mpsd

Nonequilibrium Materials Engineering

Michael A. Sentef

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

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ultrafast materials science
lab.sentef.org

Emmy Noether-Programm
Deutsche Forschungsgemeinschaft
DFG
Funded through DFG Emmy Noether Programme (SE 2558/2-1)

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MPI for the Structure and Dynamics of Matter

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Condensed Matter Dynamics

Andrea Cavalleri

Atomically Resolved Dynamics

Dwayne Miller

Theory

Angel Rubio

+2

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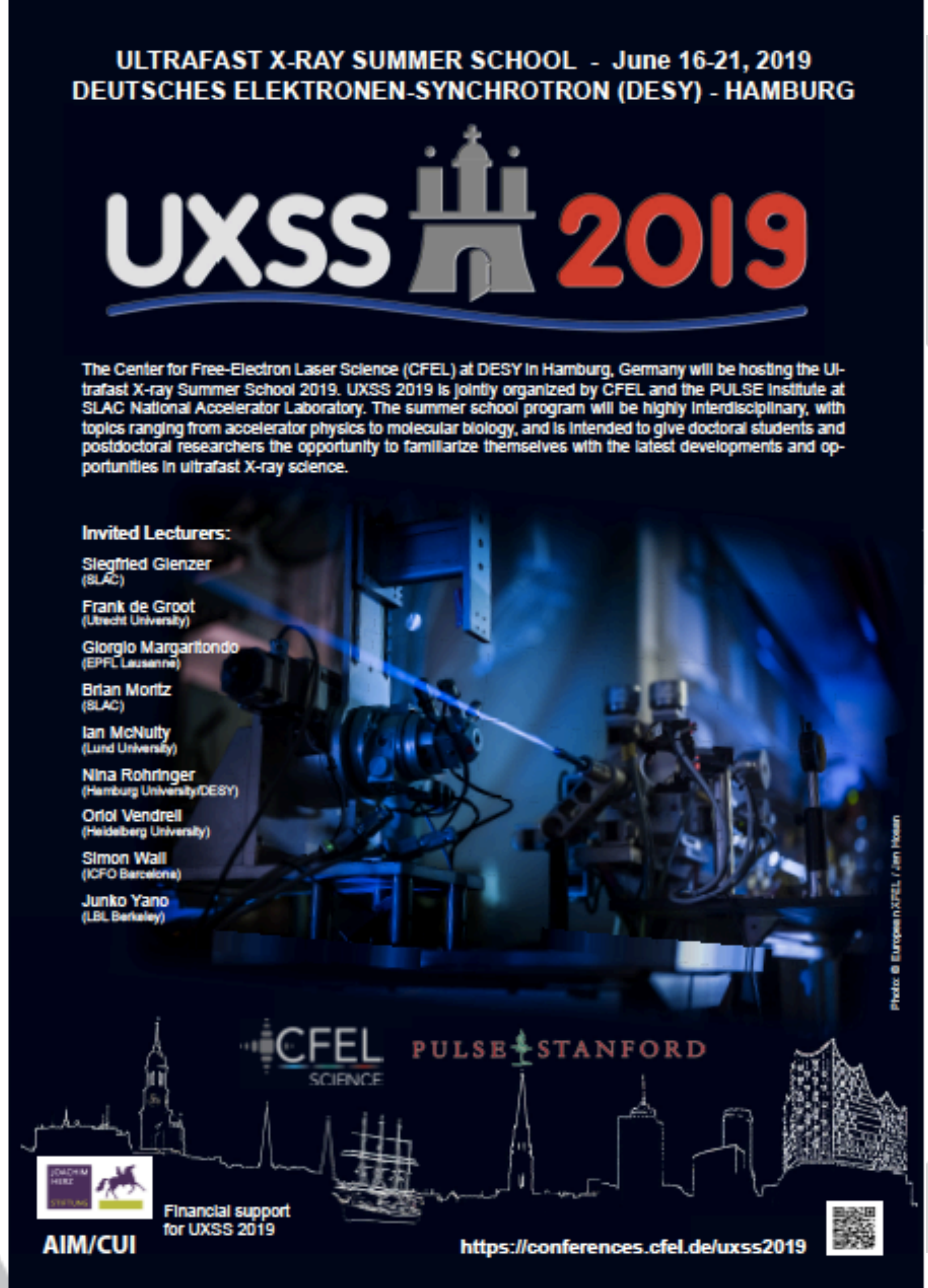

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Quantum materials

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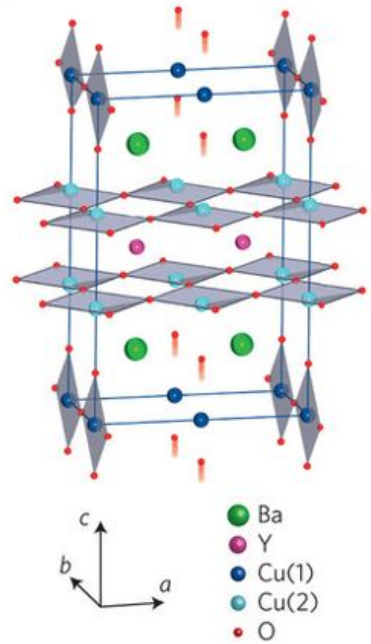
crystal structure

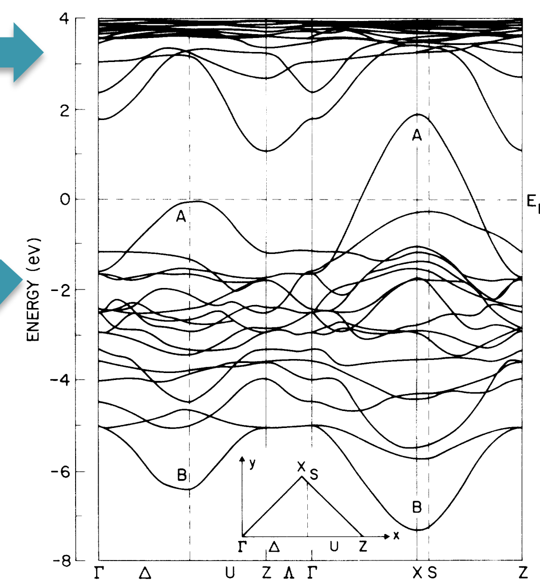


W. Hu et al., Nature Materials 13, 705 (2014)

couplings

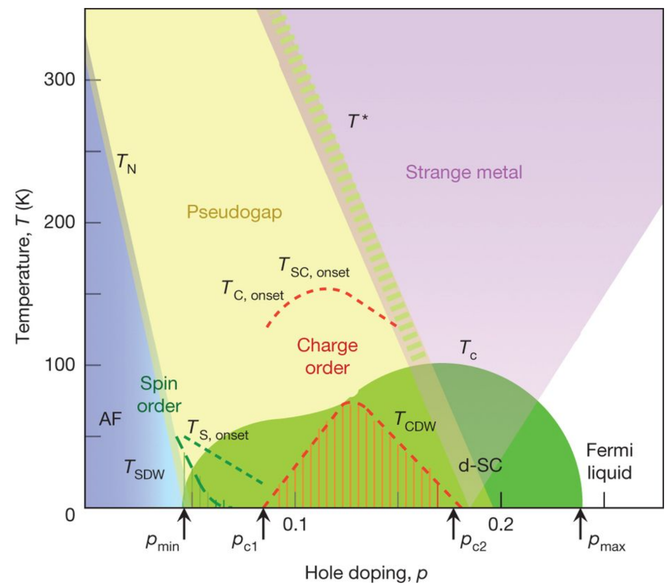
electron-electron
electron-phonon
electron-magnon
...

electron band structure



L. F. Mattheis, Phys. Rev. Lett. 58, 1028 (1987)

complex phase diagram



B. Keimer et al., Nature 518, 179 (2015)

Image Credit:
Department of Theoretical Physics at Ural University

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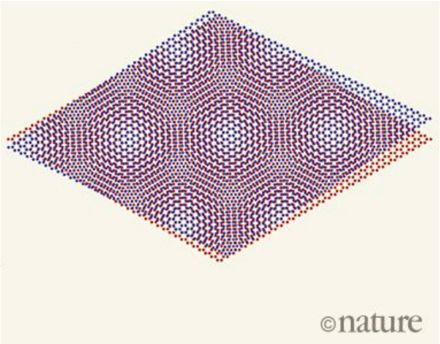
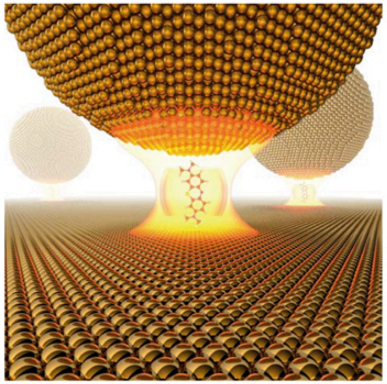
Engineering materials with light

condensed matter
quantum materials
atomic-scale control



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

nonequilibrium materials engineering



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

quantum optics
nanoplasmonics
polaritonic chemistry
QED: vacuum fluctuations

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

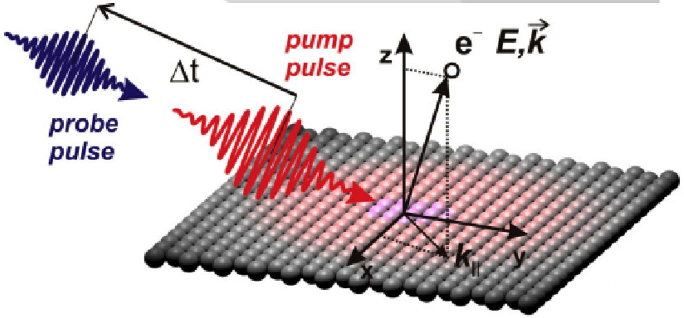


Image courtesy: J. Sobota

pump-probe: strong classical fields

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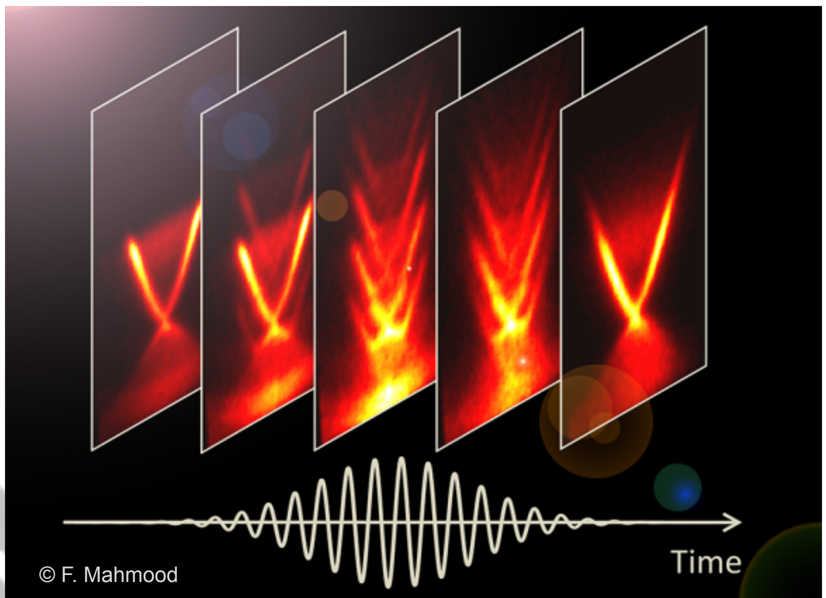
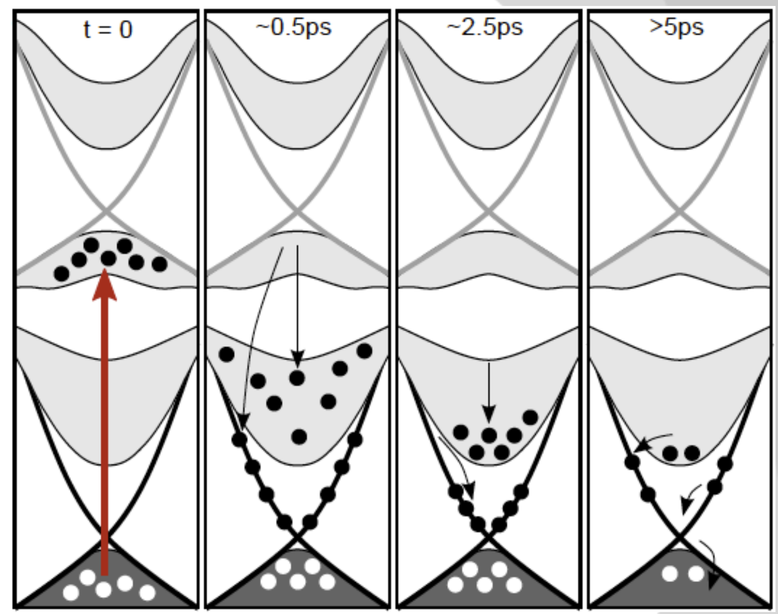
Hamiltonian engineering
e.g., Floquet-Bloch bands



F. Mahmood et al., Nature Physics 12, 306 (2016)

Distributional engineering



J. Sobota et al., JESRP 195, 249 (2014)

many ingredients, hard to disentangle

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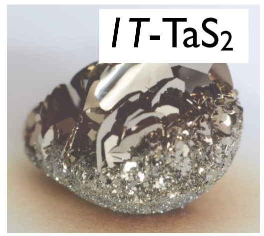
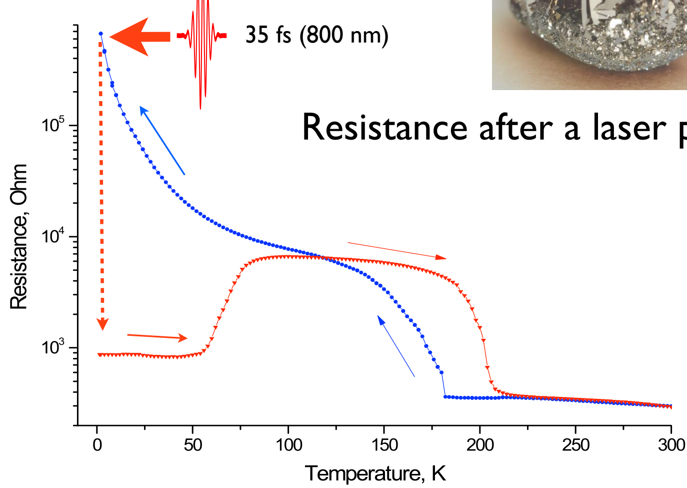
Engineering materials with light

Exposing hidden states

nonthermal switching process



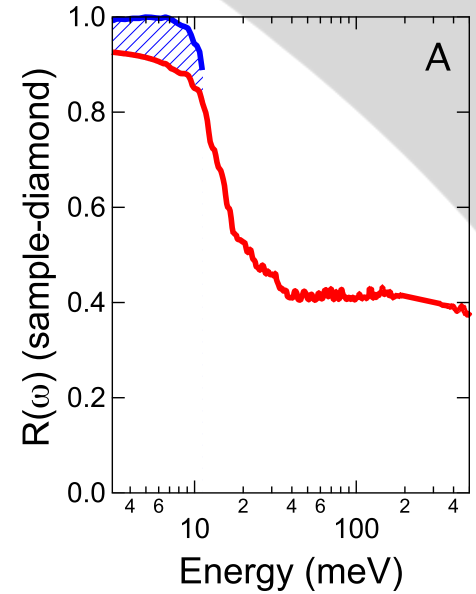


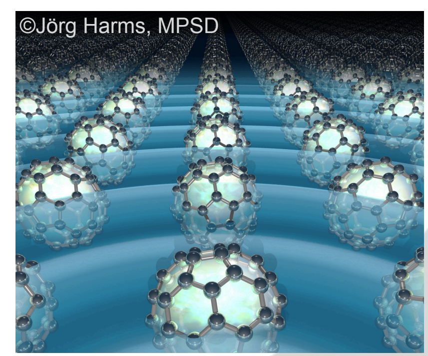
L. Stojchevska et al., Science 344, 177 (2014)

microscopic understanding?

Light-induced new states

transient superconductivity?





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

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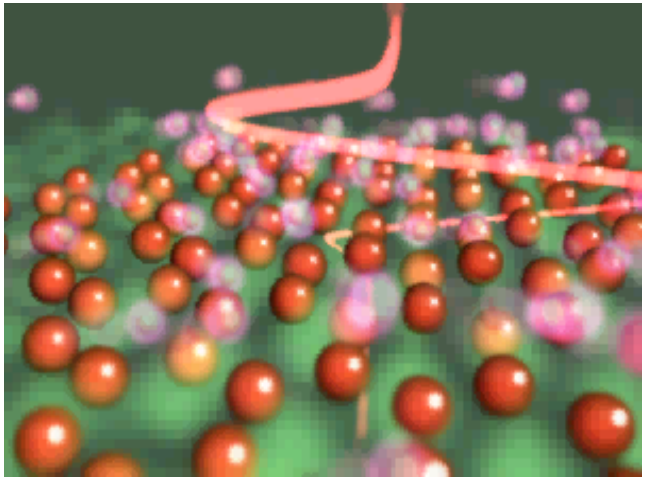
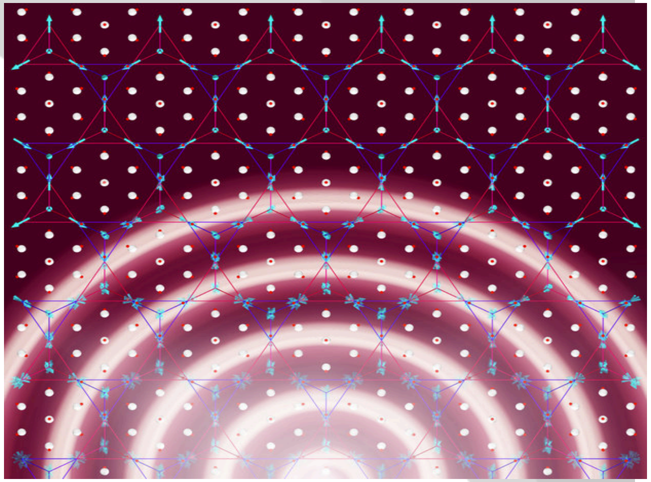
Research profile

Images:
Koichiro Tanaka (Kyoto U)
Jörg Harms (MPSD)





G. E. Topp et al., Nature Comm. 9, 4452 (2018)

nonequilibrium dynamics

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

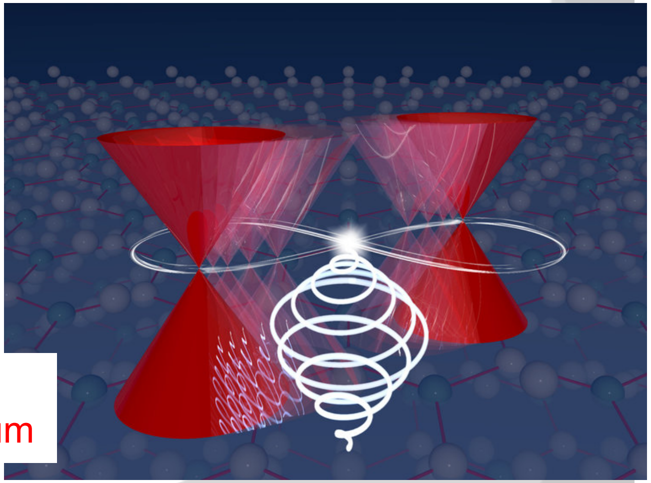
materials science

- 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 equilbrium



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

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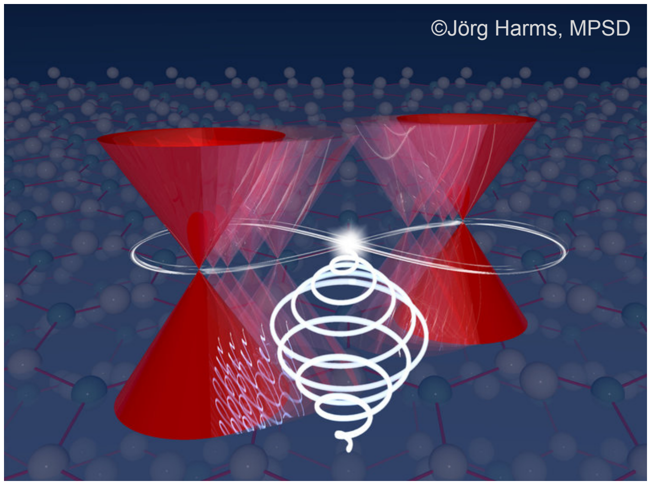
Engineering topology with light



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

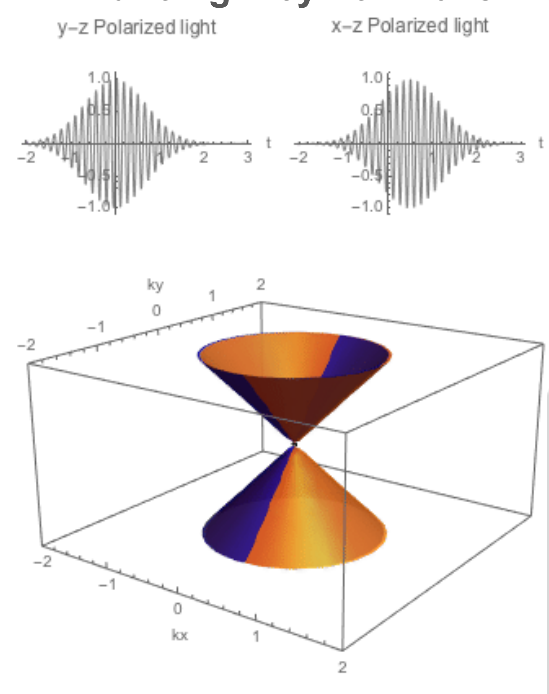
Hamiltonian engineering

Light-induced Weyl fermions in Na_3Bi

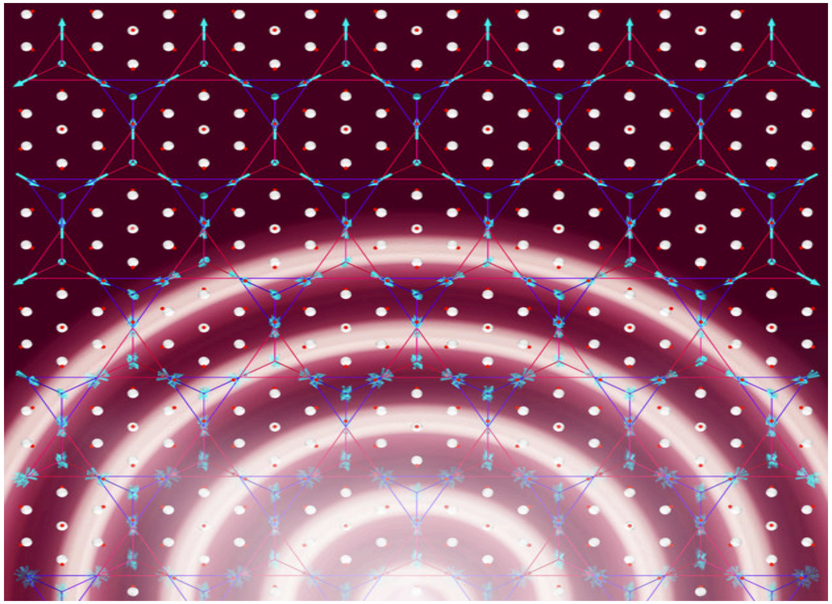
Floquet time-dependent density functional theory

Kapitza pendulum

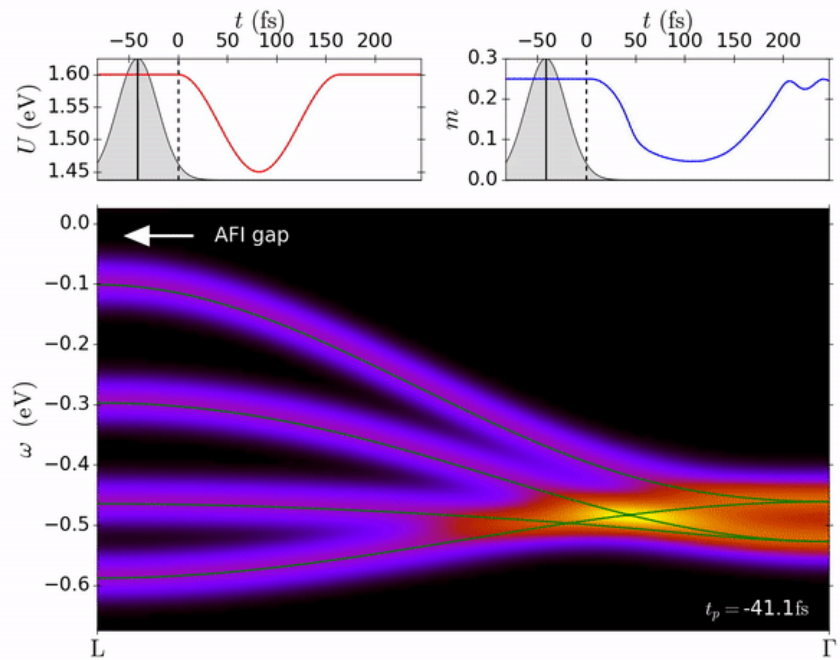
Dancing Weyl fermions



Engineering topology with light



G. E. Topp et al., Nature Comm. 9, 4452 (2018)
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

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Ultrafast transport

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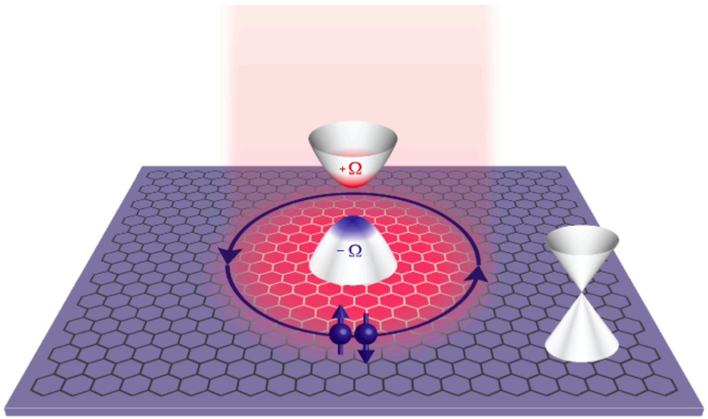
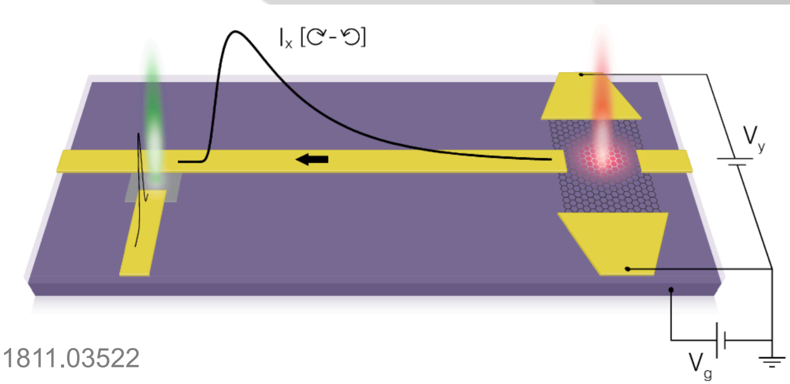


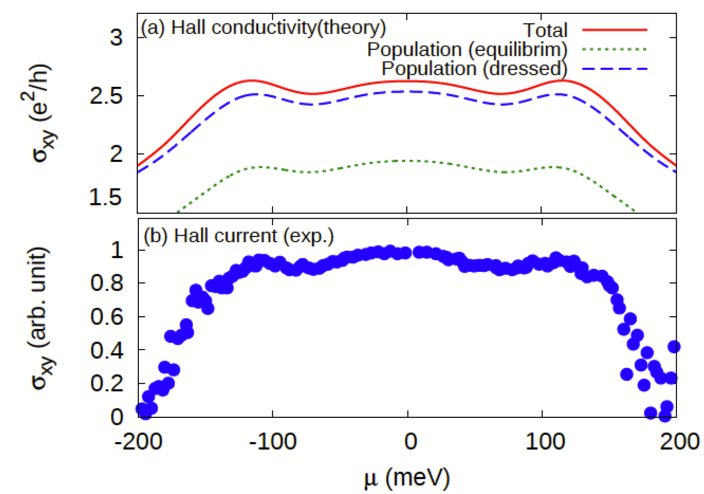


J. W. McIver et al., arXiv:1811.03522

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)

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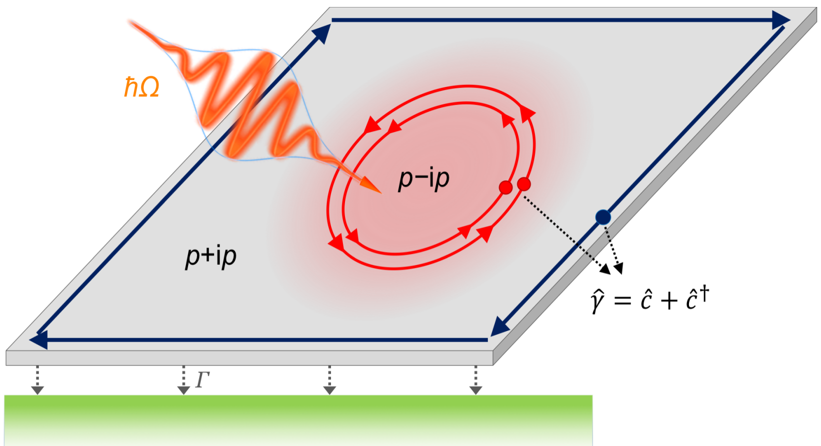
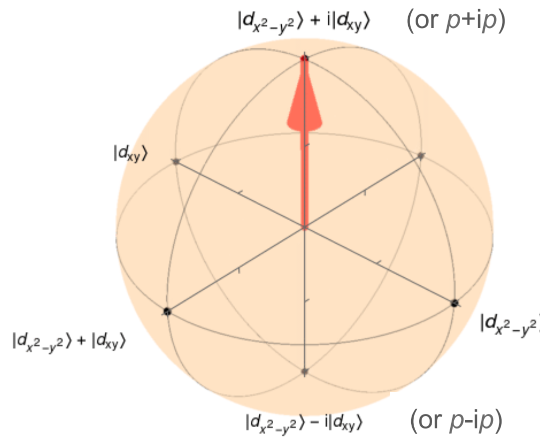
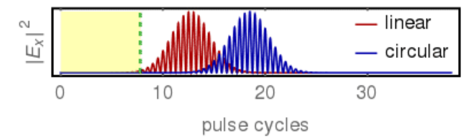
Optical control of chiral condensates



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



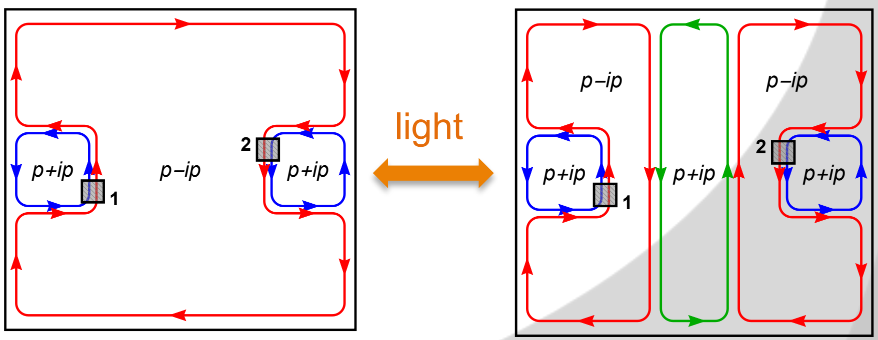


Switching a topological superconductor

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., in preparation
cf. B. Lian et al., PNAS 115, 10938 (2018)

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From classical to quantum light

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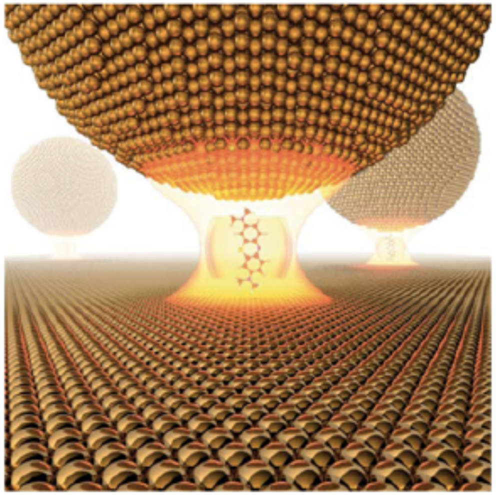
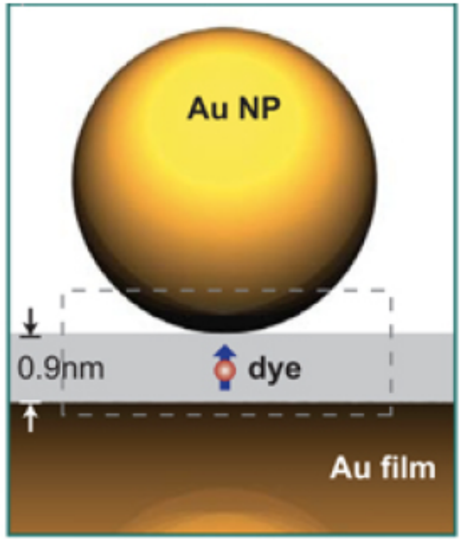
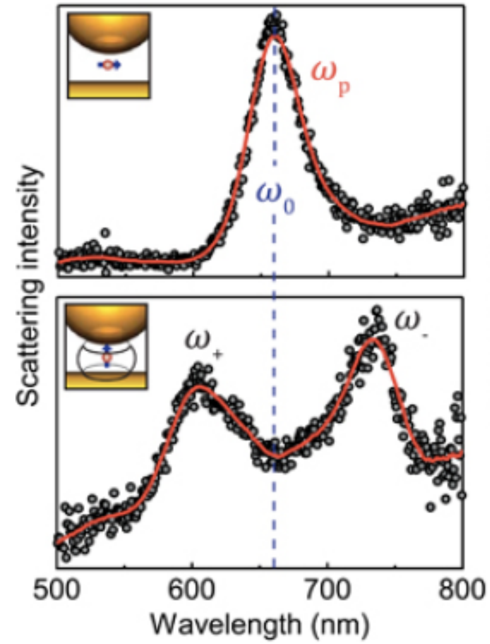




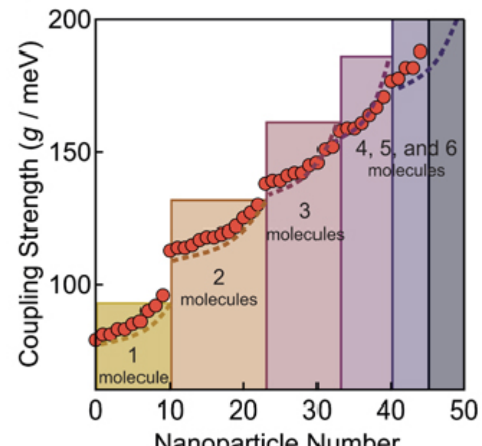
R. Chikkaraddy et al., Nature 535, 127 (2016)



Rabi splitting

collective strong light-matter coupling

what about cavity materials?



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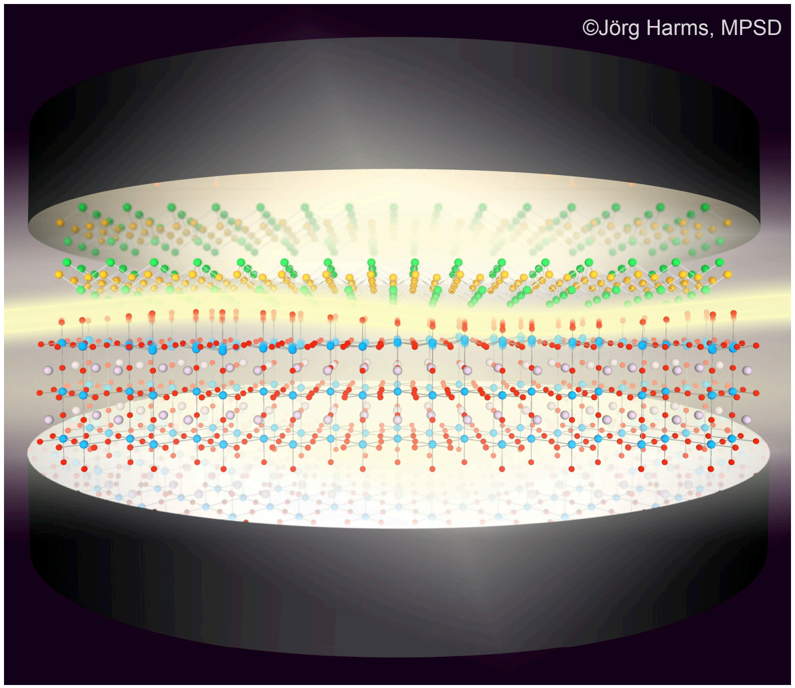
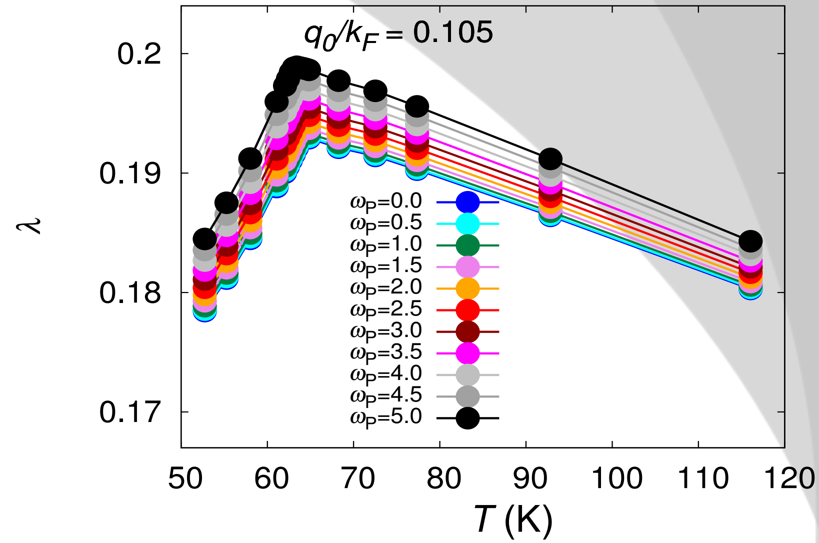
Cavity materials





MAS, M. Ruggenthaler, A. Rubio, Science Advances 4, eaau6969 (2018)

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

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Ongoing and outlook

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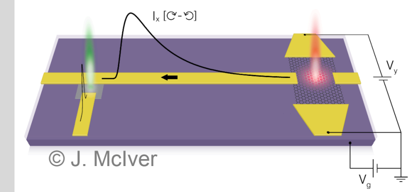
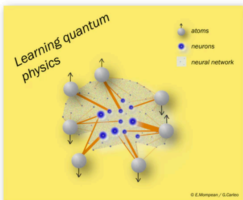
Method development for ultrafast transport and condensates

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

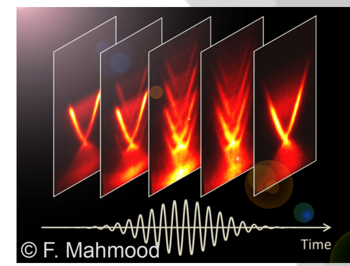
time-dependent density matrix renormalization group (M. Kalthoff, D. Kennes)

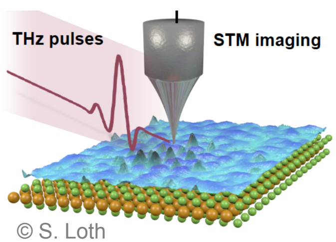
machine learning variational Monte Carlo for driven systems (D. Hofmann, G. Carleo)

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

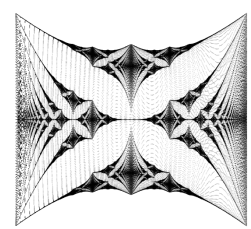
real-space imaging of 2D ordered phases (D. Kennes, S. Loth)

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)



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... and more!

Team and collaborators

thank you for your attention!

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Funded through DFG
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Emmy Noether-Programm
Deutsche Forschungsgemeinschaft
DFG

Ultrafast spectroscopy

Stanford running horse

Muybridge 1887

pump-probe spectroscopy today

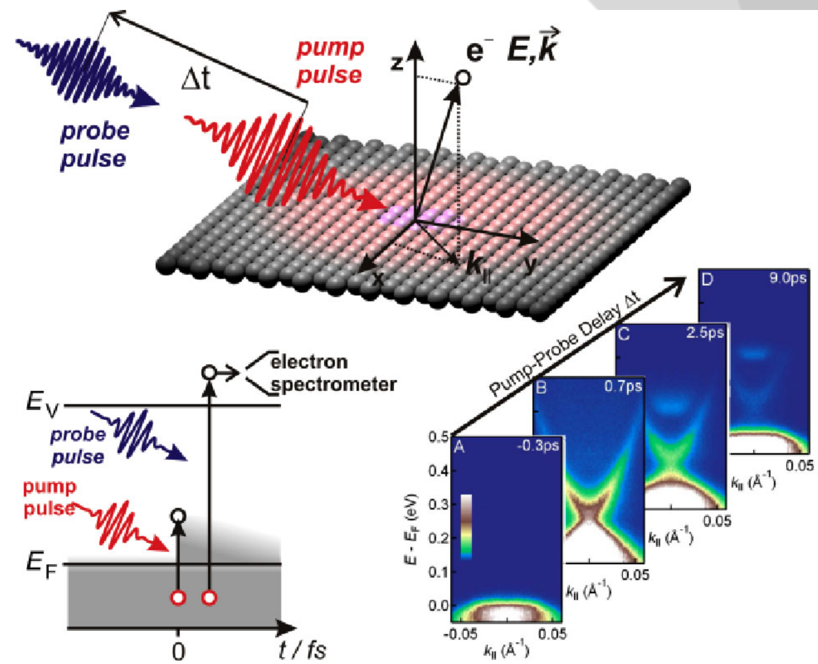

Image courtesy: J. Sobota

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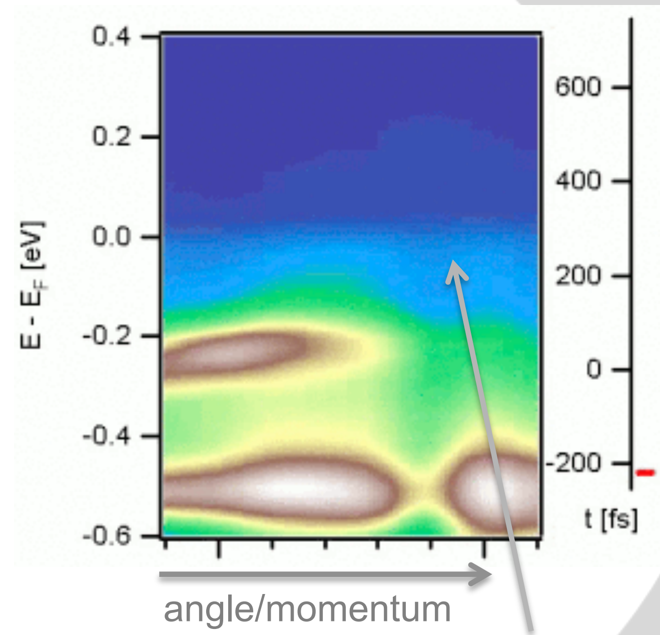
Ultrafast spectroscopy

Stanford running horse

Muybridge 1887

$TbTe_3$ charge-density wave



F. Schmitt et al., Science 321, 1649 (2008)
Image courtesy: F. Schmitt

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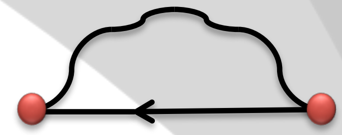
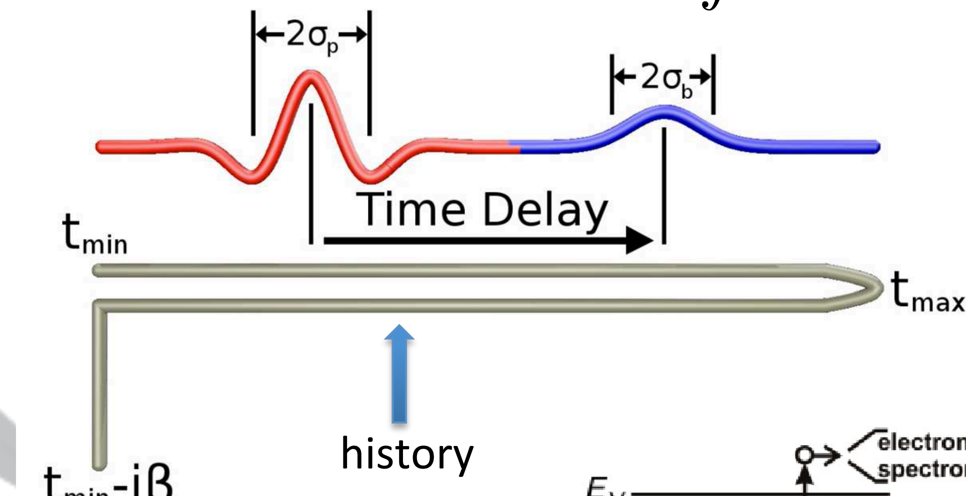
Method: Keldysh Green functions

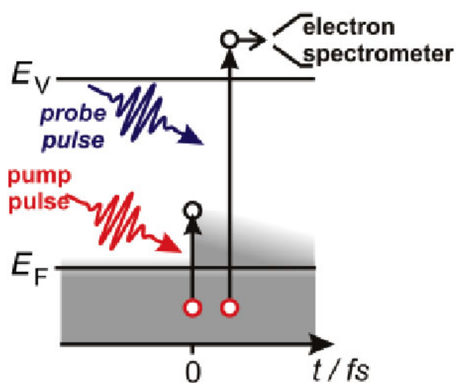
$$G_k(\omega) = G_k^0(\omega) + G_k^0(\omega)\Sigma(\omega)G_k(\omega)$$



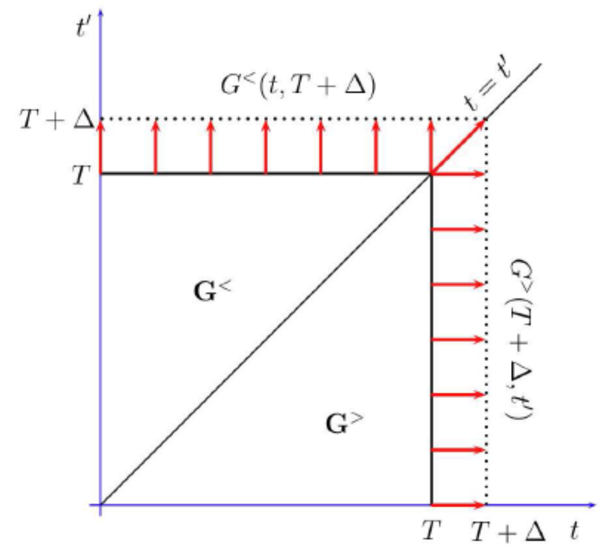
$$G_{\mathbf{k}}(t,t') = G_{\mathbf{k}}^0(t,t') + \oint dt_1 dt_2 G_{\mathbf{k}}^0(t,t_1)\underline{\Sigma(t_1,t_2)}G_{\mathbf{k}}(t_2,t')$$

self-energy Σ:
electron-electron scattering
electron-phonon scattering
...





pump-probe photoemission



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