Nonequilibrium Materials Engineering

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Max-Planck Institute for the Structure and Dynamics of Matter, Hamburg

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DFG

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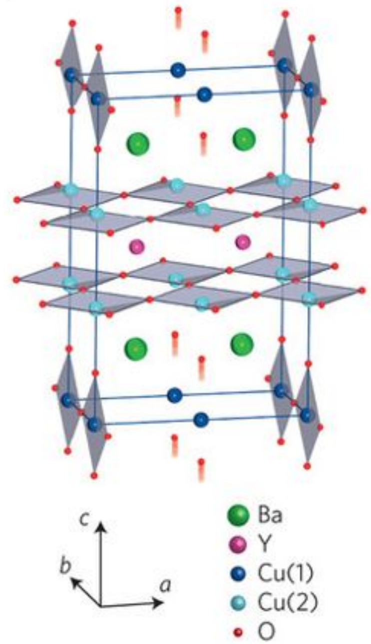
Emmy Noether Programme (SE 2558/2-1)

mpsd

Max Planck Institute for the Structure and Dynamics of Matter

Quantum materials

crystal structure

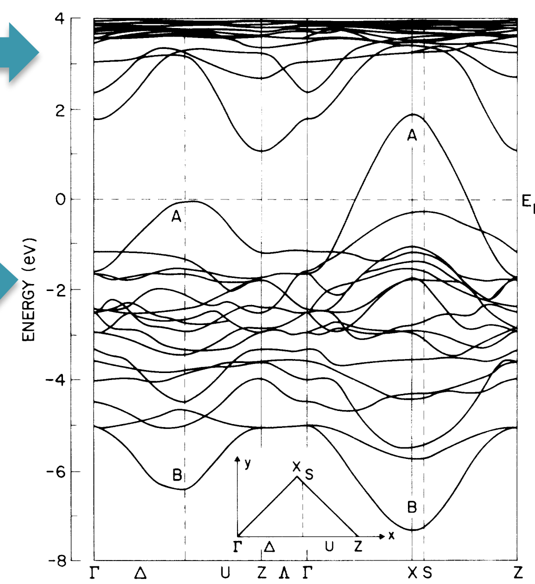


W. Hu et al., Nature Materials 13, 705 (2014)

couplings

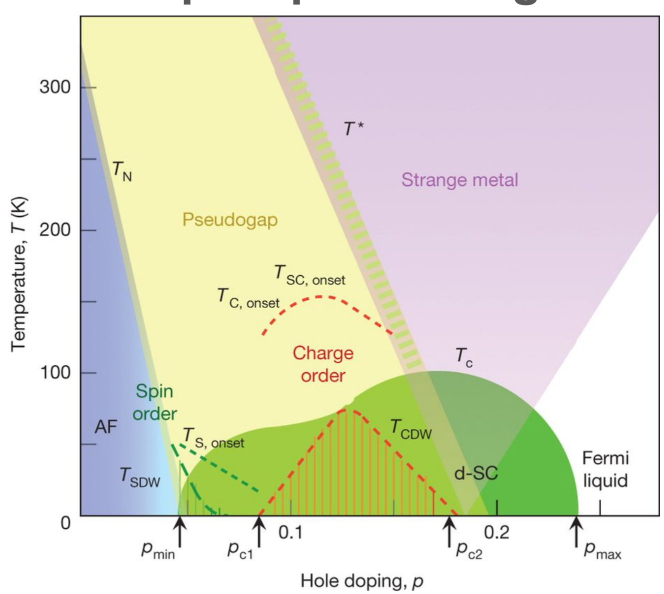
electron-electron
electron-phonon
electron-magnon
...

electron band structure



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

complex phase diagram

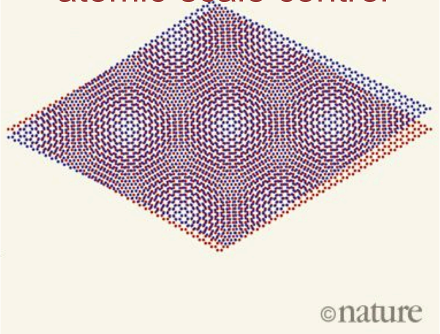


B. Keimer et al., Nature 518, 179 (2015)

Image Credit:
Department of Theoretical Physics at Ural University

Engineering materials with light

condensed matter
quantum materials
atomic-scale control



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

nonequilibrium materials engineering

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

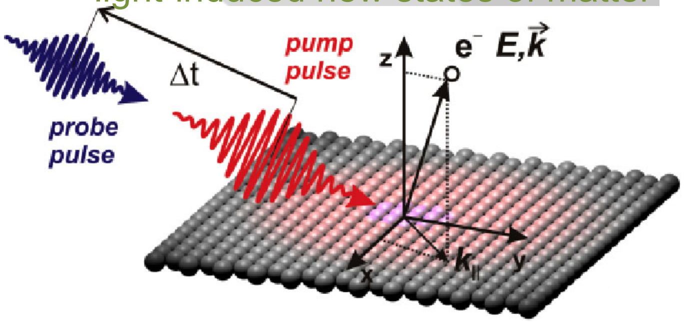
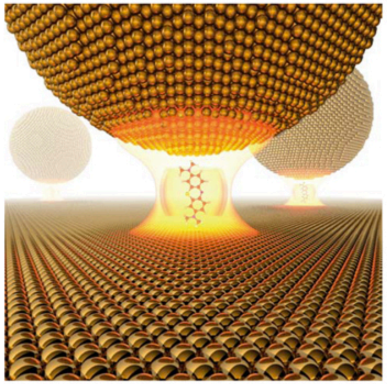


Image courtesy: J. Sobota

pump-probe: strong classical fields



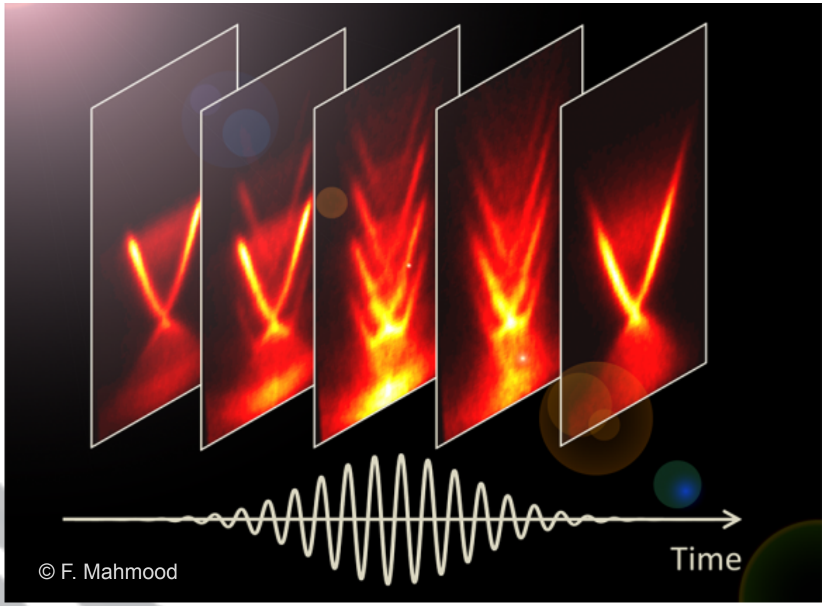
R. Chikkaraddy et al., Nature 535, 127 (2016)

quantum optics
nanoplasmonics
polaritonic chemistry

QED: vacuum fluctuations

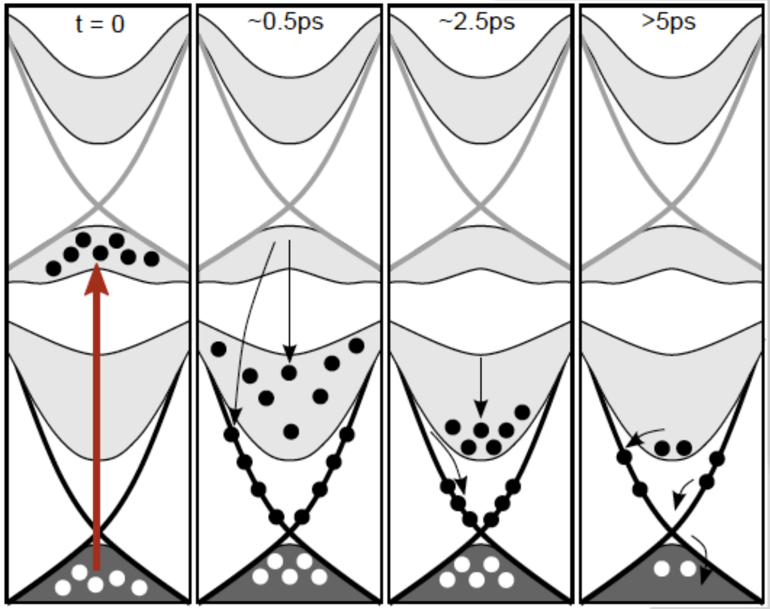
Engineering materials with light

Hamiltonian engineering
e.g., Floquet-Bloch bands



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

Distributional engineering



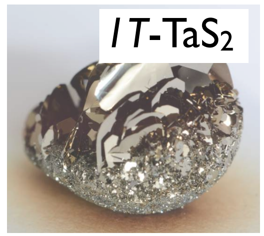
J. Sobota et al., JESRP 195, 249 (2014)

many ingredients, hard to disentangle

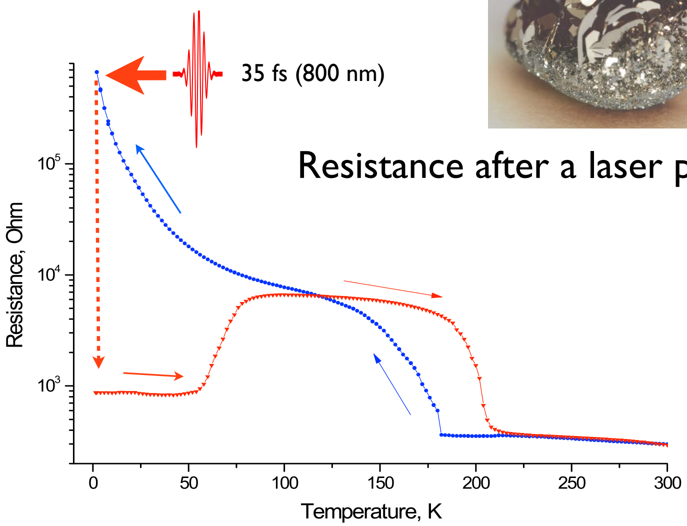
Engineering materials with light

Exposing hidden states

nonthermal switching process



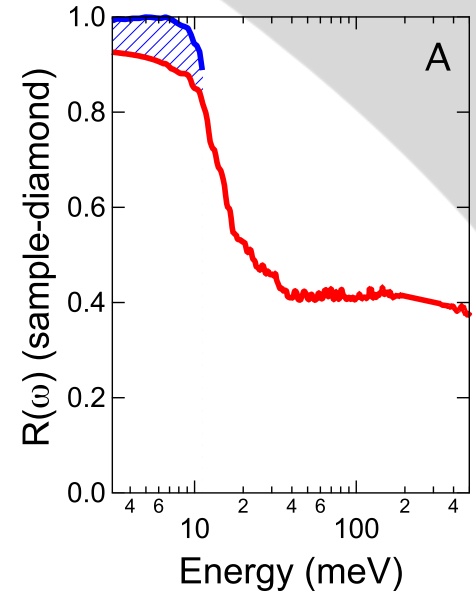
Resistance after a laser pulse

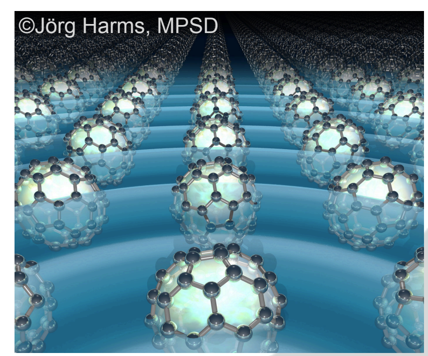


L. Stojchevska et al., Science 344, 177 (2014)

Light-induced new states

transient superconductivity?



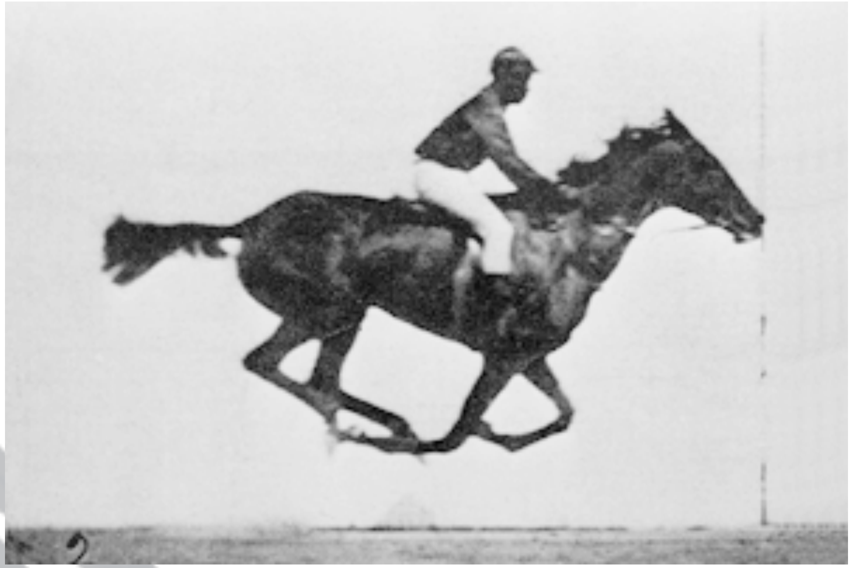


M. Mitrano et al., Nature 530, 461 (2016)

microscopic understanding?

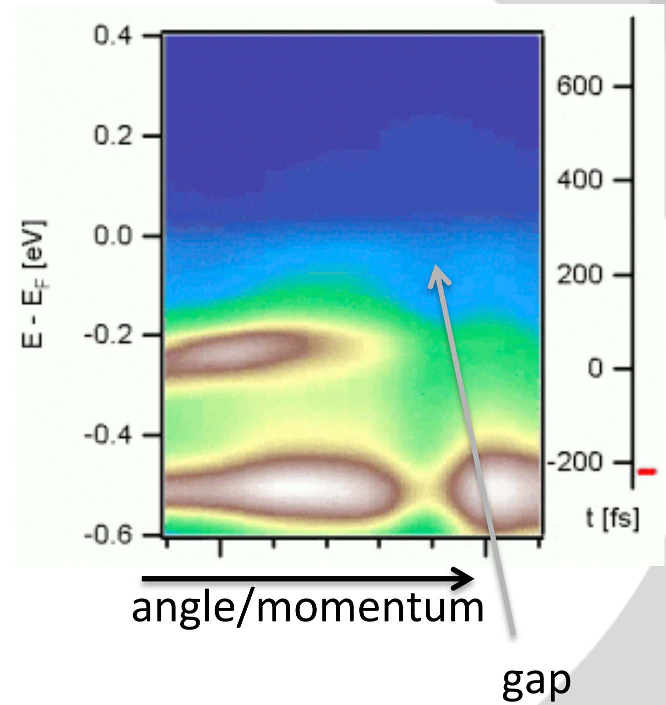
Pump-probe spectroscopy

- stroboscopic investigations of dynamic phenomena



Muybridge 1887

TbTe3 CDW metal



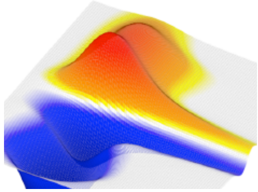
F. Schmitt et al., Science 321, 1649 (2008)
Image courtesy: J. Sobota / F. Schmitt

Ultrafast Materials Science today

Understanding the nature of quasiparticles

- Relaxation dynamics
- Control of couplings

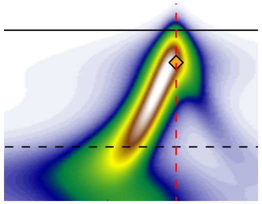
PRL 111, 077401 (2013)
PRX 3, 041033 (2013)
PRB 87, 235139 (2013)
PRB 90, 075126 (2014)
Nat. Comm. 7, 13761 (2016)
PRB 95, 024304 (2017)
PRB 95, 205111 (2017)
PRL 121, 097402 (2018)
arXiv:1802.09437, Sci. Adv.
arXiv:1808.02389



Understanding ordered phases

- Collective oscillations
- Competing orders

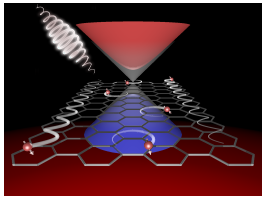
PRB 92, 224517 (2015)
PRB 93, 144506 (2016)
PRL 118, 087002 (2017)
arXiv:1806.08187
arXiv:1808.00712
arXiv:1808.04655
arXiv:1810.06536



Creating new states of matter

- nonequilibrium topological states

Nature Comm. 6, 7047 (2015)
Nature Comm. 8, 13940 (2017)
Nature Comm. 9, 4452 (2018)



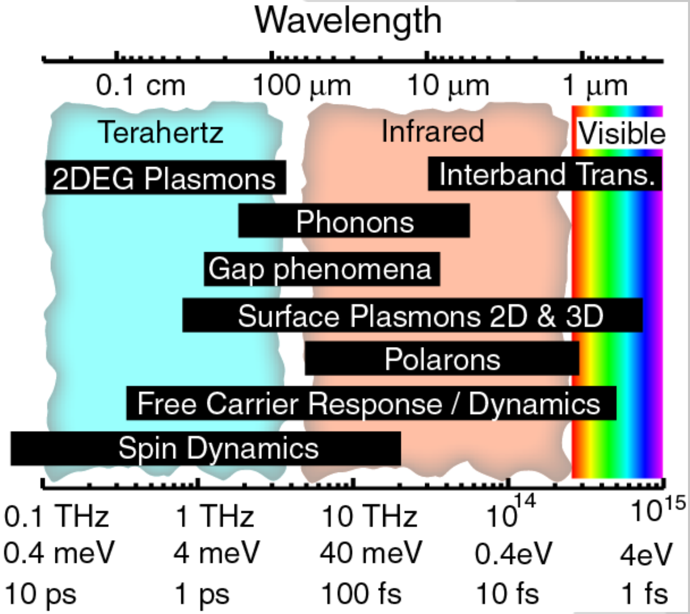


Image courtesy: D. Basov

Electron-boson coupling

Holstein model (minimal version):

$$H = \sum_{k} \epsilon(k) c_k^\dagger c_k + \Omega \sum_i b_i^\dagger b_i - g \sum_i c_i^\dagger c_i (b_i + b_i^\dagger)$$

Electrons
(Fermi gas/liquid)

Bosons
(e.g., Einstein phonon)

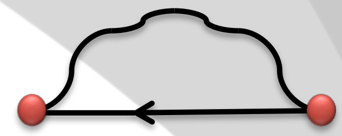
Electron-boson
coupling

Pump laser:

$$\varepsilon(k) \rightarrow \varepsilon(k,t)$$

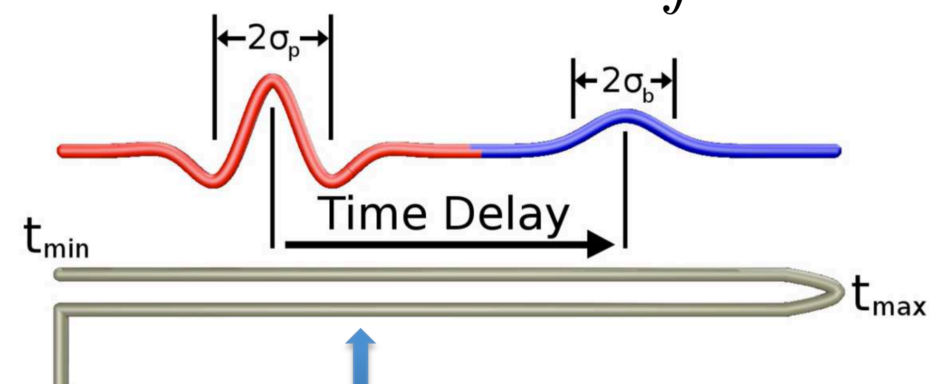
Method: Keldysh Green functions

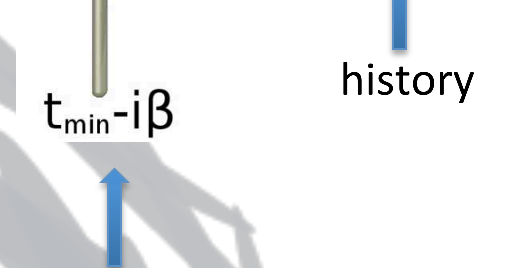
$$~~G_k(\omega) = G_k^0(\omega) + G_k^0(\omega)\Sigma(\omega)G_k(\omega)~~$$

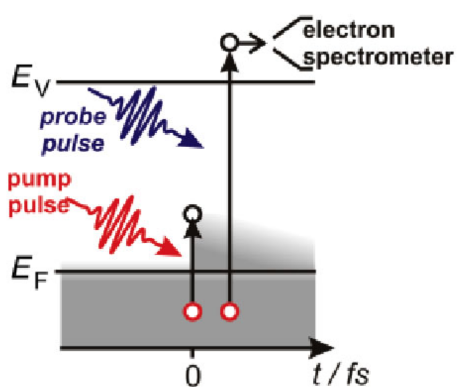


$$G_{\mathbf{k}}(t,t') = G^0_{\mathbf{k}}(t,t') + \oint dt_1 dt_2 G^0_{\mathbf{k}}(t,t_1)\underline{\Sigma(t_1,t_2)}G_{\mathbf{k}}(t_2,t')$$

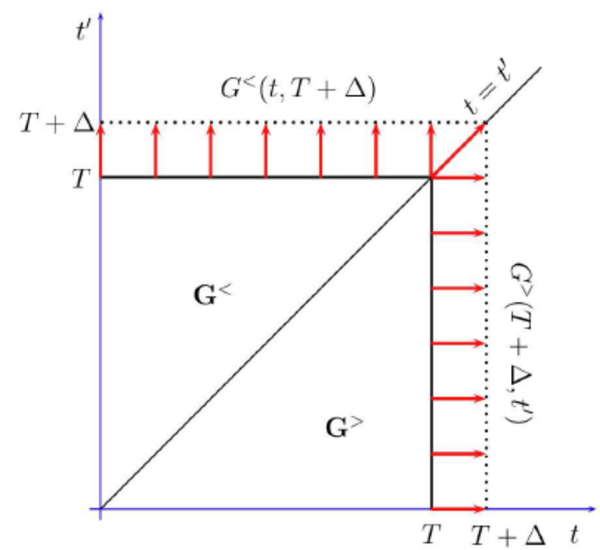
self-energy Σ:
electron-electron scattering
electron-phonon scattering
...







pump-probe photoemission

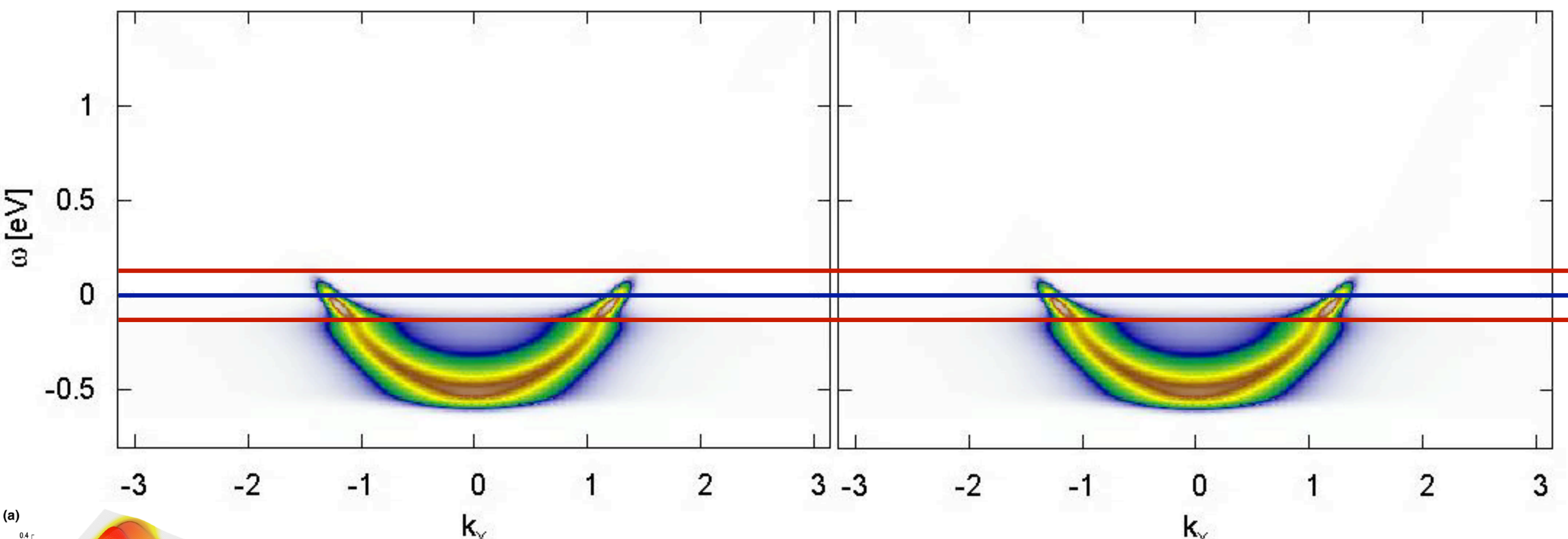


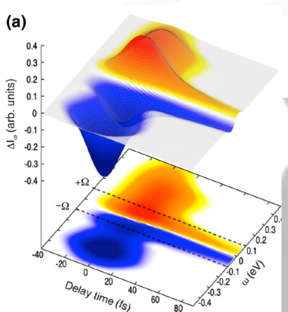
Electron-boson coupling

PRX 3, 041033 (2013)

Weak pump | Strong pump

t = -65.00 time unit = 0.66 fs t = -65.00



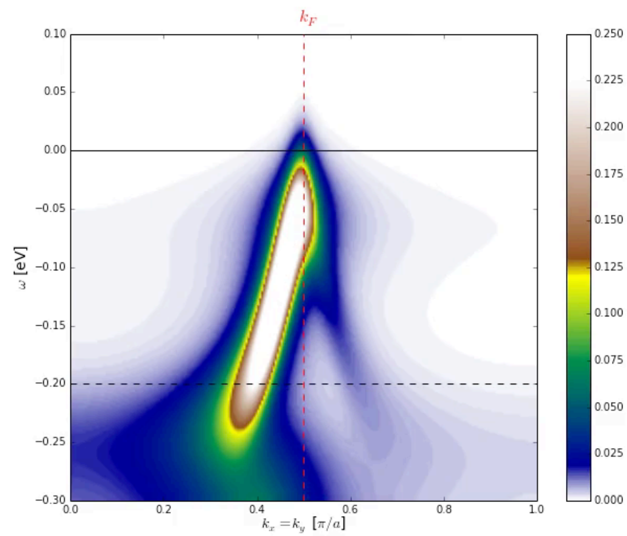


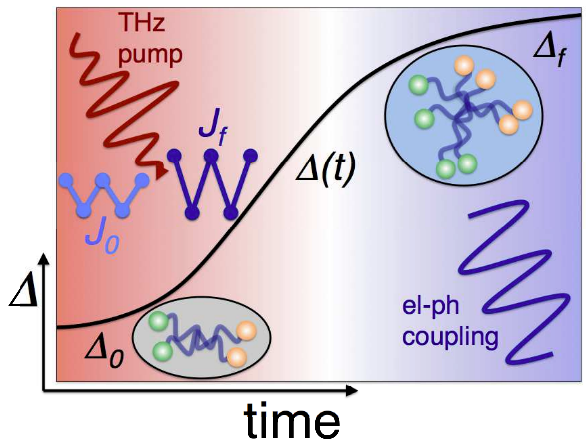
Rameau et al., Nat. Comm. 7, 13761 (2016)

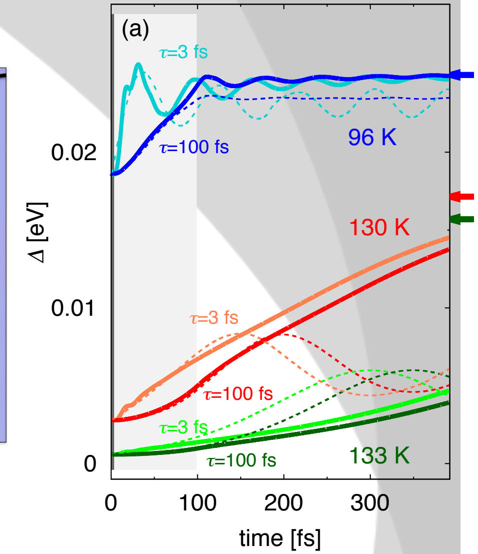
boson window effect for fast versus slow relaxation

nonlinear response for strong pump

Ordered phases







PRB 92, 224517 (2015)

Higgs amplitude mode oscillations in pump-probe photoemission spectroscopy

PRB 93, 144506 (2016)

Light-enhanced superconductivity: electron-phonon scattering versus collective order parameter dynamics

(many others: Murakami, Eckstein, Werner, Knap, Demler, Thorwart, Mitra, Kennes, Millis, ...)

Some recent key results

How to engineer materials with light?

Part I: Optical control of chiral superconductors

Short laser pulses allow for switching of Majorana modes

M. Claassen et al., arXiv:1810.06536

Part II: From classical to quantized photon fields

Materials engineering in an optical cavity using vacuum fluctuations

M. A. Sentef et al., Science Advances 4, eaau6969 (2018)

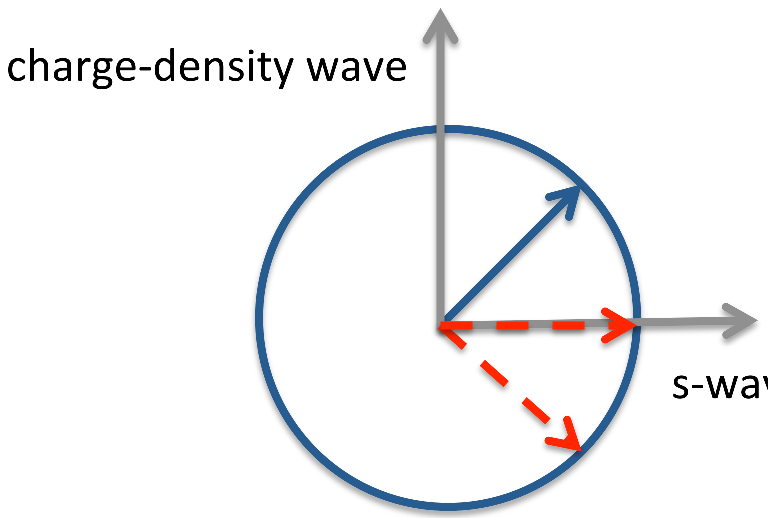
I Optical control of Majoranas

- prior work: optical control of competing orders

Theory of Laser-Controlled Competing Superconducting and Charge Orders

M. A. Sentef, A. Tokuno, A. Georges, and C. Kollath
Phys. Rev. Lett. **118**, 087002 – Published 21 February 2017

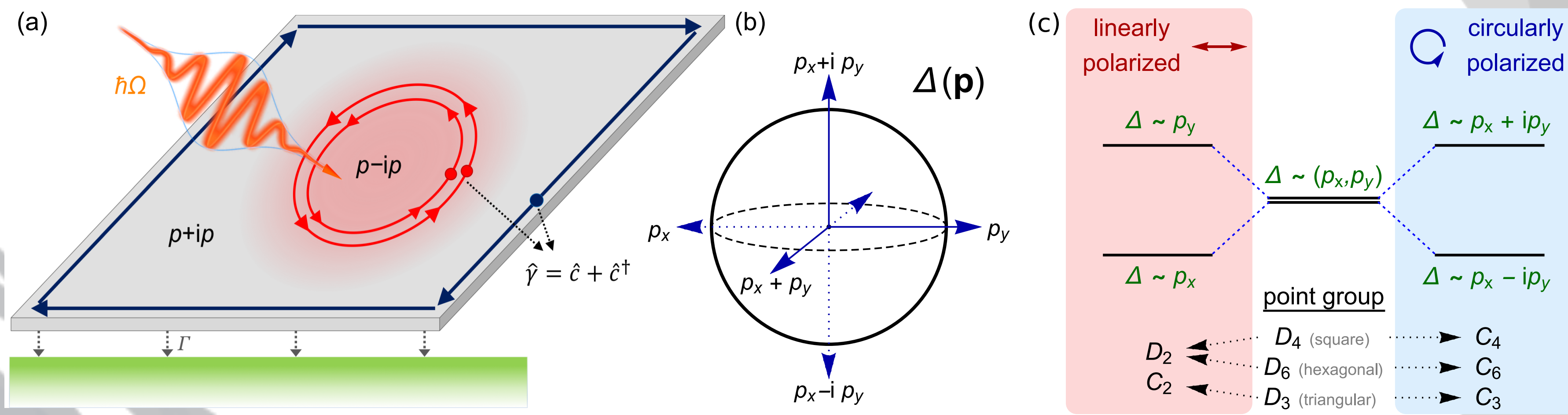
  - near-resonant laser driving switches between phases



I Optical control of Majoranas

- can one switch the chirality of a 2D topological superconductor?

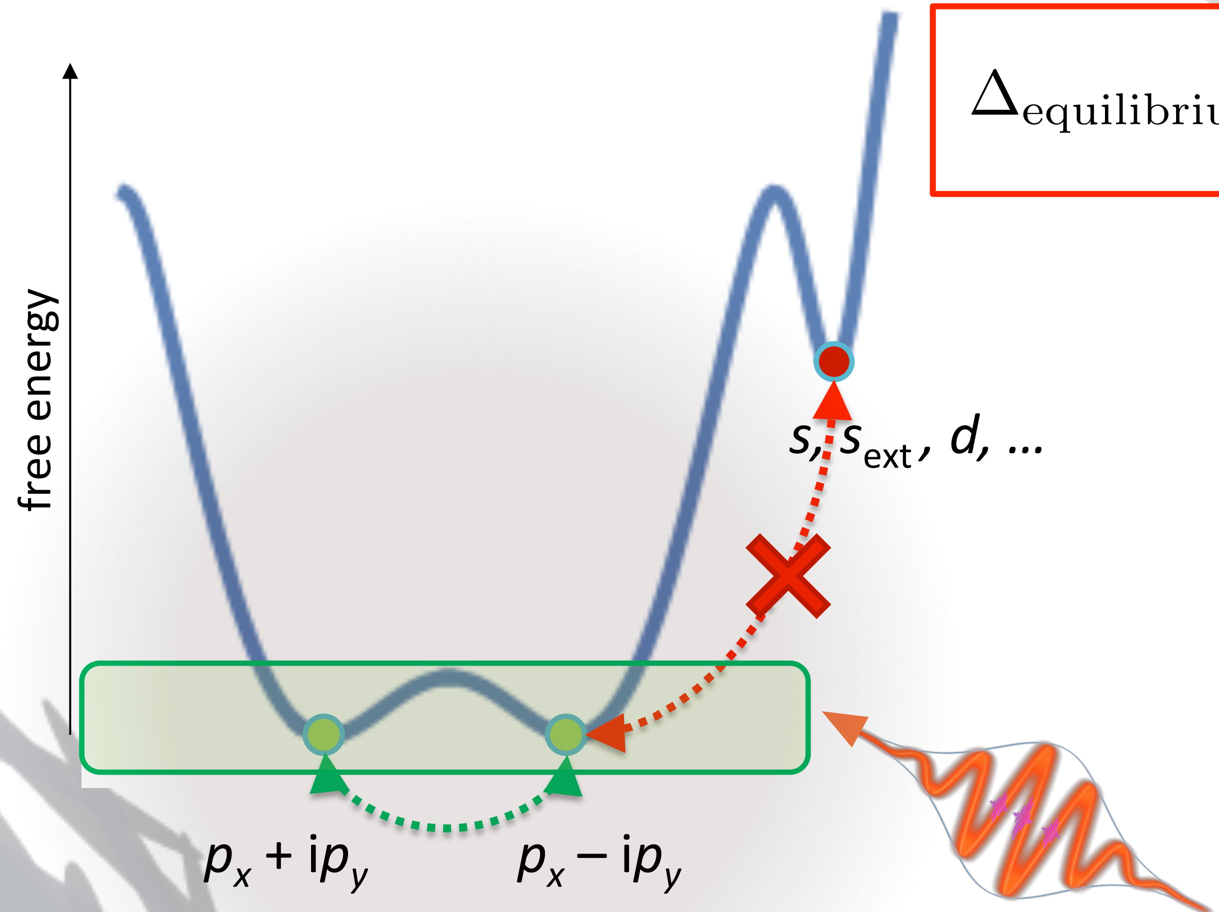
Sr_2RuO_4, highly doped graphene, twisted bilayer graphene, ...?



key idea: use two-pulse sequence with linearly and circularly polarized light

Nonequilibrium pathway to switching

$$\Delta_{\text{equilibrium}} \sim \begin{cases} p_x + ip_y \\ p_x - ip_y \end{cases}$$



$$\Delta_{\text{non-eq}}(t) \sim \cos(\theta)\ \text{“}p_x + ip_y\text{”}\ +\ \sin(\theta)e^{i\phi}\ \text{“}p_x - ip_y\text{”}$$

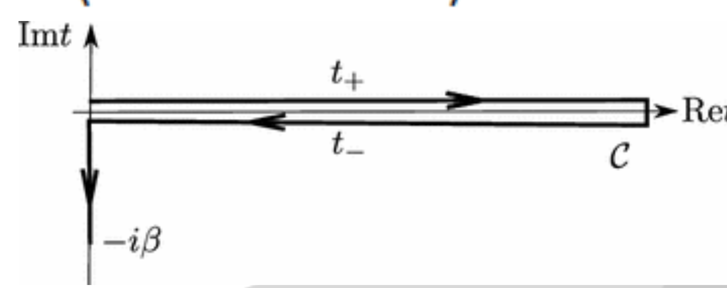
Model and Method

multiband Bogoliubov-de-Gennes Hamiltonians for doped graphene (d+id) and Sr2RuO4 (p+ip)
coupling to fermionic reservoir to dissipate energy
laser driving via Peierls substitution

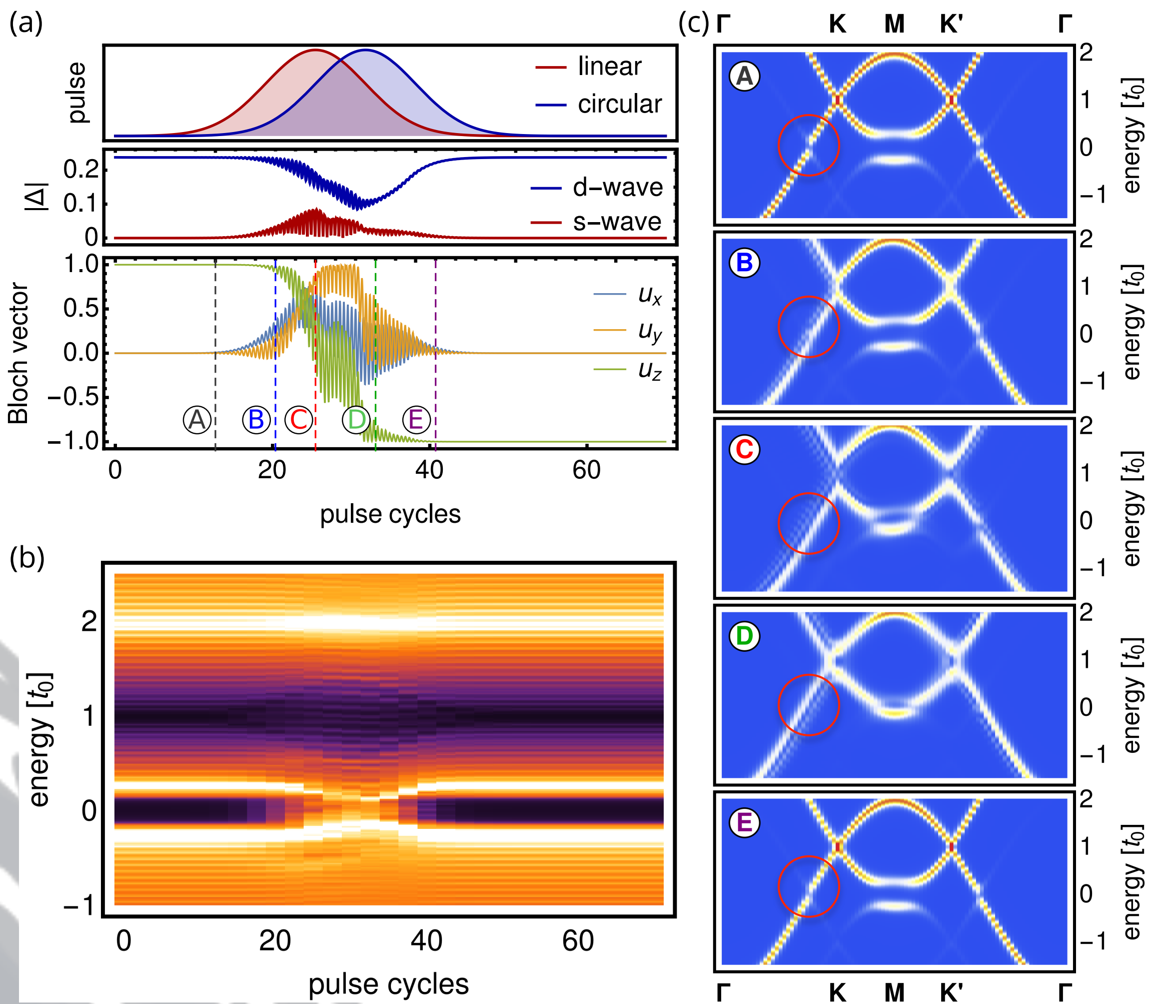
self-consistent Keldysh equations of motion for Nambu Green's functions:

$$i\partial_t \mathcal{G}_{\mathbf{k}}(t,t') = \mathcal{H}_{\mathbf{k}}(t, \boxed{\mathbf{\Delta}_{\mathbf{k}}(t)})\, \mathcal{G}_{\mathbf{k}}(t,t') + \int d\tau\, \boxed{\hat{\Sigma}_{\mathbf{k}}(t,\tau)}\, \mathcal{G}_{\mathbf{k}}(\tau,t')$$

$$\mathbf{\Delta}_{\mathbf{k}}(t) = \frac{1}{L}\sum_{j} v^{(j)} \hat{\eta}^{(j)}_{\mathbf{k}} \sum_{\substack{\mathbf{k}'\\ \alpha\beta}} \hat{\eta}^{(j)}_{\mathbf{k}'\alpha\beta} \left\langle \hat{c}_{-\mathbf{k}',\beta\downarrow} \hat{c}_{\mathbf{k}',\alpha\uparrow} \right\rangle$$



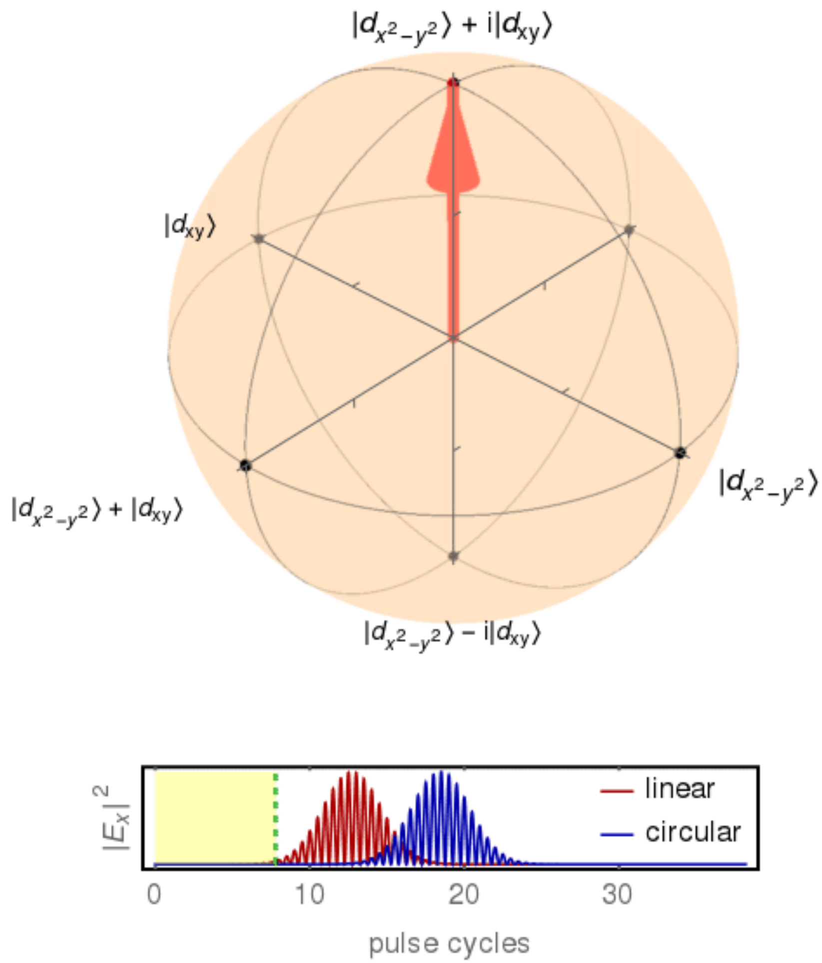
Optical control of Majoranas



two-pulse sequence reverses d+id state in graphene

time-resolved spectroscopy tracks chirality reversal

Bloch vector rotation

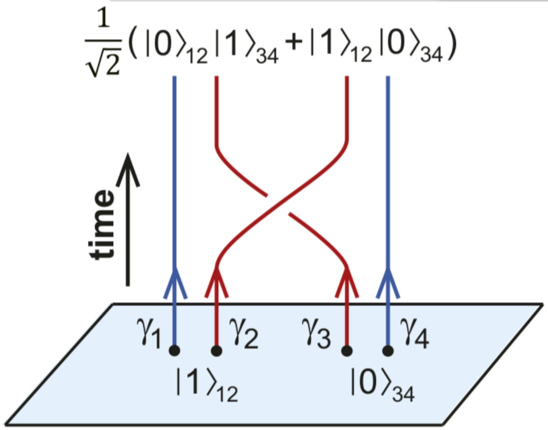


A „programmable“ topological quantum computer?

<u>non-Abelian statistics of Majorana fermions:</u>

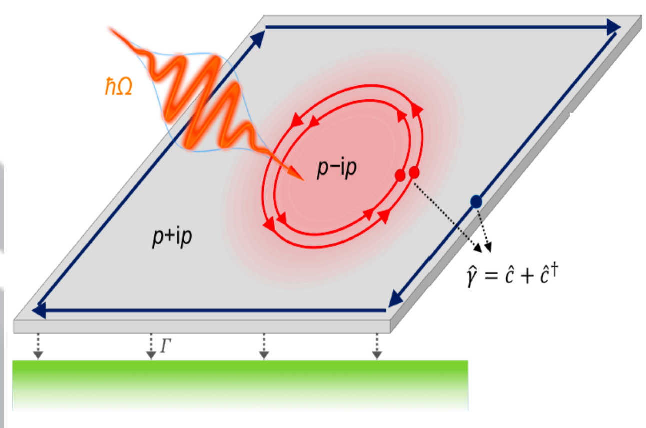
- half-quantum vortices of chiral superconductors host single Majorana fermions
- Two Majoranas represent one electron: **½ + ½ = 1**

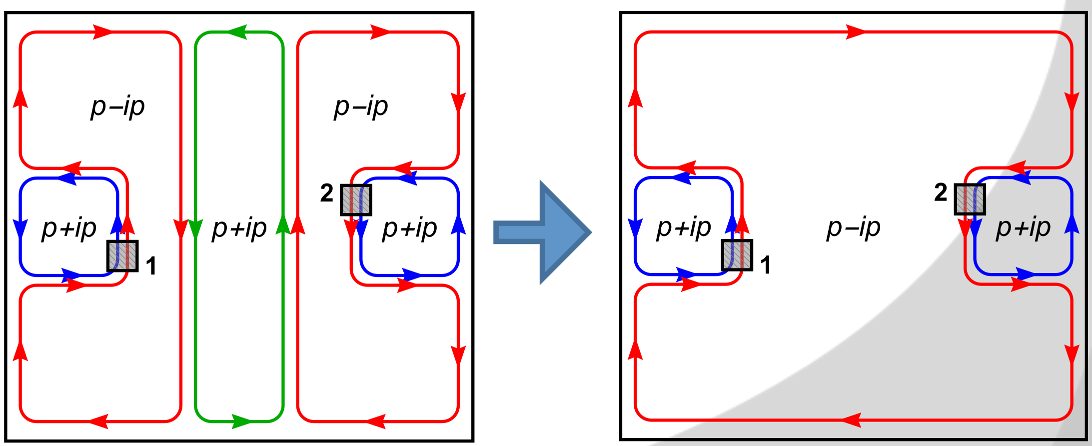
  → Braiding between Majoranas is a non-Abelian operation in electron (charge) basis!



Ivanov, PRL 86, 268 (2001)
B. Lian et al., PNAS 115, 10938 (2018)

simplest operation: a **<u>switchable Hadamard gate</u>**





Summary I

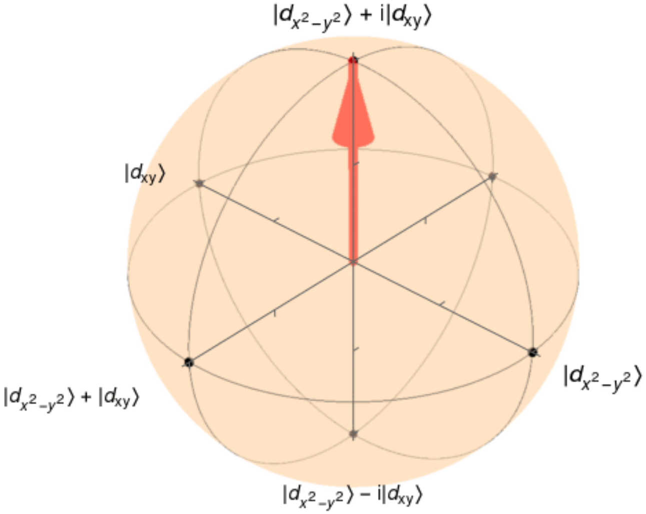
- All-optical control of chiral Majorana modes
- towards arbitrarily programmable quantum computer?

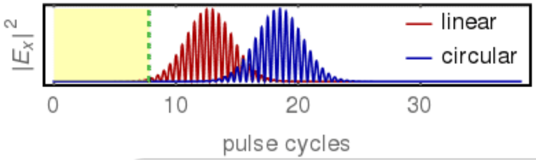
„program the gate optically, read it out electrically“

M. Claassen et al., arXiv:1810.06536, submitted to Nat. Phys.

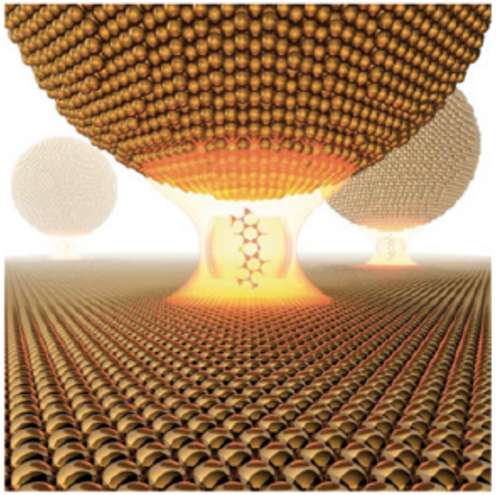
M. Claassen

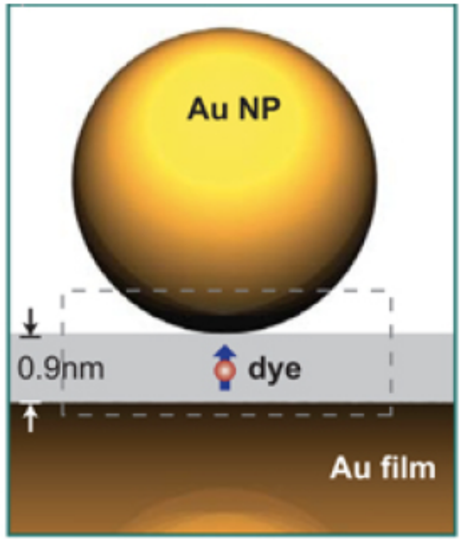
D. Kennes



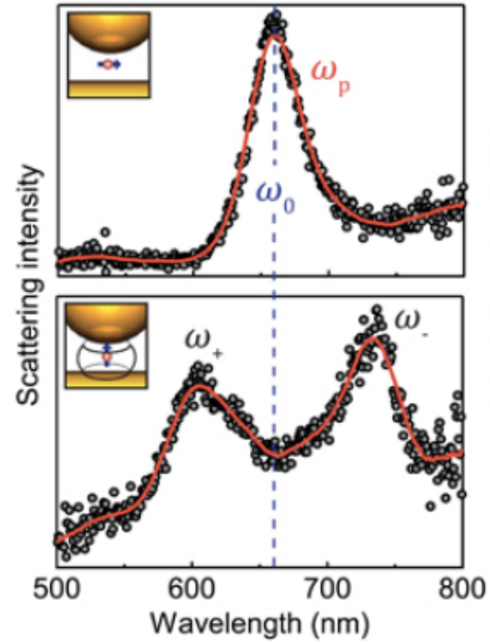


From classical to quantum light





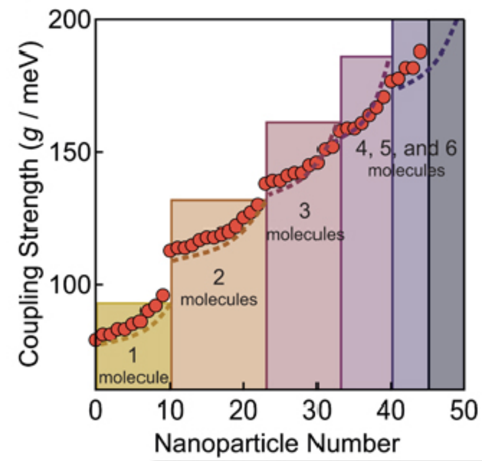
R. Chikkaraddy et al., Nature 535, 127 (2016)



Rabi splitting

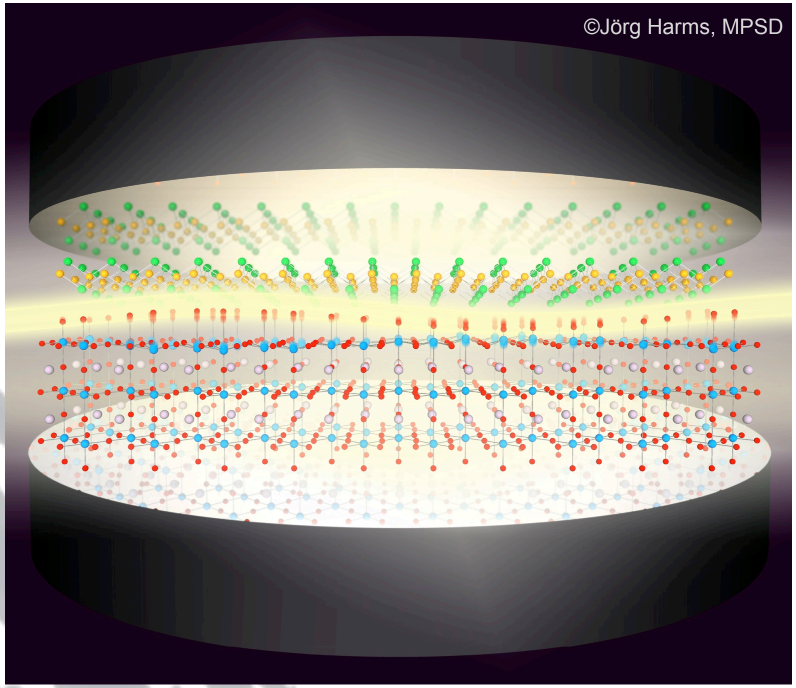
collective strong light-matter coupling

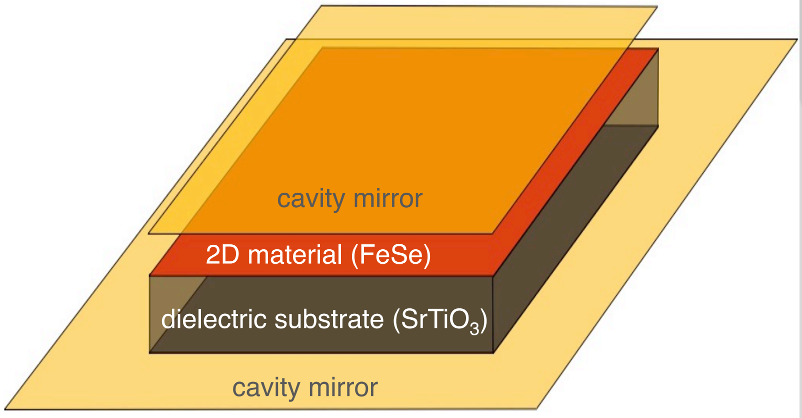
what about cavity materials?



II Cavity materials

- can one use enhanced vacuum fluctuations to change materials properties?





Cavity materials

BCS superconductors: phonon-mediated superconductivity
Ginzburg, Phys. Lett. 13, 101 (1964): exciton-mediated superconductivity?
Ruvalds, Phys. Rev. B 35, 8869(R) (1987): plasmon-mediated superconductivity?

PRL 104, 106402 (2010) PHYSICAL REVIEW LETTERS week ending 12 MARCH 2010

Exciton-Polariton Mediated Superconductivity

Fabrice P. Laussy,[1] Alexey V. Kavokin,[1,2] and Ivan A. Shelykh[3,4]

PHYSICAL REVIEW B 93, 054510 (2016)

Superconductivity and other collective phenomena in a hybrid Bose-Fermi mixture formed by a polariton condensate and an electron system in two dimensions

Ovidiu Cotleţ,[1,*] Sina Zeytinoğlu,[1,2] Manfred Sigrist,[2] Eugene Demler,[3] and Ataç Imamoğlu[1]

Cavity-assisted mesoscopic transport of fermions: Coherent and dissipative dynamics.

Hagenmüller et al., 1801.09876

Cavity quantum-electrodynamical polaritonically enhanced electron-phonon coupling and its influence on superconductivity

M. A. Sentef,[1,*] M. Ruggenthaler,[1] and A. Rubio[1,2,3]

1802.09437

Cavity-mediated electron-photon superconductivity

Frank Schlawin[1], Andrea Cavalleri[1,2] and Dieter Jaksch[1]

1804.07142

Superradiant Quantum Materials

Giacomo Mazza[1,2,*] and Antoine Georges[2,3,1,4]

1804.08534

Cavity Quantum Eliashberg Enhancement of Superconductivity

Jonathan B. Curtis,[1,2,*] Zachary M. Raines,[1,2] Andrew A. Allocca,[1,2] Mohammad Hafezi,[1] and Victor M. Galitski[1,2]

1805.01482

Manipulating quantum materials with quantum light

Martin Kiffner[1,2], Jonathan Coulthard[2], Frank Schlawin[2], Arzhang Ardavan[2], and Dieter Jaksch[2,1]

1806.06752

Cavity superconductor-polaritons

Andrew A. Allocca,* Zachary M. Raines, Jonathan B. Curtis, and Victor M. Galitski

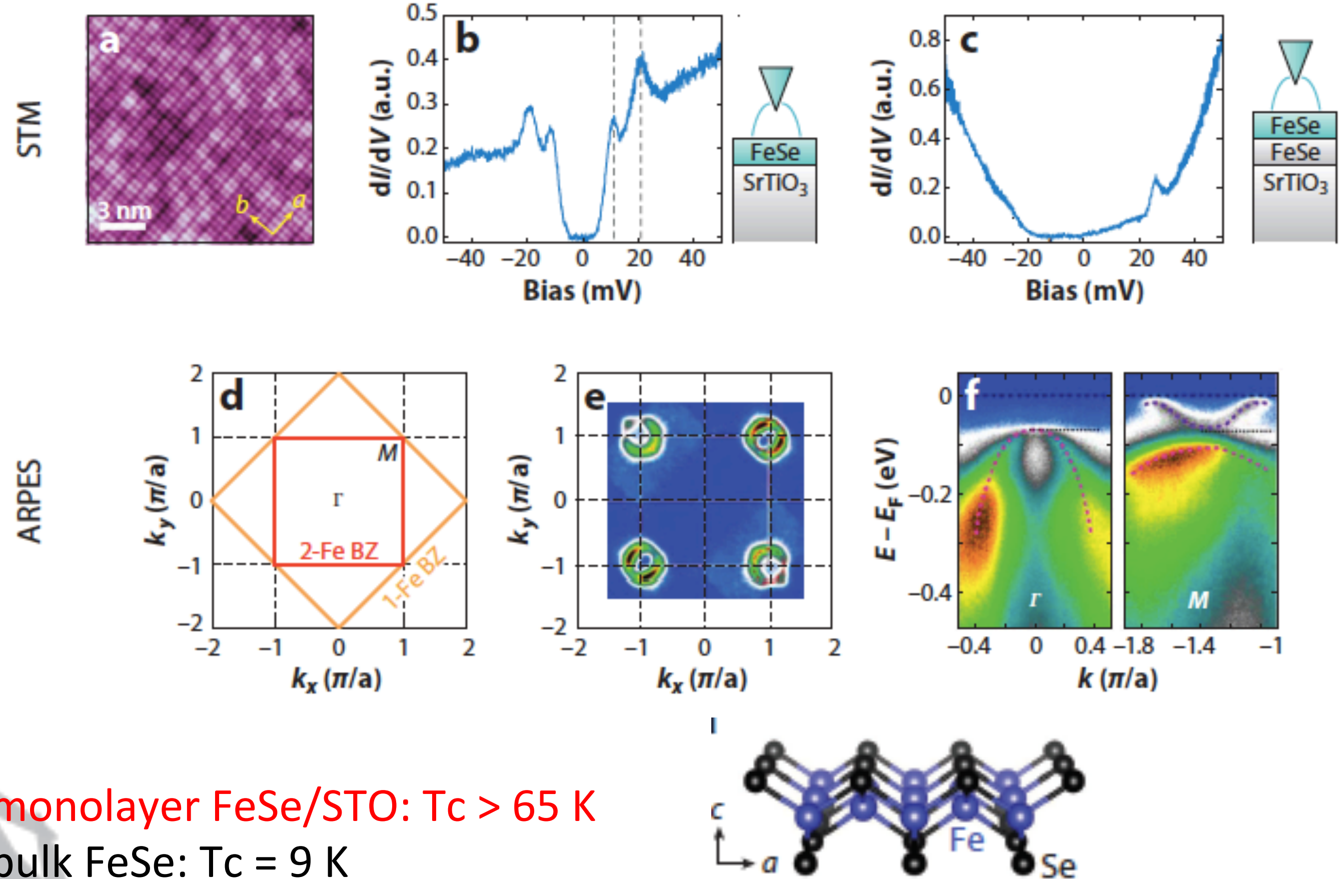
1807.06601

Ab-initio Exciton-polaritons: Cavity control of Dark Excitons in two dimensional Materials

Simone Latini,[1,*] Enrico Ronca,[1,†] Umberto De Giovannini,[1,2,‡] Hannes Hübener,[1,§] and Angel Rubio[1,3,¶]

1810.02672

monolayer FeSe/STO



monolayer FeSe/STO: Tc > 65 K

bulk FeSe: Tc = 9 K

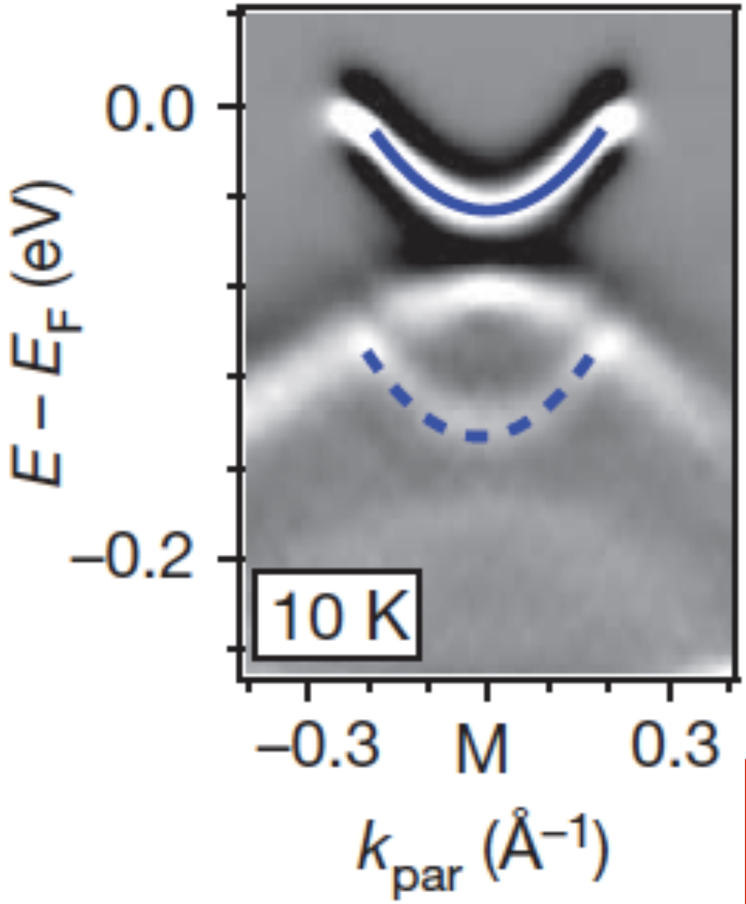
Wang QY, Li Z, Zhang WH, Zhang ZC, Zhang JS, et al. 2012. *Chin. Phys. Lett.* 29:037402

Liu D, Zhang W, Mou D, He J, Ou YB, et al. 2012. *Nat. Commun.* 3:931

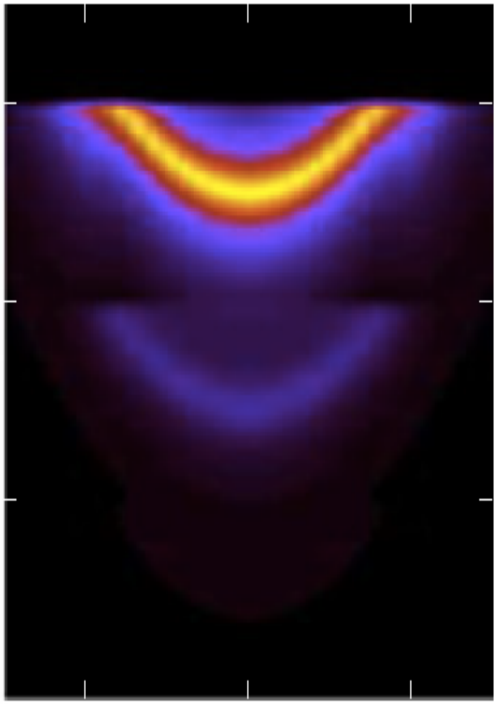
Huang and Hoffman, Annu. Rev. CMP 8, 311 (2017)

monolayer FeSe/STO: ARPES

experiment



theory



replica bands: forward (small-q) electron-phonon scattering

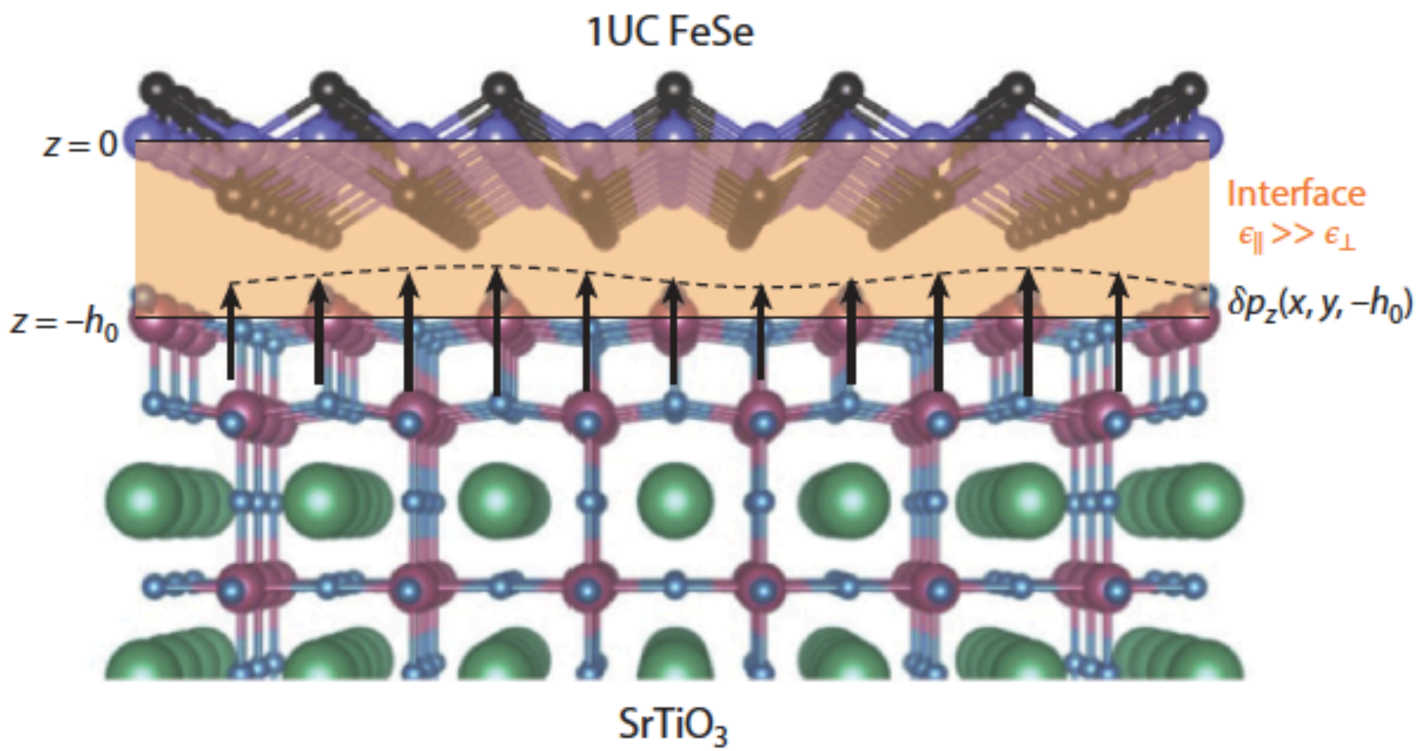
Lee et al., Nature 515, 245 (2014)

Rademaker et al., New J. Phys. 18, 022001 (2016)

monolayer FeSe/STO: interfacial phonon

bare el-phonon vertex $g(\vec{q}) = g_0 \exp(-|\vec{q}|/q_0)$ *Lee et al., Nature 515, 245 (2014)*

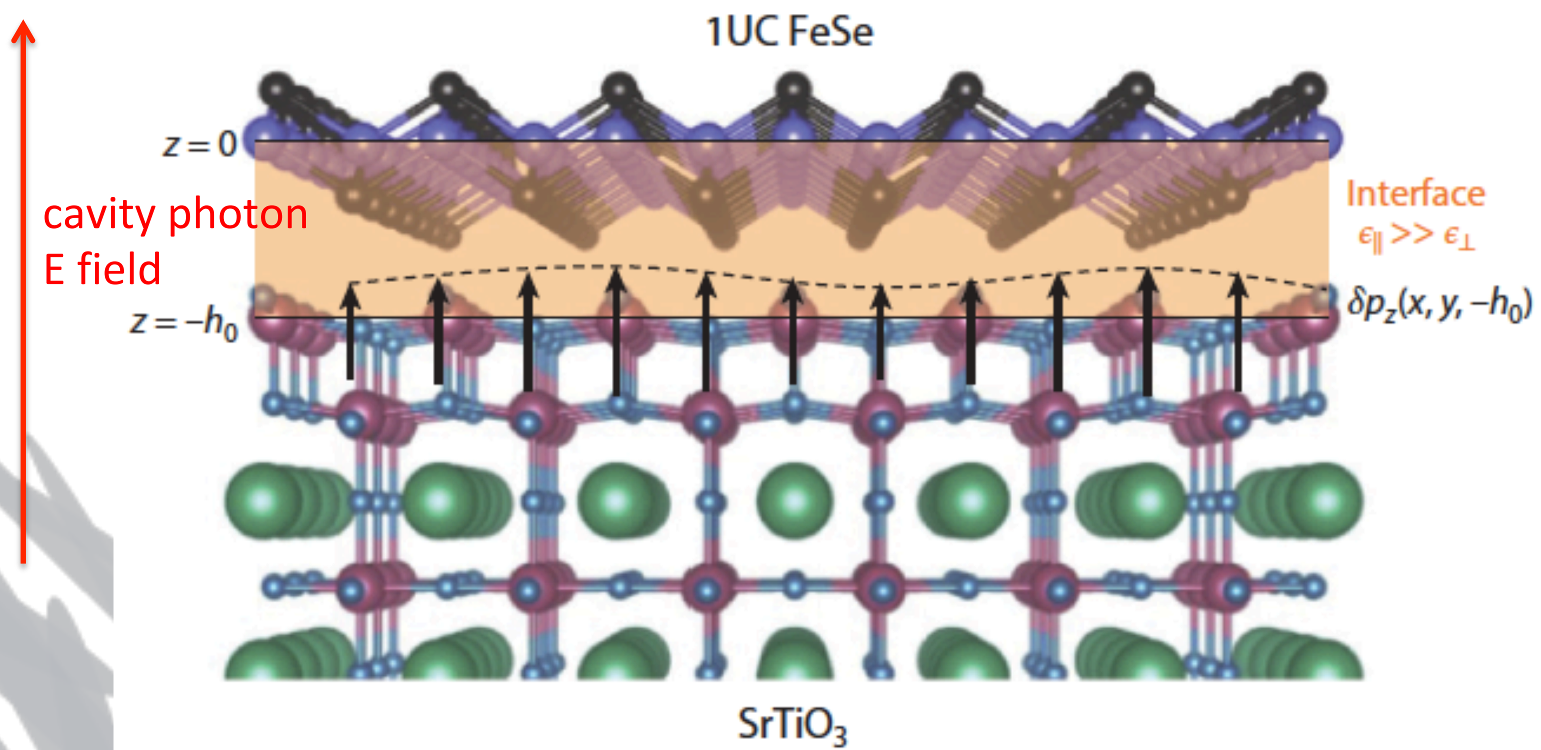
$$q_0^{-1} = h_0\sqrt{\epsilon_{\|}/\epsilon_{\perp}} \quad \epsilon_{\|}/\epsilon_{\perp} \approx 100$$



Huang and Hoffman, Annu. Rev. CMP 8, 311 (2017)

Cavity engineering

- idea: use phonon polaritons to enhance electron-phonon coupling



Huang and Hoffman, Annu. Rev. CMP 8, 311 (2017)

Model and Method

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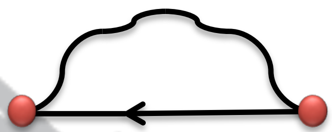
electrons / el-polariton coupling / polaritons

$$H = \sum_{\vec{k},\sigma} \epsilon_{\vec{k}} c^\dagger_{\vec{k},\sigma} c_{\vec{k},\sigma} + \frac{1}{\sqrt{N}} \sum_{\vec{k},\vec{q},\sigma,\lambda=\pm} c^\dagger_{\vec{k}+\vec{q},\sigma} c_{\vec{k},\sigma} (g^*_\lambda(\vec{q}) \alpha^\dagger_{-\vec{q},\lambda} + g_\lambda(\vec{q}) \alpha_{\vec{q},\lambda}) + \sum_{\vec{q},\lambda=\pm} \omega_\lambda(\vec{q}) \alpha^\dagger_{\vec{q},\lambda} \alpha_{\vec{q},\lambda}$$

bare el-phonon vertex $g(\vec{q}) = g_0 \exp(-|\vec{q}|/q_0) \quad q_0^{-1} = h_0 \sqrt{\epsilon_\parallel / \epsilon_\perp}$

G-self-consistent Migdal-Eliashberg diagram

$$\hat{\Sigma}(\vec{k}, i\omega_n) = \frac{-1}{N\beta} \sum_{\vec{q},m,\lambda=\pm} |g_\lambda(\vec{q})|^2 D^{(0)}_\lambda(\vec{q}, i\omega_n - i\omega_m) \hat{\tau}_3 \hat{G}(\vec{k}+\vec{q}, i\omega_m) \hat{\tau}_3$$

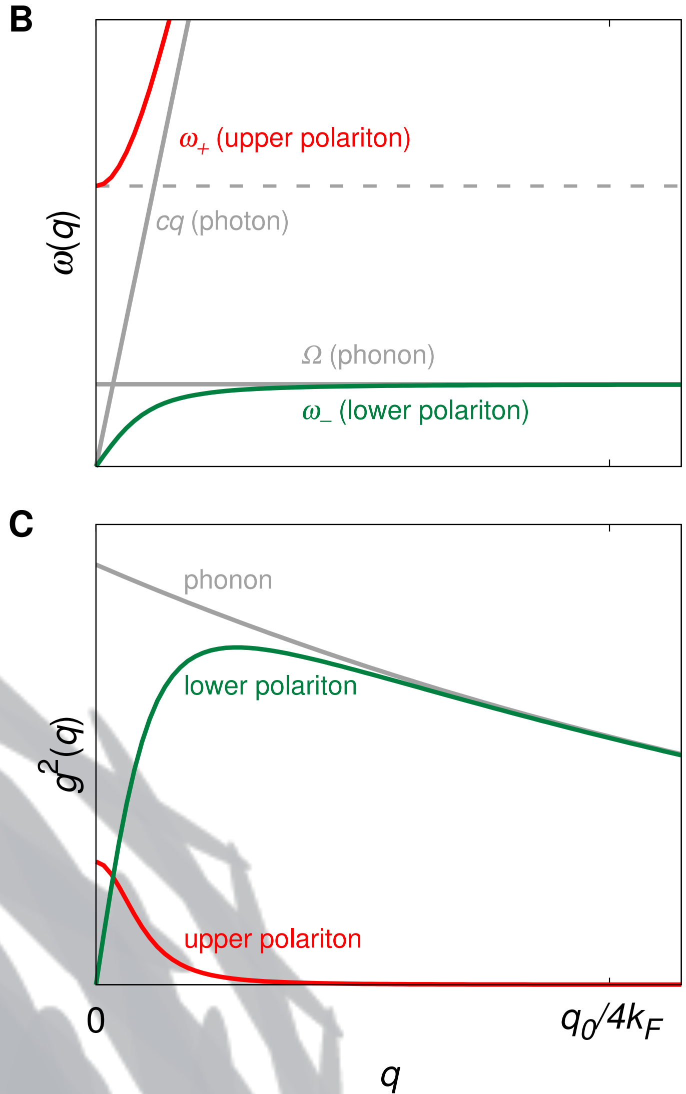


$$\hat{\Sigma}(\vec{k}, i\omega_n) = i\omega_n[1 - Z(\vec{k}, i\omega_n)]\hat{\tau}_0 + \chi(\vec{k}, i\omega_n)\hat{\tau}_3 + \phi(\vec{k}, i\omega_n)\hat{\tau}_1$$

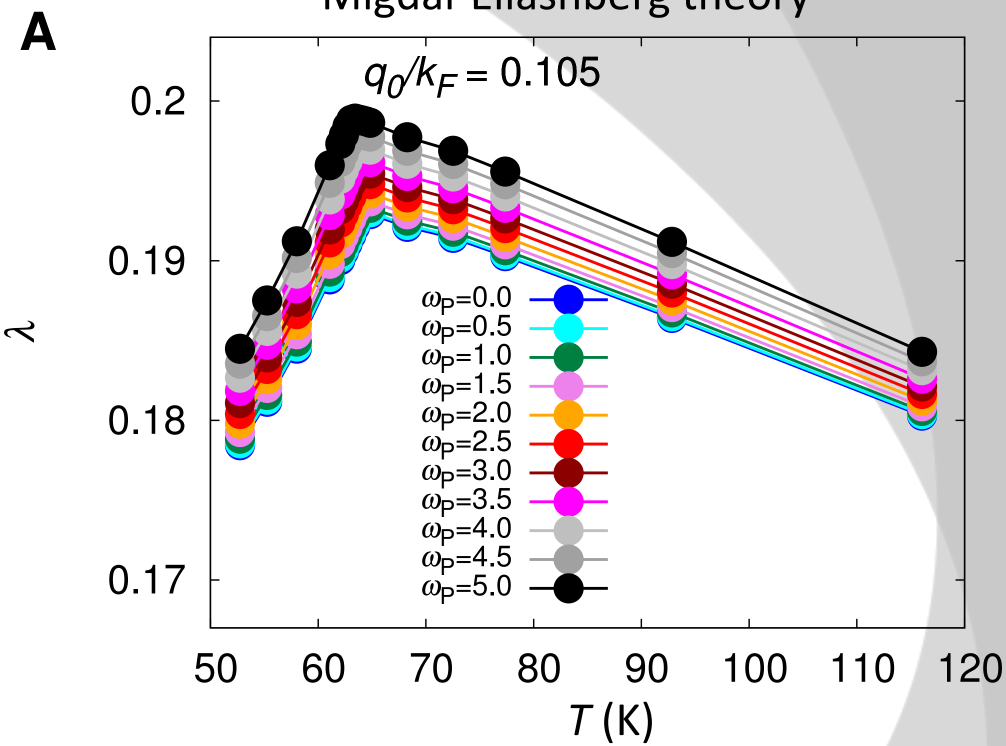
$$\lambda \equiv Z(\vec{k}_F, i\pi/\beta) - 1$$

Mass enhancement: $m^*/m = 1 + \lambda$

Cavity materials: Phonon polaritons

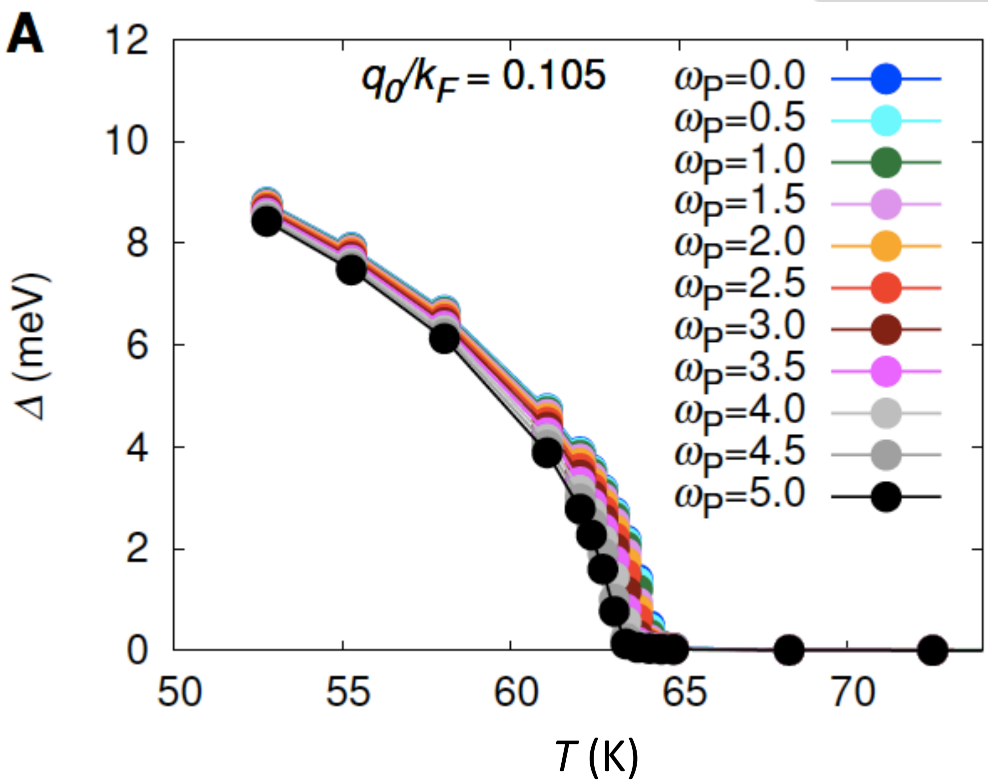


Migdal-Eliashberg theory



enhanced electron-phonon coupling, controlled by cavity volume

Superconductivity



suppressed superconductivity despite enhanced el-ph coupling

forward scattering

$$\boxed{T_C \approx \frac{\lambda\Omega}{2+3\lambda}}$$

vs.

$$T_{C,\mathrm{BCS}} \approx 1.13\Omega \exp(-\tfrac{1}{\lambda})$$

q-independent scattering

Summary II

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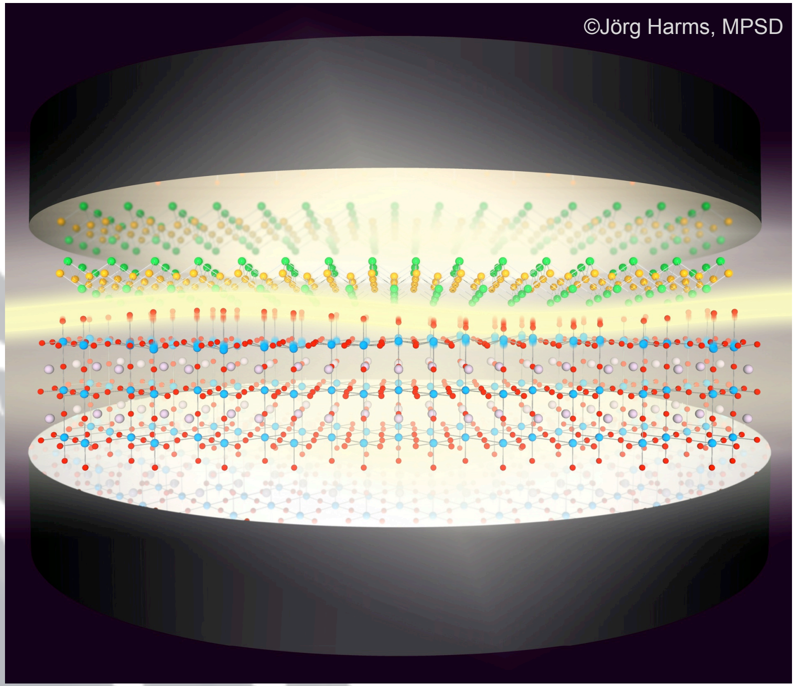
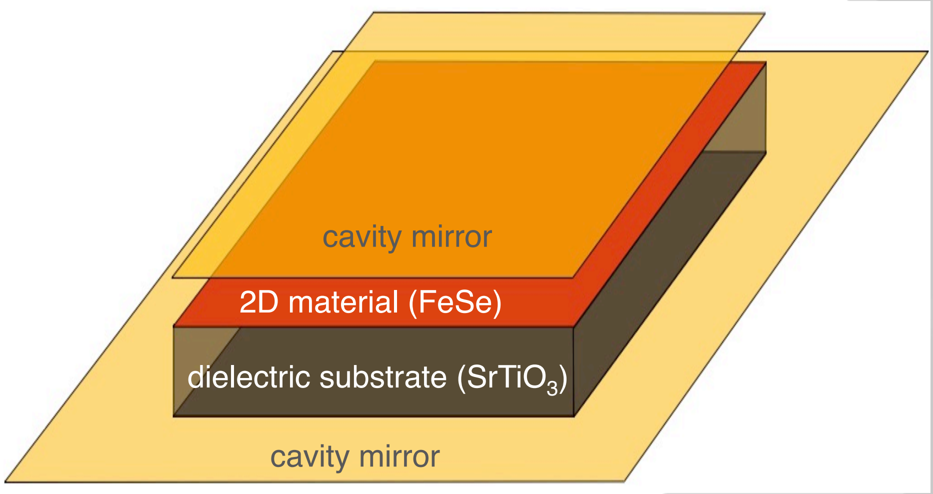
- cavity leads to enhanced electron-phonon coupling
- can one also enhance superconductivity?

M. A. Sentef, M. Ruggenthaler, A. Rubio, arXiv:1802.09437
Science Advances 4, eaau6969 (2018)





Team and collaborators

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thank you for your attention!

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