Nonequilibrium Materials Engineering

Michael A. Sentef

New Tools for Emergence and Non-Equilibrium Physics
Teddington, December 18, 2018

lab.sentef.org
Condensed Matter Dynamics
Andrea Cavalleri
Atomically Resolved Dynamics
Dwayne Miller
Theory
Angel Rubio
+2
ULTRAFAST X-RAY SUMMER SCHOOL - June 16-21, 2019
DEUTSCHES ELEKTRONEN-SYNCHROTRON (DESY) - HAMBURG

UXSS 2019

The Center for Free-Electron Laser Science (CFEL) at DESY in Hamburg, Germany will be hosting the Ultrastar X-ray Summer School 2019. UXSS 2019 is jointly organized by CFEL and the PULSE Institute at SLAC National Accelerator Laboratory. The summer school program will be highly interdisciplinary, with topics ranging from accelerator physics to molecular biology, and is intended to give doctoral students and postdoctoral researchers the opportunity to familiarize themselves with the latest developments and opportunities in ultrastar X-ray science.

Invited Lecturers:
Siegfried Gliener (SLAC)
Frank de Groot (Leiden University)
Giorgio Margaritondo (EPFL, Lausanne)
Bjørn Mortz (SLAC)
Ian McNulty (Lund University)
Nina Rohringer (Hamburg University/DESY)
Ondřej Vendrell (Haidenberg University)
Simon Wall (CfFO Barcelona)
Junko Yano (LBL Berkeley)

CFEL
PULSE	STANFORD

Financial support for UXSS 2019
https://conferences.cfel.de/uxss2019

SENTEFLAB
ultrafast materials science
Quantum materials

Crystal structure

Couplings

- electron-electron
- electron-phonon
- electron-magnon

Electron band structure

Complex phase diagram

- Temperature, T (K)
- Hole doping, p


W. Hu et al., Nature Materials 13, 705 (2014)


Image Credit: Department of Theoretical Physics at Ural University
**Engineering materials with light**

- **condensed matter**
  - quantum materials
  - atomic-scale control

- **quantum optics**
  - nanoplasmonics
  - polaritonic chemistry

- **nonequilibrium materials engineering**

- **ultrafast spectroscopy**
  - revealing elementary couplings
  - light-induced new states of matter

- **pump-probe: strong classical fields**

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R. Chikkaraddy et al., Nature 535, 127 (2016)

Y. Cao et al., Nature 556, 43 (2018)

QED: vacuum fluctuations

Image courtesy: J. Sobota
Engineering materials with light

Hamiltonian engineering
e.g., Floquet-Bloch bands

Distributional engineering

many ingredients, hard to disentangle


J. Sobota et al., JESRP 195, 249 (2014)
Engineering materials with light

Exposing hidden states
nonthermal switching process

Light-induced new states
transient superconductivity?

Resistance after a laser pulse

Resistance change after a (single) 35 fs pulse

Switching to a hidden state in $1T$-TaS$_2$:

L. Stojchevska et al., Science 344, 177 (2014)

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Microscopic understanding?

M. Mitrano et al., Nature 530, 461 (2016)
Research profile

nonequilibrium dynamics
   Keldysh Green's functions
   time-dependent density functional theory

materials science
   lattice models
   effective models
   ab initio

pump-probe spectroscopy
   bridge to experiments

**mission statement**: to understand and predict emergent properties of quantum materials interacting with light away from their thermal equilibrium
Engineering topology with light

H. Hübener et al., Nature Comm. 8, 13940 (2017)

Hamiltonian engineering
Light-induced Weyl fermions in Na$_3$Bi
Floquet time-dependent density functional theory

Kapitza pendulum

Dancing Weyl fermions
y–z Polarized light
x–z Polarized light

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Engineering topology with light

N. Tancogne-Dejean, MAS, A. Rubio, PRL 121, 097402 (2018)

Coupling engineering
Dynamical ab initio Hubbard U
Light-induced Weyl fermions in pyrochlore iridates

Time-resolved photoemission
nonthermal effects
bands + distributions important
Ultrafast transport

Optical control of transport and topology

Light-induced anomalous Hall effect in graphene

Theory: bands + distributions important!

S. A. Sato et al., in preparation
MAS et al., Nature Comm. 6, 7047 (2015)
Optical control of chiral condensates

Switching a topological superconductor
Universal optical switching of chiral Majoranas
Dynamical BCS-Keldysh
Towards programmable quantum gate?

program the gate optically, read it out electrically

M. Claassen et al., arXiv:1810.06536, Nat. Phys. in review

M. Claassen et al., in preparation
cf. B. Lian et al., PNAS 115, 10938 (2018)
From classical to quantum light

R. Chikkaraddy et al., Nature 535, 127 (2016)

collective strong light-matter coupling

what about cavity materials?
Cavity materials

Polaritonic materials engineering
Light-enhanced electron-phonon coupling in monolayer FeSe/SrTiO$_3$
Migdal-Eliashberg theory

no heating
no need for strong lasers
long lifetime of light-induced states
Ongoing and outlook

**Method development for ultrafast transport and condensates**
- **ultrafast transport in 2D materials** (G. Topp, S. Sato, L. Xian, J. McIver, B. Schulte, G. Jotzu)
- bridging Boltzmann and Keldysh, excitonic insulators (R. Tuovinen et al., 1808.00712)

**Driven low-dimensional correlated systems**
- time-dependent density matrix renormalization group (M. Kalthoff, D. Kennes)
- machine learning variational Monte Carlo for driven systems (D. Hofmann, G. Carleo)

**Dynamical band structure engineering**
- Subgap melting of charge density wave in quantum wires (M. Chávez-Cervantes et al., 1810.09731)
- Floquet versus subcycle spectroscopy in time-resolved ARPES (G. Topp, I. Gierz)

**Inhomogeneous systems and THz STM**
- real-space imaging of 2D ordered phases (D. Kennes, S. Loth)
- chiral domains and programmable quantum gates (M. Claassen, D. Kennes)

**Cavity materials**
- cavity topology engineering (X. Wang, E. Ronca, S. Latini, ...)
- polaritonic 2D materials (V. Rokaj et al., arXiv:1808.02389)

... and more!
Team and collaborators

thank you for your attention!

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Ultrafast spectroscopy

Stanford running horse

Muybridge 1887

Image courtesy: J. Sobota
Ultrafast spectroscopy

Stanford running horse

Muybridge 1887

TbTe$_3$ charge-density wave

Image courtesy: F. Schmitt
Method: Keldysh Green functions

\[ G_k(\omega) = G_k^0(\omega) + G_k^0(\omega) \Sigma(\omega) G_k(\omega) \]

\[ G_k(t, t') = G_k^0(t, t') + \int dt_1 dt_2 G_k^0(t, t_1) \Sigma(t_1, t_2) G_k(t_2, t') \]

self-energy \( \Sigma \): electron-electron scattering, electron-phonon scattering...

initial state

pump-probe photoemission

\[ E_V \]

probe pulse

\[ E_F \]

pump pulse

\[ T \]

\[ T + \Delta \]

\[ t = t' \]

\[ t' \]

\[ T \]

\[ T + \Delta \]

\[ t \]