFT and various theoretical modeling
Publication with exp group submitted (2023): Intercalation-induced states at the Fermi level and the coupling of intercalated magnetic ions to conducting layers in Ni1/3NbS2

Paradigm shifting.
Mostly @IFS driven!

No Forro: Forro Zuppiroli, Berner, Nuesch, Lebental, IF/Zagreb

More elaborate list at: https://www.dropbox.com/s/xhvf57rhv0mr8kq/ET-methods-w-experimentalists.docx?dl=0