Nonequilibrium Materials Engineering

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Quantum materials

**crystal structure**

![Crystal structure diagram](Image Credit: W. Hu et al., Nature Materials 13, 705 (2014))

**couplings**
- electron-electron
- electron-phonon
- electron-magnon

![Couplings diagram](Image Credit: B. Keimer et al., Nature 518, 179 (2015))

**complex phase diagram**

![Phase diagram](Image Credit: B. Keimer et al., Nature 518, 179 (2015))

**electron band structure**

![Band structure](Image Credit: L. F. Mattheis, Phys. Rev. Lett. 58, 1028 (1987))

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


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**

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

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

Image courtesy: J. Sobota

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Engineering materials with light

Hamiltonian engineering
e.g., Floquet-Bloch bands

Distributional engineering

many ingredients, hard to disentangle
Engineering materials with light

Exposing hidden states
nonthermal switching process

Light-induced new states
transient superconductivity?

Microscopic understanding?

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

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

Igor Vaskivskyi

L. Stojchevska et al., Science 2014;344:177-180
Pump-probe spectroscopy

- stroboscopic investigations of dynamic phenomena

Muybridge 1887

*Image courtesy: J. Sobota / F. Schmitt*
Understanding the nature of quasiparticles

- Relaxation dynamics
- Control of couplings

PRX 3, 041033 (2013)  PRB 95, 205111 (2017)

Understanding ordered phases

- Collective oscillations
- Competing orders

PRB 93, 144506 (2016)  arXiv:1808.00712
   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:

\[ \epsilon(k) \rightarrow \epsilon(k, t) \]
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-phononon scattering
...

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Electron-boson coupling

PRX 3, 041033 (2013)

Weak pump

Strong pump

t = -65.00  

time unit = 0.66 fs

t = -65.00

boson window effect for fast versus slow relaxation

nonlinear response for strong pump

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

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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

charge-density wave

s-wave superconductor
I Optical control of Majoranas

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

Sr$_2$RuO$_4$, highly doped graphene, twisted bilayer graphene, ...?

key idea: use two-pulse sequence with linearly and circularly polarized light
Nonequilibrium pathway to switching

\[ \Delta_{\text{equilibrium}} \sim \{ p_x + ip_y, p_x - ip_y \} \]

\[ \Delta_{\text{non-eq}}(t) \sim \cos(\theta) \, "p_x + ip_y" + \sin(\theta) e^{i\phi} \, "p_x - ip_y" \]
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:

\[ i \partial_t G_k(t, t') = \mathcal{H}_k(t, \Delta_k(t)) G_k(t, t') + \int d\tau \sum_{k'} \langle \hat{\Sigma}_k(t, \tau) G_k(\tau, t') \rangle \]

\[ \Delta_k(t) = \frac{1}{L} \sum_j \nu^{(j)}(j) \sum_{k', \alpha, \beta} \hat{\eta}^{(j)}_{k'} \hat{\eta}^{(j)}_k \left\langle \hat{c}_{-k', \beta} \hat{c}_{k, \alpha} \right\rangle \]
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?

**non-Abelian statistics of Majorana fermions:**
- half-quantum vortices of chiral superconductors host single Majorana fermions
- Two Majoranas represent one electron: $\frac{1}{2} + \frac{1}{2} = 1$

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

**simplest operation:** a **switchable Hadamard gate**

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

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

„program the gate optically, read it out electrically“


M. Claassen  D. Kennes
From classical to quantum light

Collective strong light-matter coupling

What about cavity materials?

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

• can one use enhanced vacuum fluctuations to change materials properties?
Cavity materials

BCS superconductors: phonon-mediated superconductivity

Cavity-assisted mesoscopic transport of fermions:
Coherent and dissipative dynamics.
Hagenmüller et al., 1801.09876

Cavity-mediated electron-photon superconductivity
Frank Schlawiń, Andrea Cavalleri and Dieter Jaksch
1804.07142

Cavity Quantum Eliashberg Enhancement of Superconductivity
Jonathan B. Curtis, Zachary M. Raines, Andrew A. Allocca, Mohammad Hafezi, and Victor M. Galitski
1805.01482

Manipulating quantum materials with quantum light
Martin Kiffner, Jonathan Coulthard, Frank Schlawin, Arzhang Ardavan, and Dieter Jaksch
1806.06752

Cavity superconductor-polaritons
Andrew A. Allocca, Zachary M. Raines, Jonathan B. Curtis, and Victor M. Galitski
1807.06601

Superradiant Quantum Materials
Giacomo Mazza and Antoine Georges
1804.08534

Ab-initio Exciton-polaritons:
Cavity control of Dark Excitons in two dimensional Materials
Simone Latini, Enrico Ronca, Umberto De Giovannitti, Hannes Hübscher, and Angel Rubio
1810.02672
monolayer FeSe/STO: \( T_c > 65 \) K
bulk FeSe: \( T_c = 9 \) K

**Huang and Hoffman, Annu. Rev. CMP 8, 311 (2017)**
monolayer FeSe/STO: ARPES

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

Lee et al., Nature 515, 245 (2014)  
Rademaker et al., New J. Phys. 18, 022001 (2016)
bare el-phonon vertex

\[ g(\vec{q}) = g_0 \exp(-|\vec{q}|/q_0) \]

\[ q_0^{-1} = h_0 \sqrt{\epsilon_\parallel/\epsilon_\perp} \]

\[ \epsilon_\parallel/\epsilon_\perp \approx 100 \]

\textit{Lee et al., Nature 515, 245 (2014)}

\textit{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

$$H = \sum_{k,\sigma} \epsilon_k c_{k,\sigma}^{\dagger} c_{k,\sigma} + \frac{1}{\sqrt{N}} \sum_{\bar{k},\bar{q},\sigma, \lambda = \pm} c_{\bar{k}+\bar{q},\sigma}^{\dagger} c_{\bar{k},\sigma} (g_{\lambda}^*(\bar{q}) \alpha_{\bar{q},\lambda}^{\dagger} + g_{\lambda}(\bar{q}) \alpha_{\bar{q},\lambda}) + \sum_{\bar{q},\lambda = \pm} \omega_{\lambda}(\bar{q}) \alpha_{\bar{q},\lambda}^{\dagger} \alpha_{\bar{q},\lambda}$$

G-self-consistent Migdal-Eliashberg diagram

$$g(\bar{q}) = g_0 \exp(-|\bar{q}|/q_0) \quad q_0^{-1} = \hbar_0 \sqrt{\epsilon_\parallel / \epsilon_\perp}$$

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

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

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

Mass enhancement: $$m^*/m = 1 + \lambda$$
Cavity materials: Phonon polaritons

Migdal-Eliashberg theory

enhanced electron-phonon coupling, controlled by cavity volume
Suppressed superconductivity despite enhanced el-ph coupling

Forward scattering

\[ T_C \approx \frac{\lambda \Omega}{2 + 3 \lambda} \]

vs.

\[ T_{C, BCS} \approx 1.13 \Omega \exp\left(-\frac{1}{\lambda}\right) \]

q-independent scattering
Summary II

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

Science Advances 4, eaau6969 (2018)
Team and collaborators

thank you for your attention!