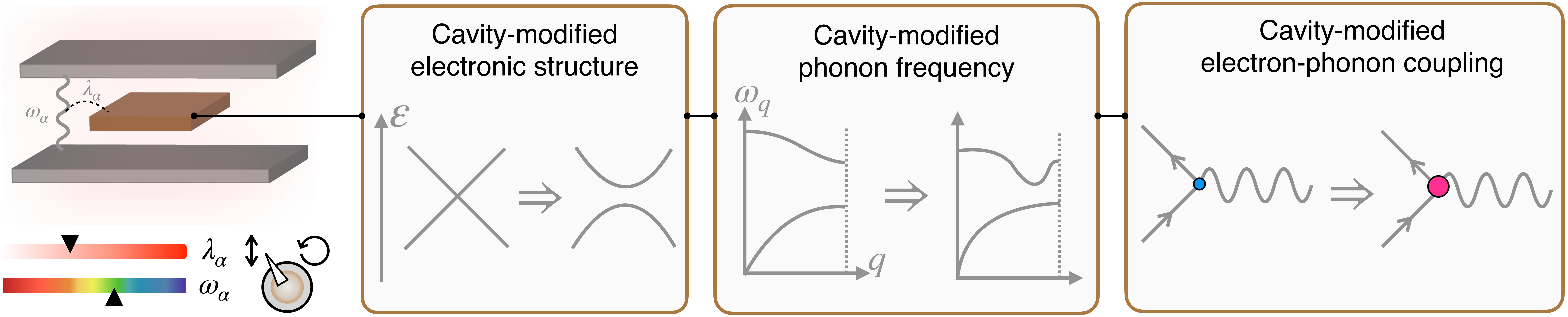
Cavity materials engineering: QEDFT electron-photon exchange approximation for solid-state materials applications



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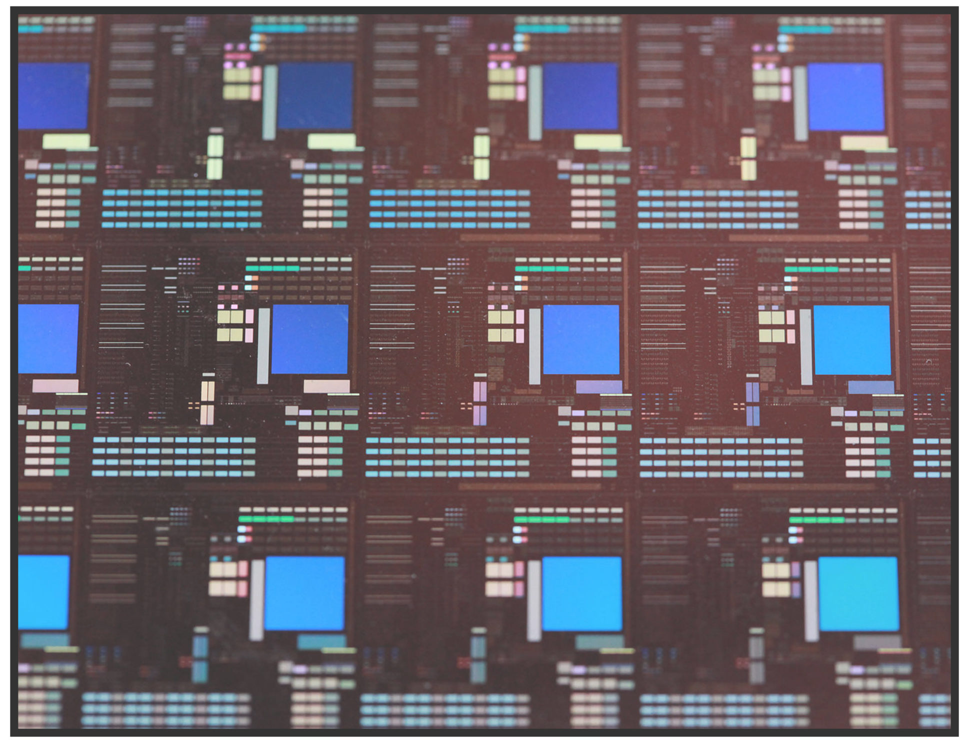
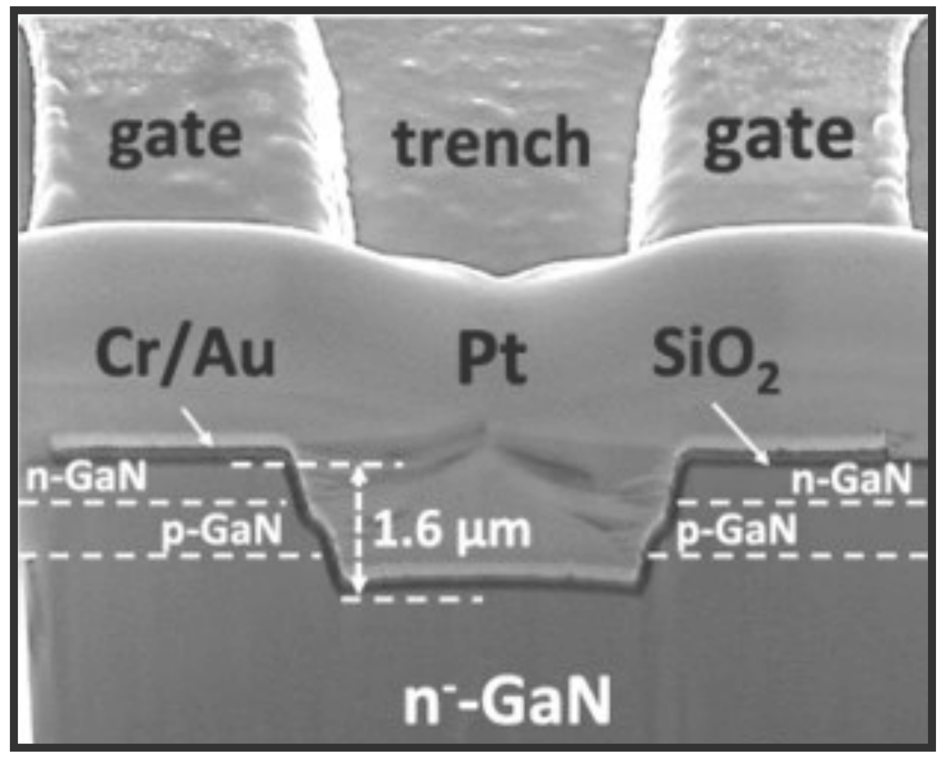
Atomic structure: the fundamental building blocks of materials for many applications

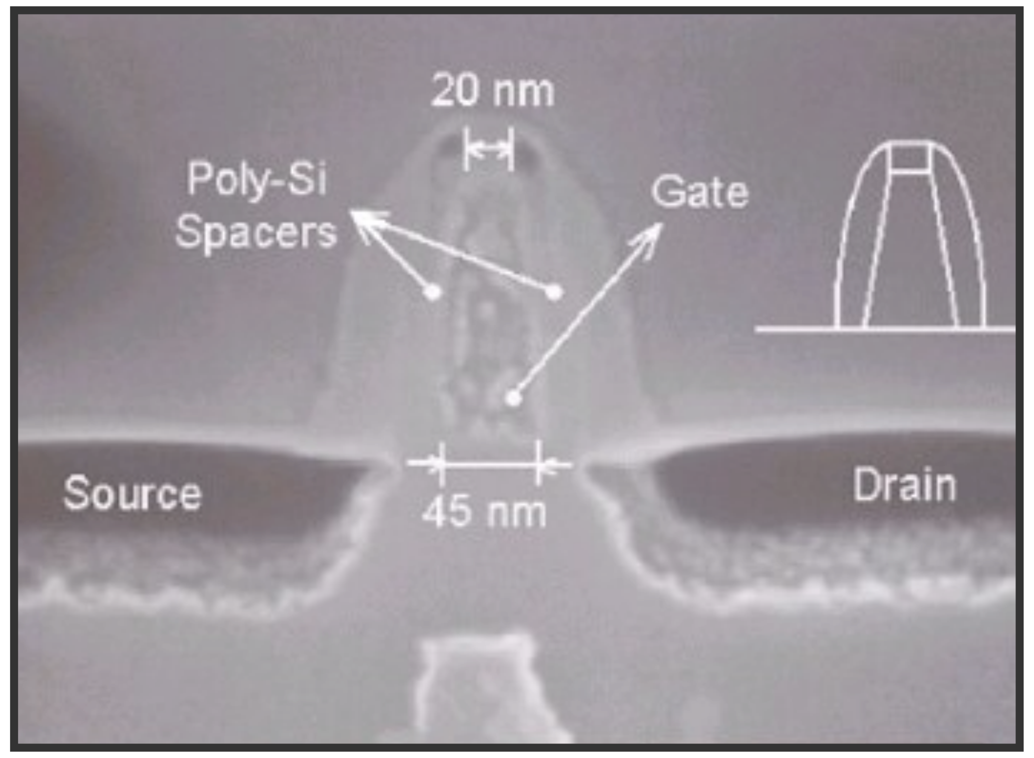
Macroscale



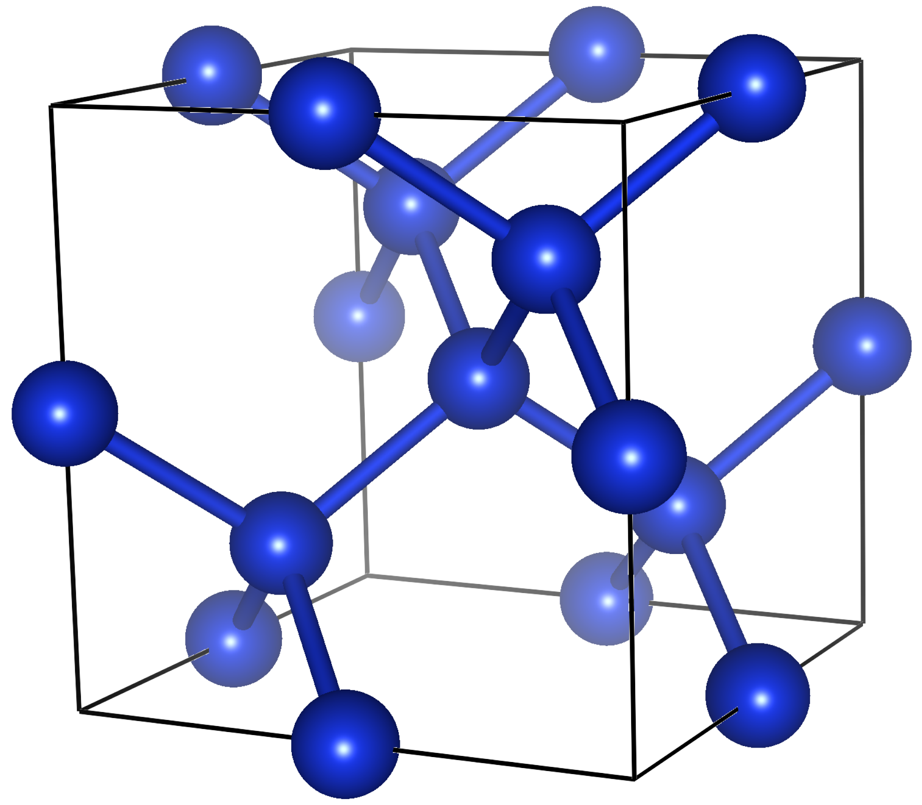
Microscale



Nanoscale



Atomic scale



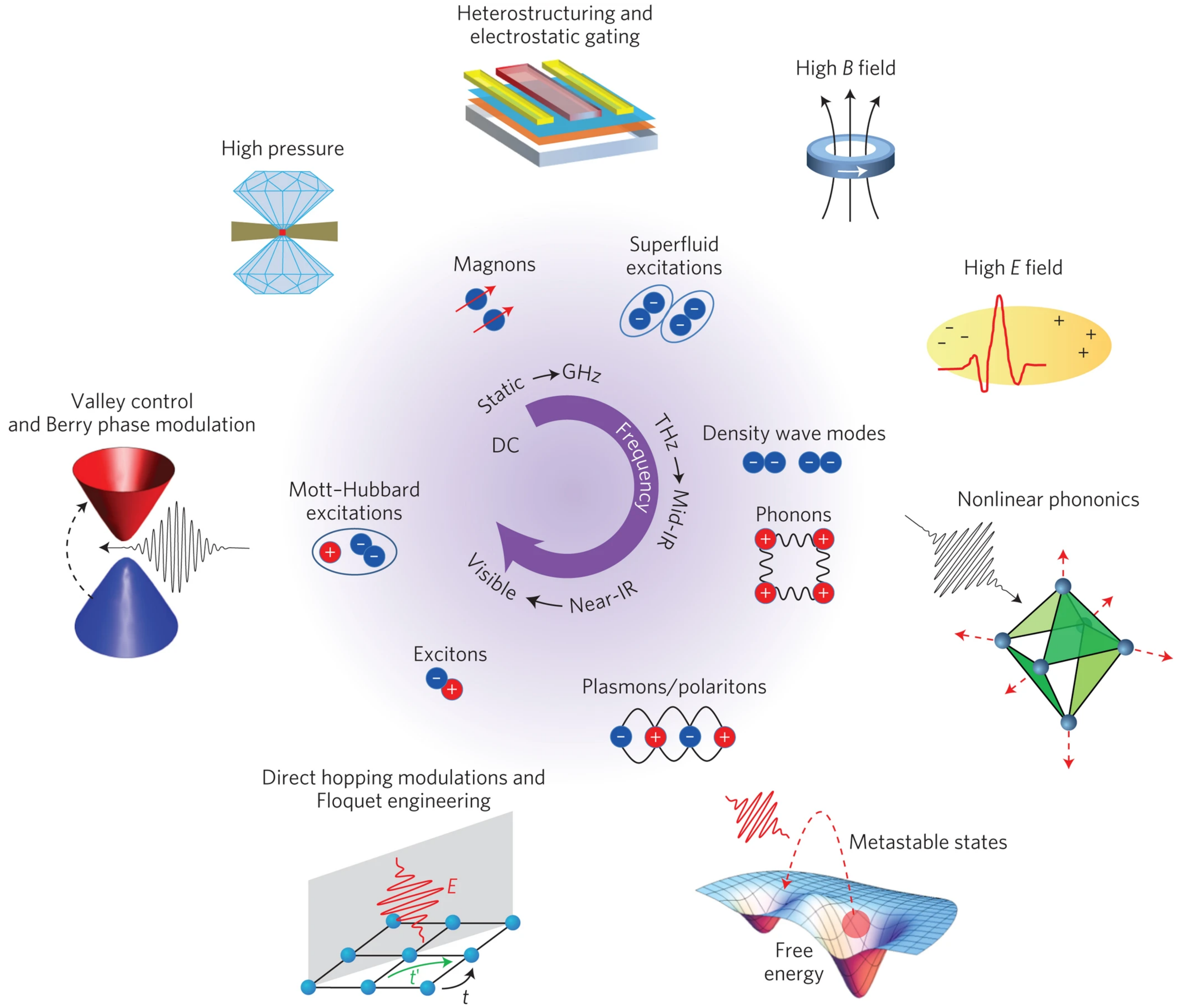
Atomistic structure

Coulomb interaction
(longitudinal EM fields)

$$\hat{H}_{\mathrm{M}} = \sum_{i=1}^{N_e} \frac{\hat{\mathbf{p}}_i^2}{2m_e} + \frac{1}{2}\sum_{i\neq j}^{N_e}\frac{e^2}{|\mathbf{r}_i-\mathbf{r}_j|} - \sum_{i}^{N_e}\sum_{I=1}^{N_n}\frac{Z_I e^2}{|\mathbf{r}_i-\mathbf{R}_I|} - \sum_{I=1}^{N_n}\frac{\hat{\mathbf{P}}_I^2}{2M_I} + \frac{1}{2}\sum_{I\neq J}^{N_n}\frac{Z_I Z_J e^2}{|\mathbf{R}_I-\mathbf{R}_J|}$$

Doping, strain (stress), temperature, gating, twisting… ⇒ materials phases & properties

Use external (classical) electromagnetic (EM) fields to engineer materials properties on demand



D. N. Basov, R. D. Averitt, & D. Hsieh, *Nature materials*, *16*(11), 1077-1088 (2017)

Atomistic structure + transverse EM field

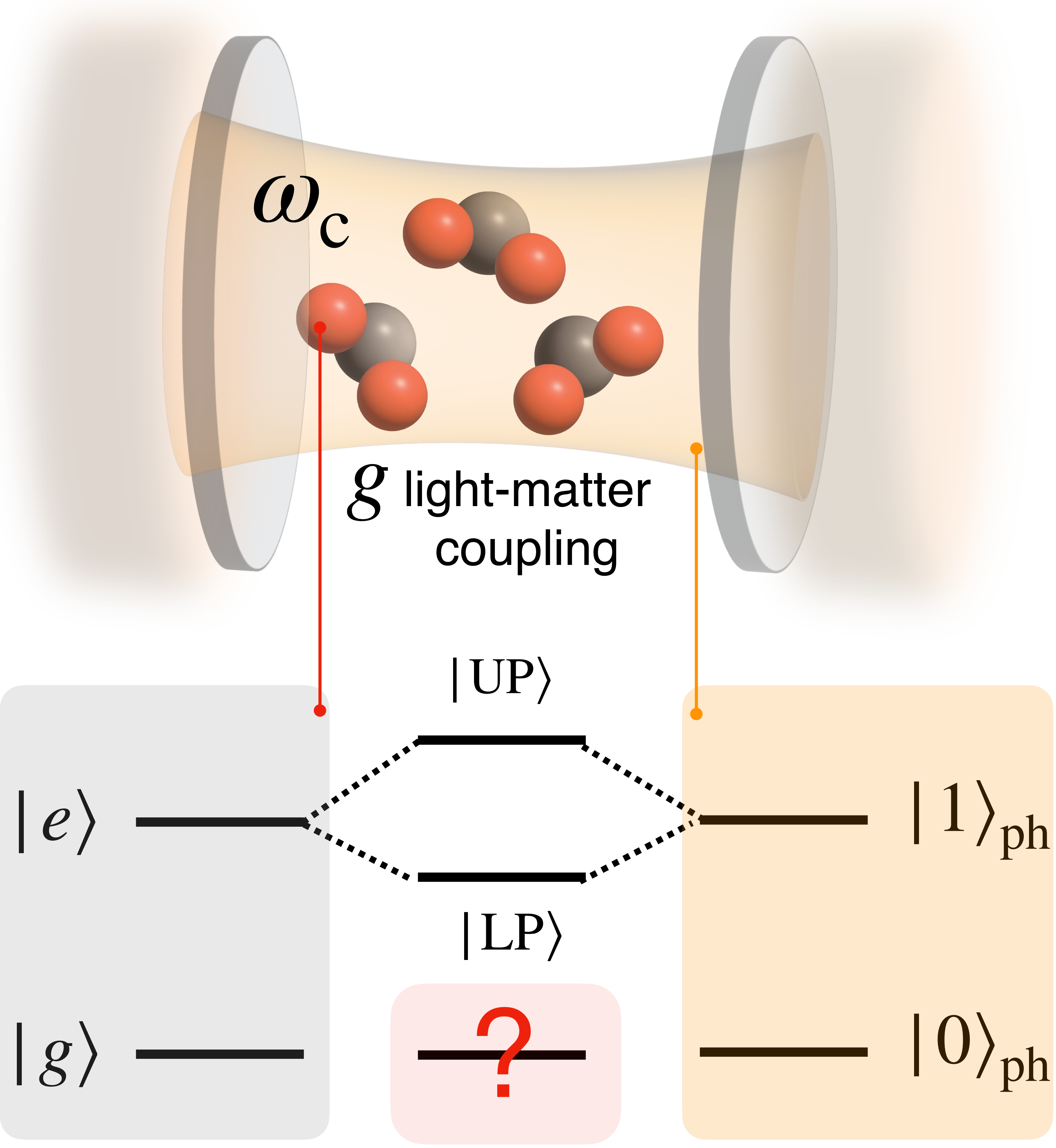
$$\hat{H}_{\mathrm{M}} = \hat{T}_{\mathrm{e}} + \hat{W}_{ee} + \hat{W}_{en} + \hat{T}_{n} + \hat{W}_{nn}$$

$$\hat{T}_e = \sum_{i=1}^{N_e} \frac{[\hat{\mathbf{p}}_i + |e|\mathbf{A}_{\perp}(\mathbf{r}_i, t)]^2}{2m_e}$$

$$\hat{T}_n = \sum_{I=1}^{N_n} \frac{[\hat{\mathbf{P}}_I - Z_I|e|\mathbf{A}_{\perp}(\mathbf{R}_I, t)]^2}{2m_e}$$

Frequency, polarization, pulse (envelope),…

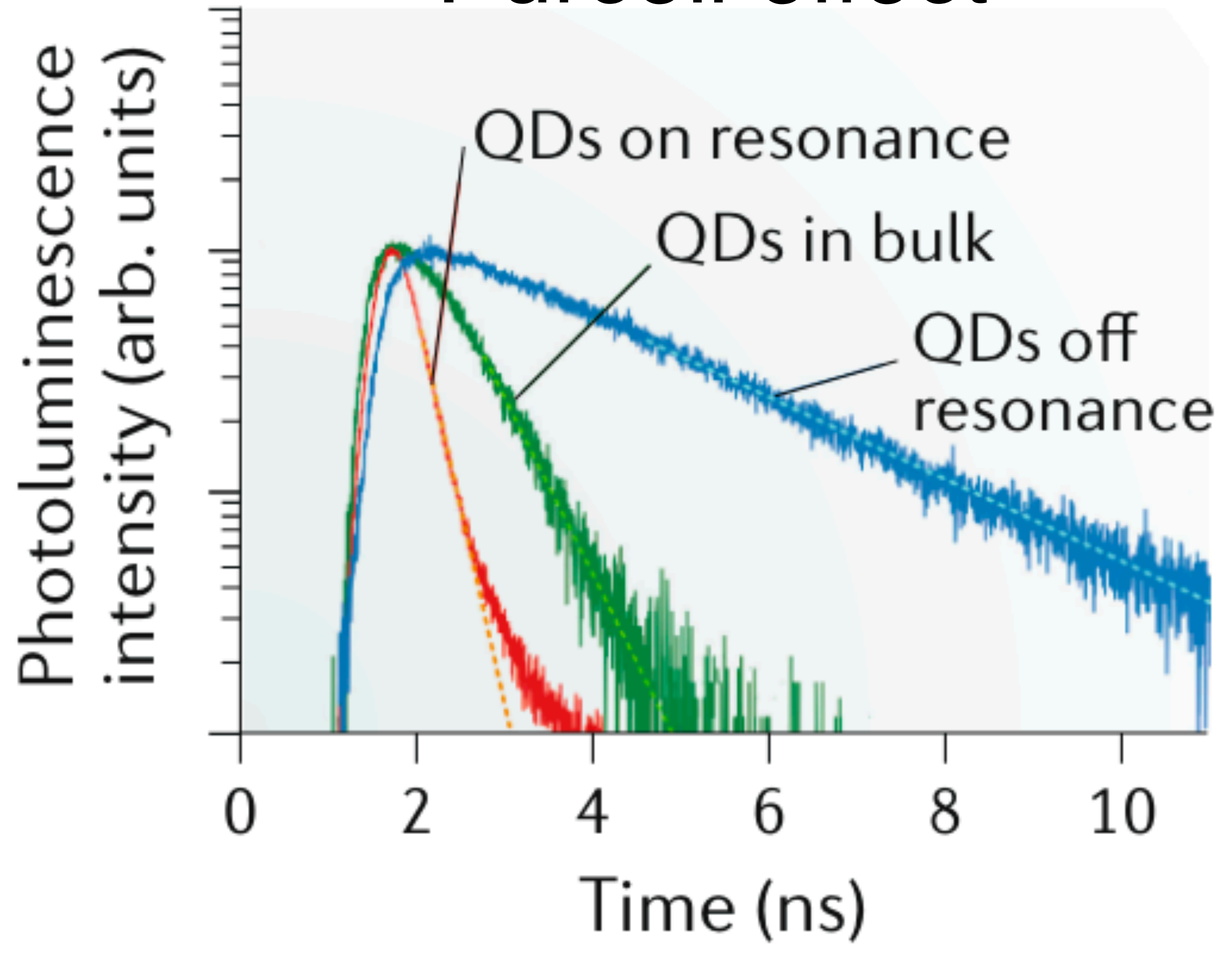
Enhance light-matter interactions using a cavity



Dark cavity - without external driving

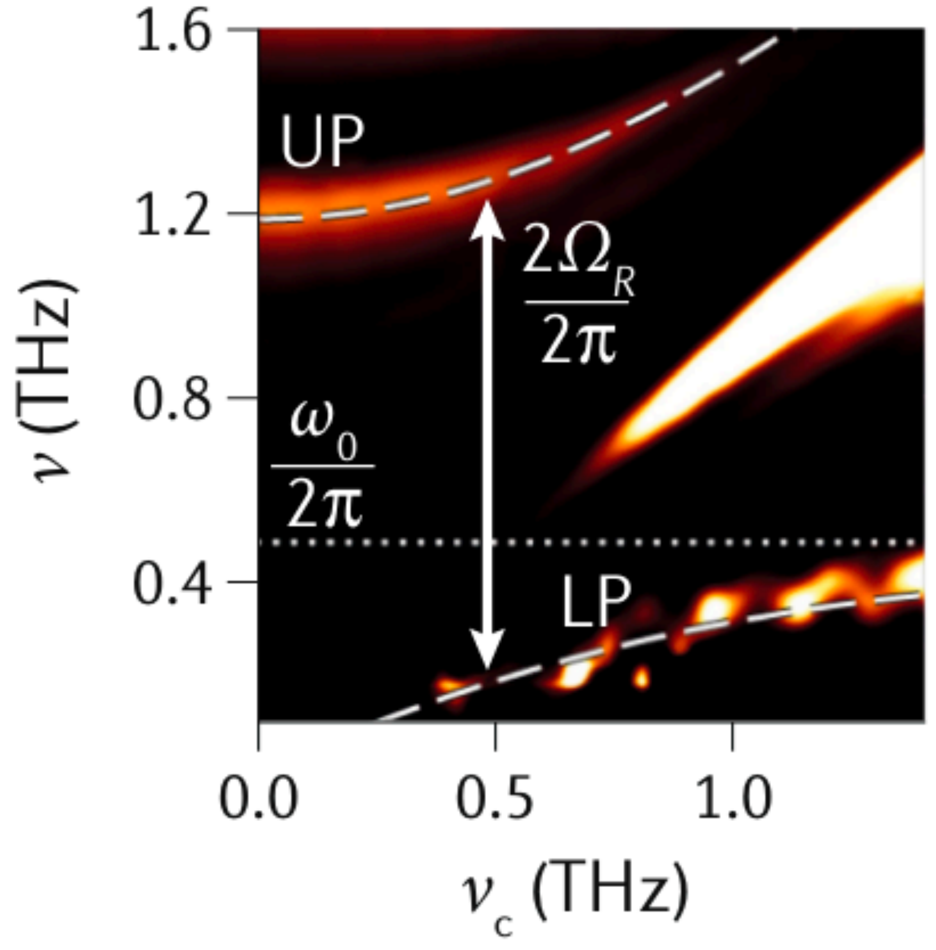
Weak coupling

Purcell effect



Strong coupling

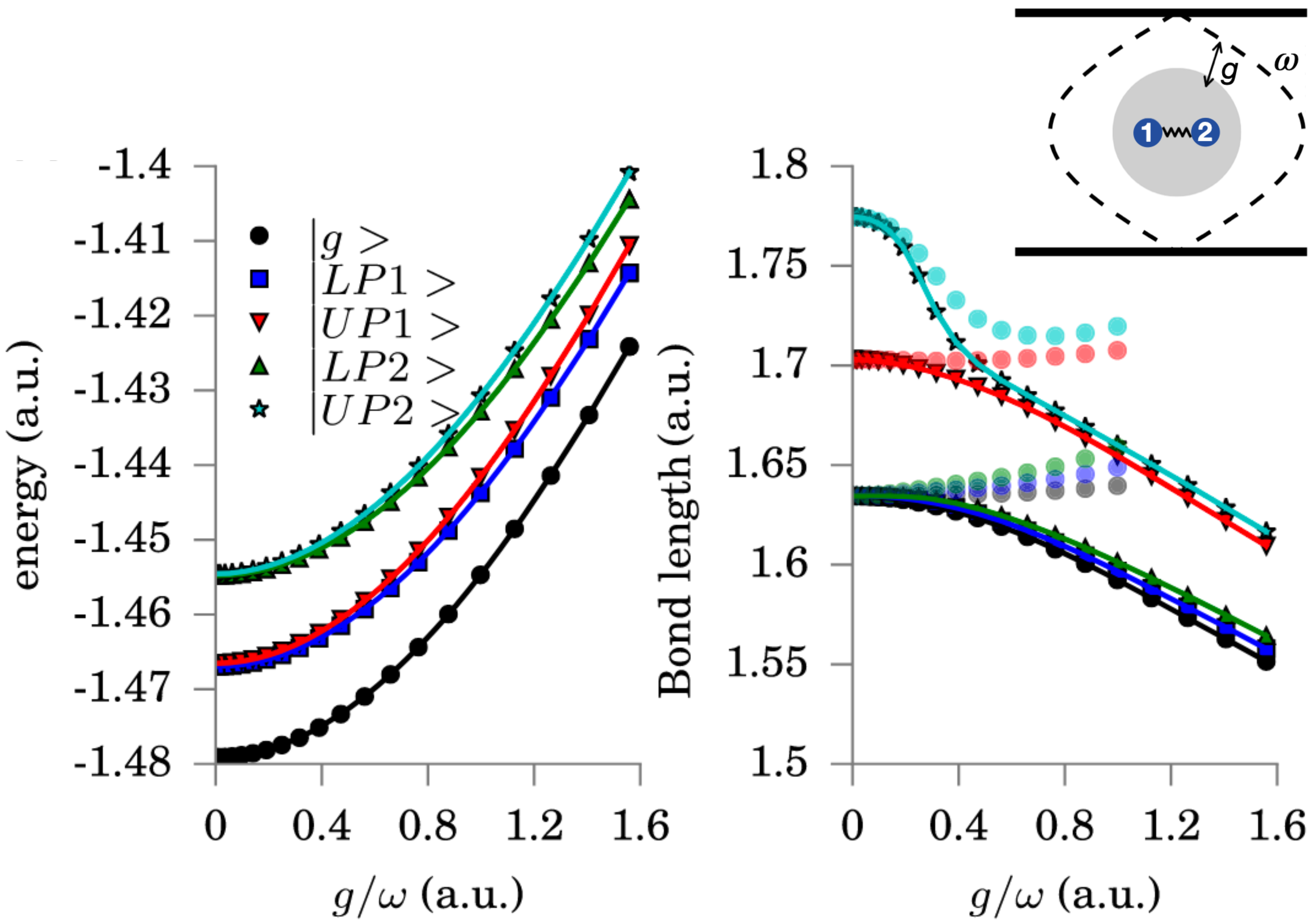
Polaritons



P. Forn-Díaz *et al.*, *Rev. Mod. Phys.* **91**, 025005 (2019)

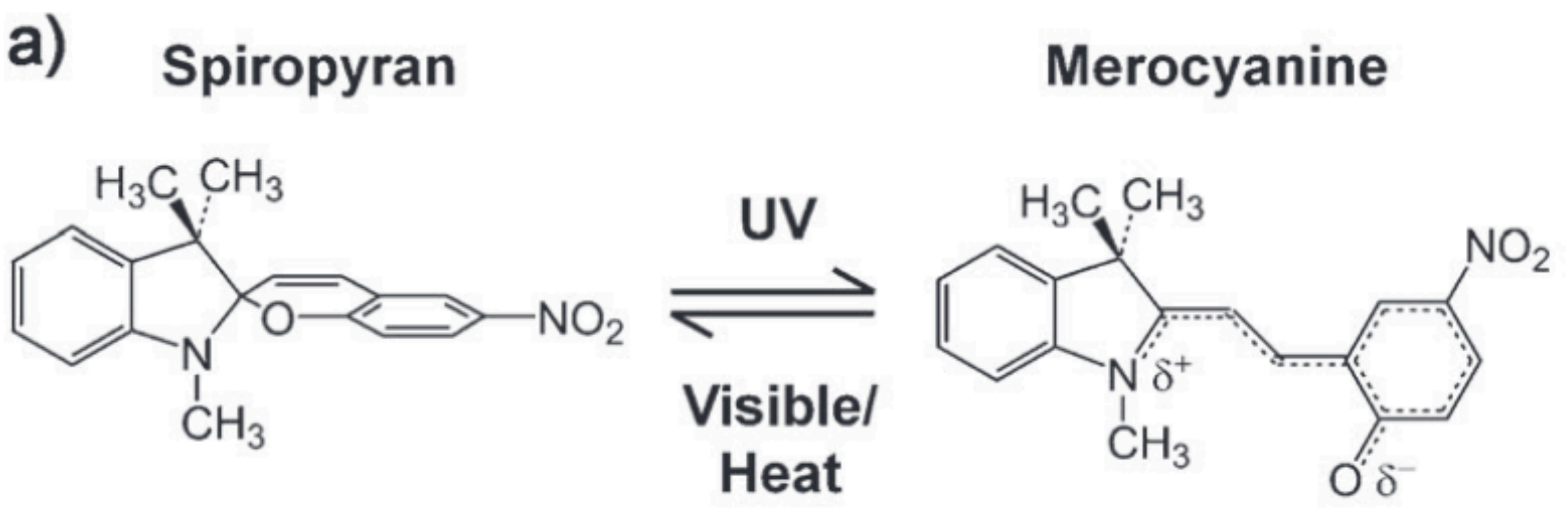
F. Kockum *et al.*, *Nat Rev Phys* **1**, 19–40 (2019)

Quantum vacuum fluctuations to modify the energy landscape of materials (molecules) inside an optical cavity

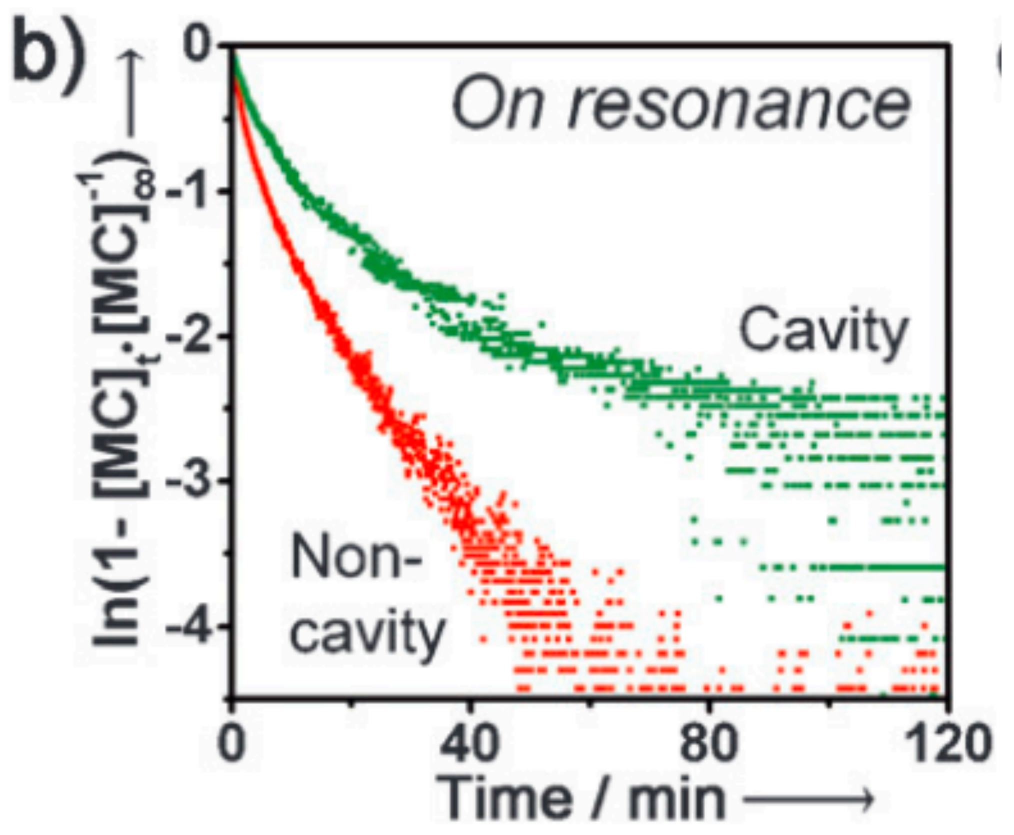


J. Flick, M. Ruggenthaler, H. Appel, & A. Rubio, *PNAS* **114**, 3026–3034 (2017)

M. Ruggenthaler, J. Flick., C. Pellegrini, H. Appel, I. V. Tokatly, & A. Rubio, PRA **90**, 012508 (2014)

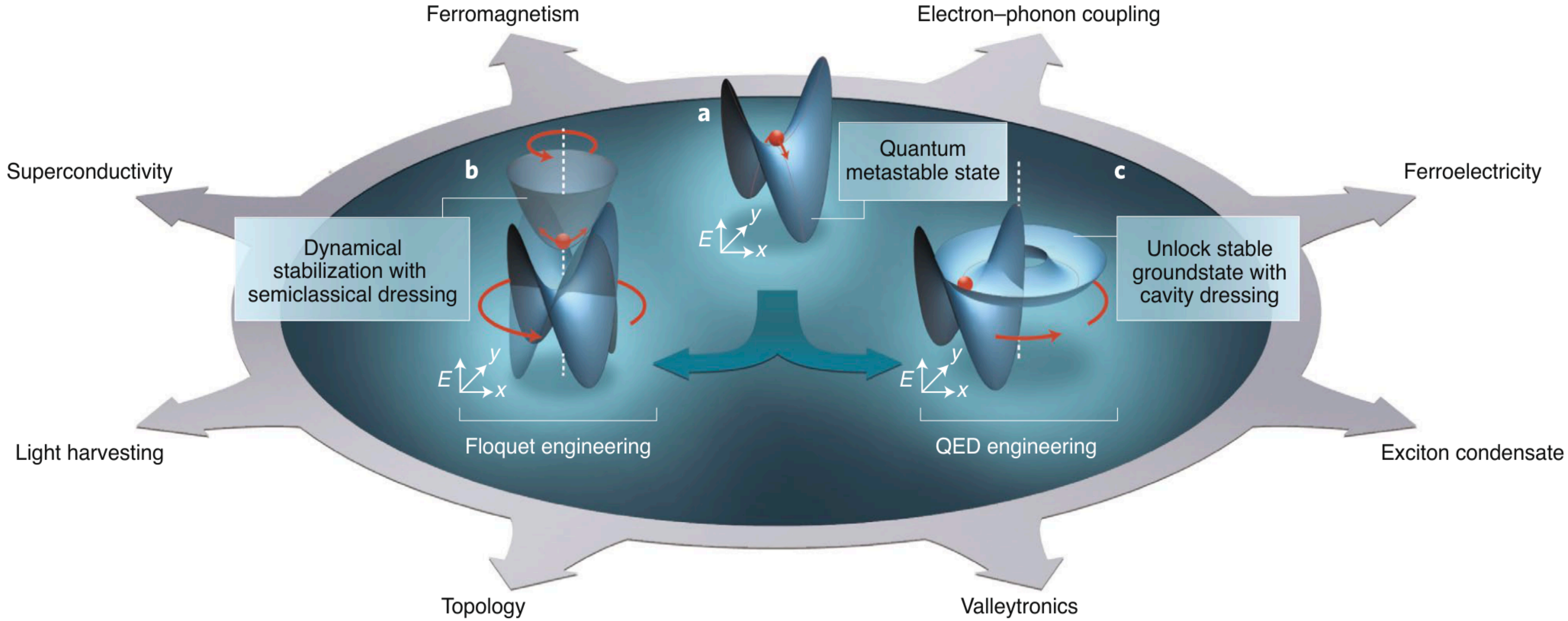


Tune chemical reaction rate using a dark cavity



J. A. Hutchison, T. Schwartz, C. Genet, E. Devaux, & T. W. Ebbesen, Angew. Chem. Int. Ed. **51**, 1592–1596 (2012)

Cavity (QED) materials engineering offers a novel route to control solid-state properties using confined quantum light



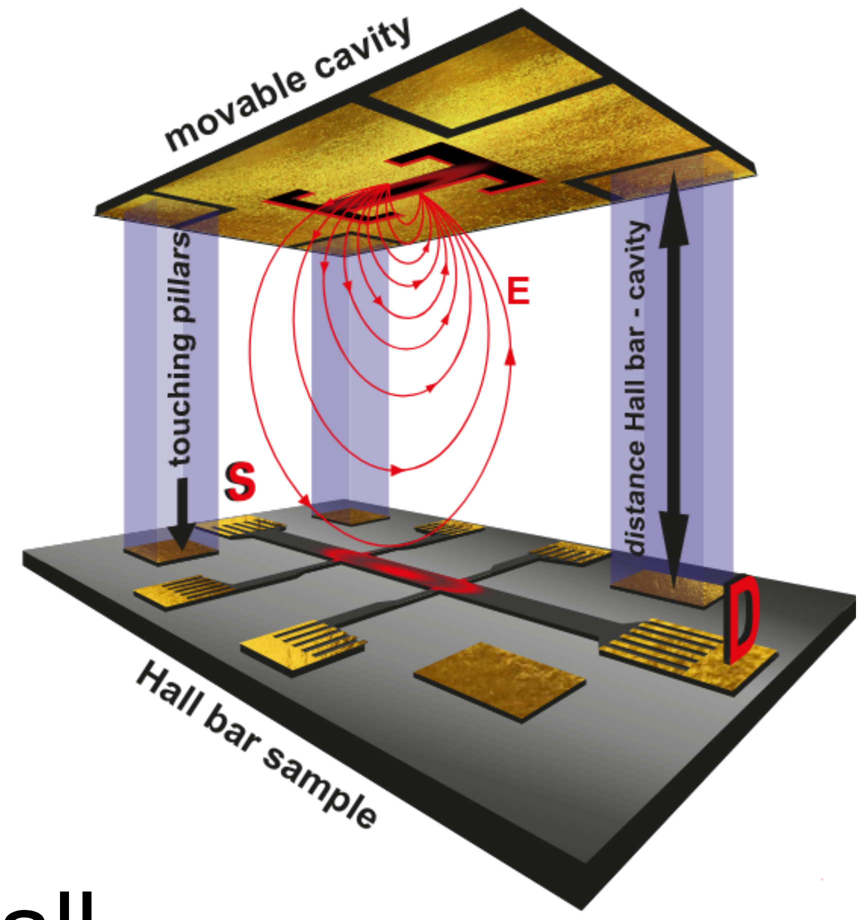
H. Hübener, H., U. De Giovannini, C. Schäfer, J. Andberger, M. Ruggenthaler, J. Faist, & A. Rubio, *Nature Materials*, *20*(4), 438–442 (2021)

Review papers

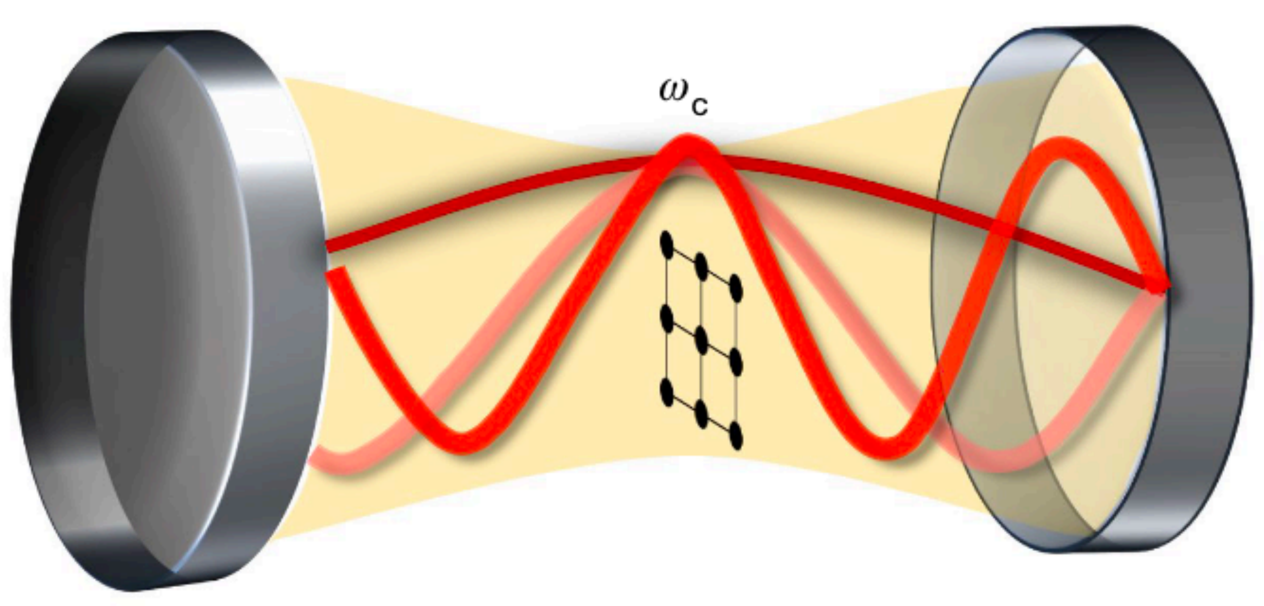
- I-T. Lu *et al.*, *arXiv:2502.03172* (2025); Accepted in AOP
- T. W. Ebbesen *et al.*, *Chemical Reviews*, *123*(21), 12037-12038 (2023)
- F. Schlawin *et al.*, *Applied Physics Reviews*, *9*(1), 011312 (2022)
- J. Bloch *et al.*, *Nature*, *606*(7912), 41-48 (2022)
- F. J. Garcia-Vidal *et al.*, *Science*, *373*(6551), eabd0336 (2021)
- N. M. Peraca *et al.*, Ch03 in Semiconductors and Semimetals, vol. 105 of Semiconductor Quantum Science and Technology, page 89–151 (2020)
- M. Ruggenthaler *et al.*, *Nature Reviews Chemistry* **2**, 1–16 (2018)

Quantum vacuum fluctuations can be used to modify a wide range of solid-state materials properties

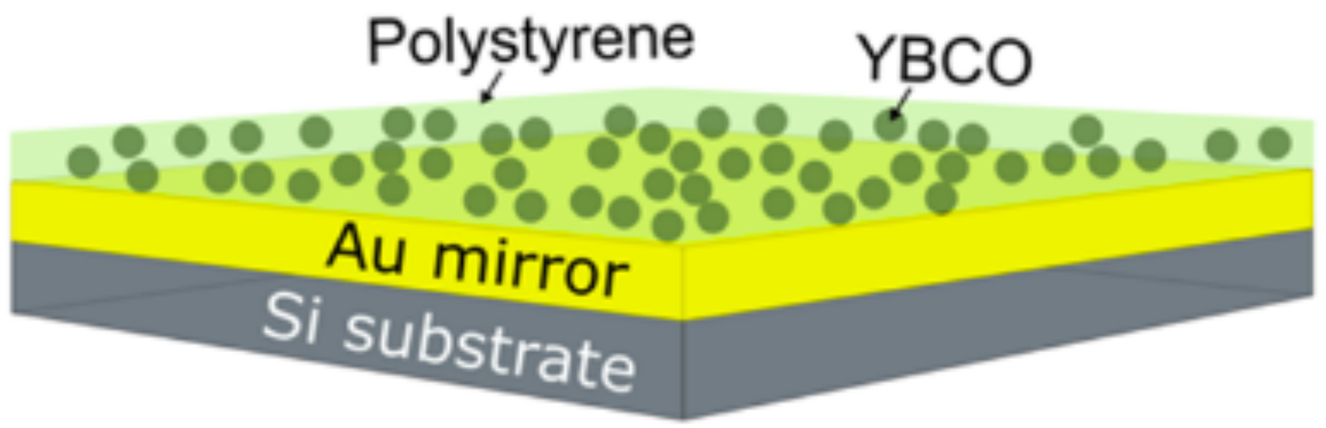
Split ring resonator



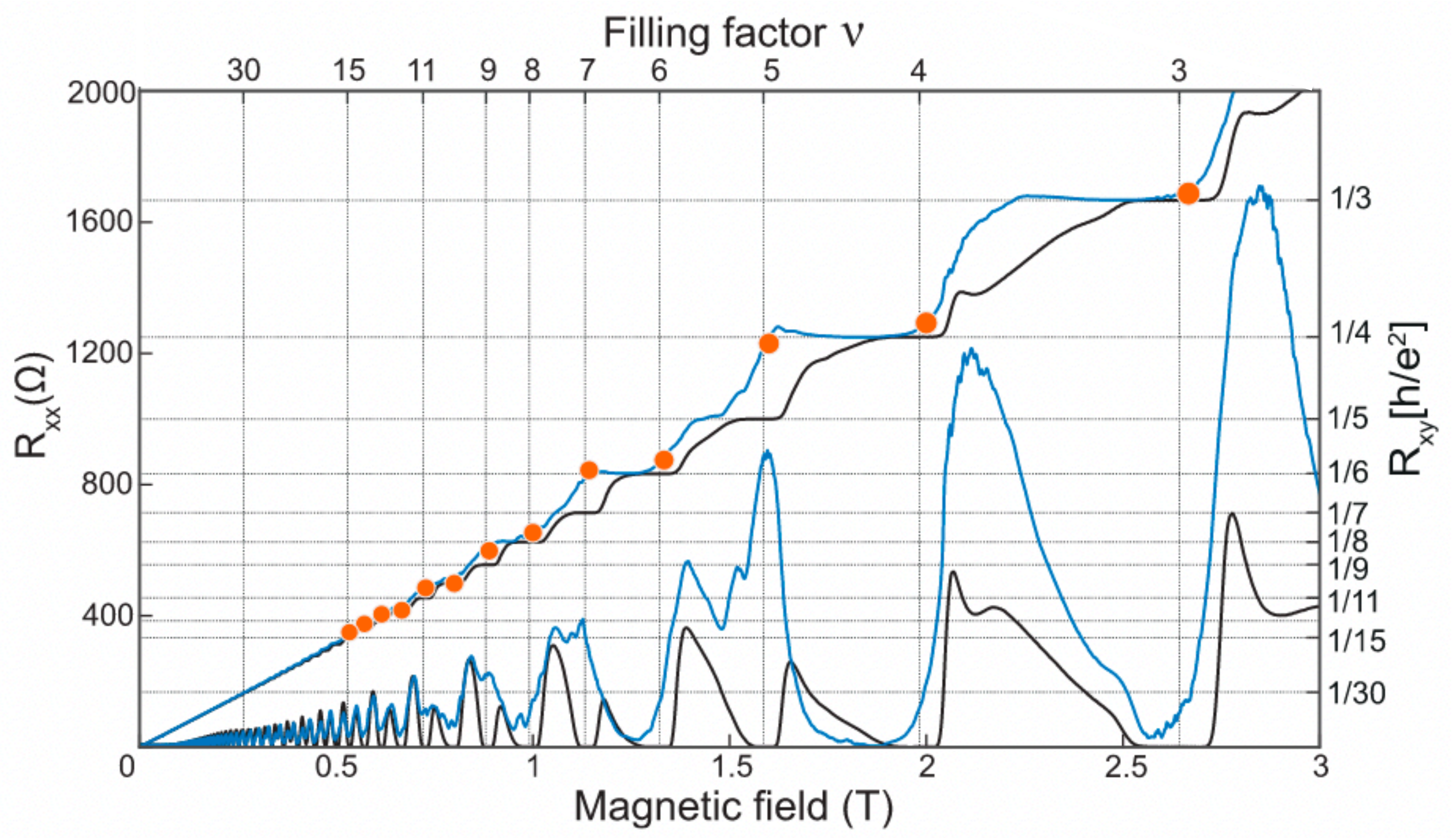
Fabry-Pérot cavity



Plasmonics



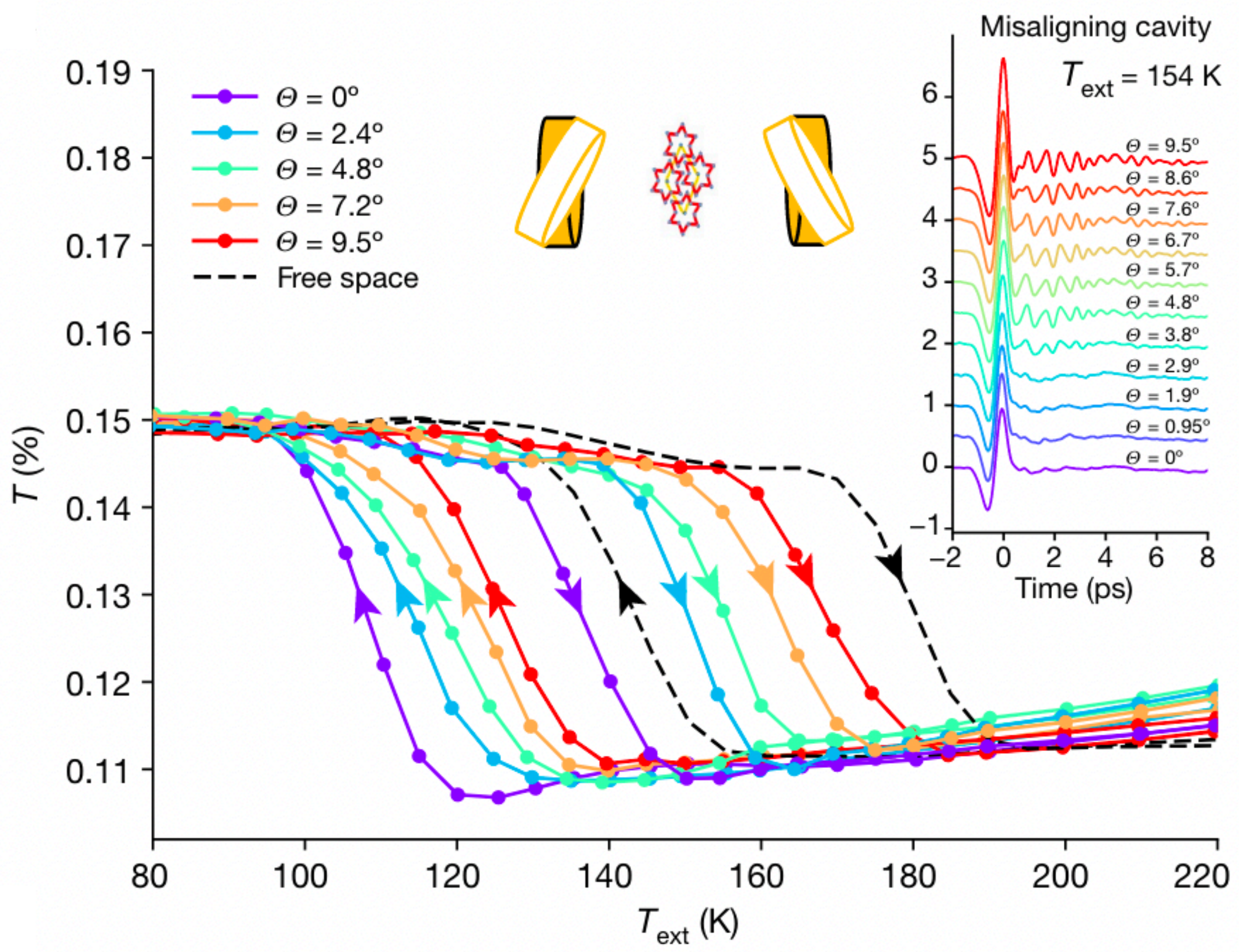
Quantum Hall



F. Appugliese *et al.*, Science 375, 1030-1034 (2022)

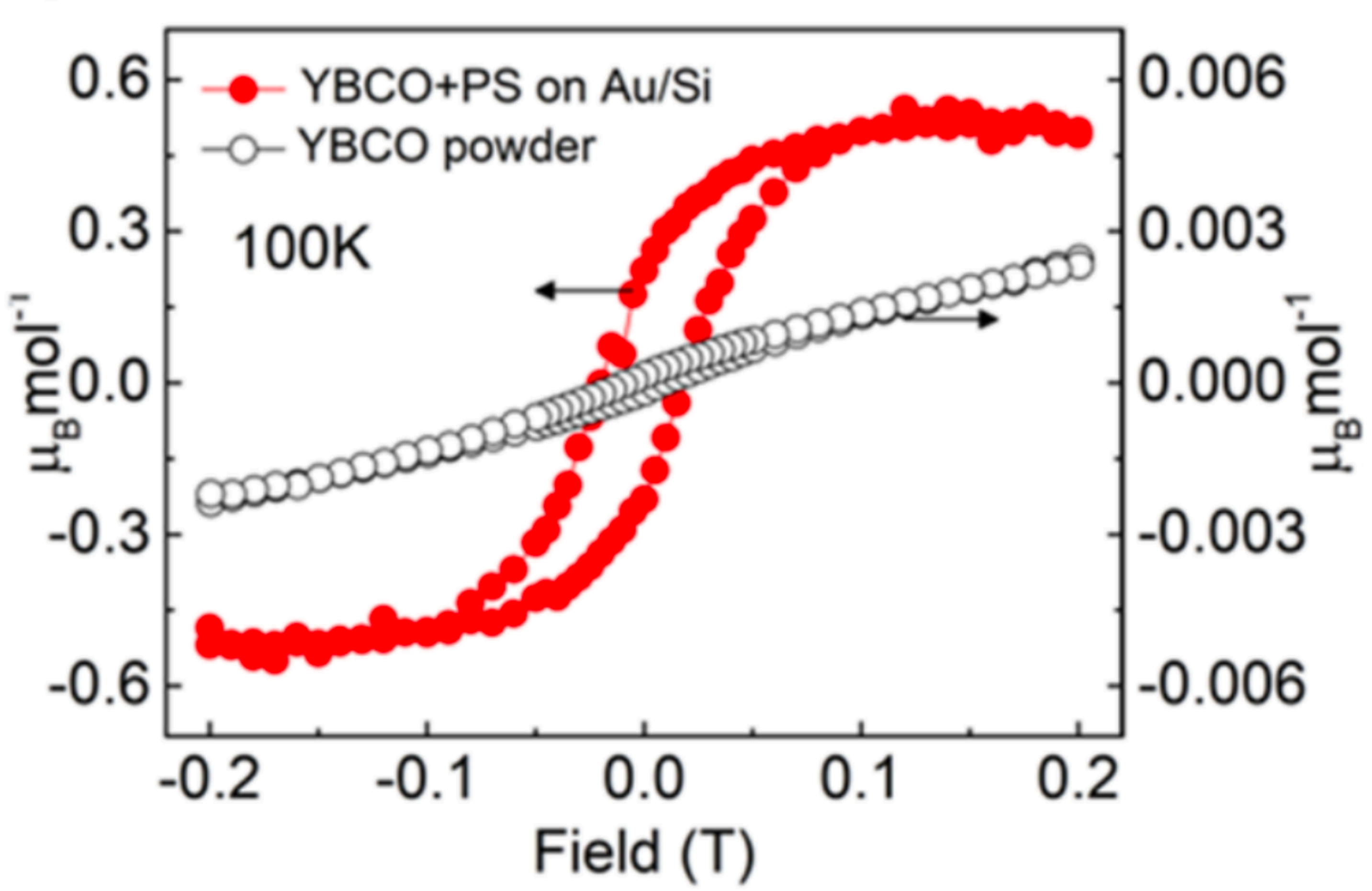
J. Enkner *et al.*, arXiv:2405.18362 (2024)

Metal-to-insulator



G. Jarc *et al.*, Nature 622, 487 (2023)

Ferromagnetism



A. Thomas *et al.*, Nano Letters 21, 4365 (2021)

First-principle framework for matter-only and light-matter coupled systems

Systems	Hamiltonians	First principles framework	Physics
Matter	$\hat{H}_{\text{Matter}}(\underline{\hat{\mathbf{r}}}, \underline{\hat{\mathbf{R}}})$	DFT	Static phenomena
Matter + **classical** transverse EM field	$\hat{H}_{\text{Matter}}(\underline{\hat{\mathbf{r}}}, \underline{\hat{\mathbf{R}}}, \mathbf{A})$	TD(C)DFT	Time dependent phenomena
Matter + **quantum** transverse EM field	$\hat{H}(\underline{\hat{\mathbf{r}}}, \underline{\hat{\mathbf{R}}}, \hat{\mathbf{A}})?$	??(C)DFT	Static, time-dependent & temperature from first principles

M. Ruggenthaler, N. Tancogne-Dejean, J. Flick, H. Appel, & A. Rubio, *Nature Reviews Chemistry* **2**, 1–16 (2018)

The Pauli-Fierz (PF) Hamiltonian serves as the foundation for (quantum) light-matter coupled systems

Coulomb kernel

$$\hat{H}_{\mathrm{PF}} = \sum_{i=1}^{N_e} \left[\frac{\left(\hat{\mathbf{p}}_i + |e|\hat{\mathbf{A}}_\perp(\mathbf{r}_i)\right)^2}{2m_{e,b}} + \frac{|e|\hbar}{2m_{e,b}}\sigma_i \cdot \hat{\mathbf{B}}(\mathbf{r}_i) \right] + \frac{1}{2}\sum_{i\neq j}^{N_e} \frac{e^2}{4\pi\epsilon_0|\mathbf{r}_i - \mathbf{r}_j|} - \sum_{i=1}^{N_e}\sum_{I=1}^{N_n} \frac{Z_I e^2}{4\pi\epsilon_0|\mathbf{r}_i - \mathbf{R}_I|}$$

$$+ \sum_{I=1}^{N_n} \left[\frac{\left(\hat{\mathbf{P}}_I - Z_I|e|\hat{\mathbf{A}}_\perp(\mathbf{R}_I)\right)^2}{2M_{I,b}} - \frac{Z_I|e|\hbar}{2M_{I,b}}\mathbf{S}_I \cdot \hat{\mathbf{B}}(\mathbf{R}_I) \right] + \frac{1}{2}\sum_{I\neq J}^{N_n} \frac{Z_I Z_J e^2}{4\pi\epsilon_0|\mathbf{R}_I - \mathbf{R}_J|} + \sum_{\mathbf{n},\lambda} \hbar\omega_{\mathbf{n}}\hat{a}^\dagger_{\mathbf{n},\lambda}\hat{a}_{\mathbf{n},\lambda}$$

- Has a well-defined ground state
- Bare mass for electrons and nuclei
- Consistent boundary conditions for both light and matter
- Equations of motion for photons obey Maxwell's equations

M. Ruggenthaler, D. Sidler, & A. Rubio, *Chem. Rev.* **123**, 11191–11229 (2023)

M. Ruggenthaler, N. Tancogne-Dejean, J. Flick, H. Appel, & A. Rubio, *Nat Rev Chem* **2**, 1–16 (2018)

QEDFT extends DFT by including the quantum nature of (transverse) electromagnetic fields

$$\hat{H}_{\text{PF}} = \frac{1}{2}\sum_{l=1}^{N_e}\left(-i\nabla_l + \frac{1}{c}\hat{\mathbf{A}}(\mathbf{r}_l)\right)^2 + \frac{1}{2}\sum_{l\neq k}^{N_e} w(\mathbf{r}_l,\mathbf{r}_k) + \sum_{l=1}^{N_e} v_{\text{ext}}(\mathbf{r}_l) + \sum_{\alpha=1}^{M_p}\omega_\alpha\left(\hat{a}_\alpha^\dagger\hat{a}_\alpha + \frac{1}{2}\right) - \frac{1}{c}\int d^3r\, \mathbf{j}_{\text{ext}}(\mathbf{r})\cdot\hat{\mathbf{A}}(\mathbf{r})$$

$$(V_{\text{ext}}, \mathbf{j}_{\text{ext}}) \quad \leftrightarrows \quad |\Psi\rangle \quad \leftrightarrows \quad (\rho(\mathbf{r}), \mathbf{A}(\mathbf{r})) \quad \leftrightarrows \quad |\Phi\rangle \quad \leftrightarrows \quad (V_{\text{KS}}, \mathbf{j}_{\text{KS}})$$

Non-interacting system

M. Ruggenthaler, arXiv:1509.01417 (2017) (Ground-state QEDFT)

M. Ruggenthaler, J. Flick., C. Pellegrini, H. Appel, I. V. Tokatly, & A. Rubio, *PRA* **90**, 012508 (2014) (Relativistic and non-relativistic QEDFT)

Maxwell-KS system $\hat{h} = \frac{1}{2}\left(-i\nabla + \frac{1}{c}\mathbf{A}_{\text{KS}}(\mathbf{r})\right)^2 + v_{\text{KS}}(\mathbf{r})$ $\quad v_{\text{KS}}(\mathbf{r}) = v_{\text{ext}}(\mathbf{r}) + v_{\text{H}}(\mathbf{r}) + v_{\text{xc}}(\mathbf{r}) + v_{\text{pxc}}(\mathbf{r})$

$\downarrow$ long-wavelength approximation: $\mathbf{A}_{\text{KS}}$

v_{xc}: electron-electron interaction

v_{pxc}: electron-photon interaction

Searching functionals for electron-photon interactions: length gauge & energy approach

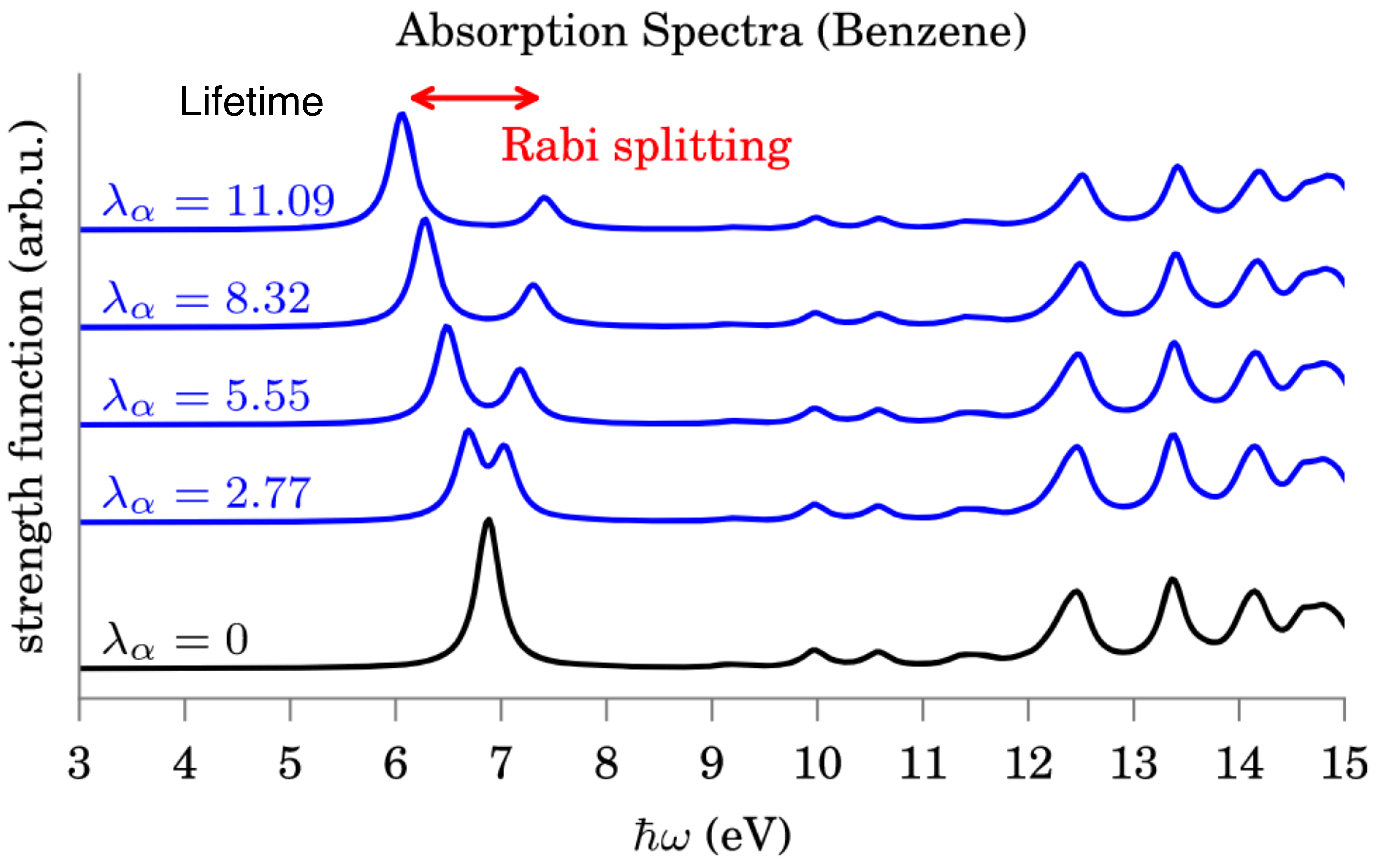
- Perturbation theory (**first functional, OEP**): C. Pellegrini, J. Flick, I. V. Tokatly, H. Appel, & A. Rubio, *PRL* **115**, 093001 (2015)

- **Linear response**: J. Flick, D. M. Welakuh, M. Ruggenthaler, H. Appel, & A. Rubio, *ACS Photonics* **6**, 2757–2778 (2019)

- **Density** approach:
  J. Flick, *PRL*, *129*(14), 143201 (2022)

- **Photon-RPA** (1D model):
  D. Novokreschenov *et al.*, *PRB* **108**, 235424 (2023)

- **Van der Waal corrections**:
  C. Tasci *et al.*, *PRL 134*(7), 073002 (2025)

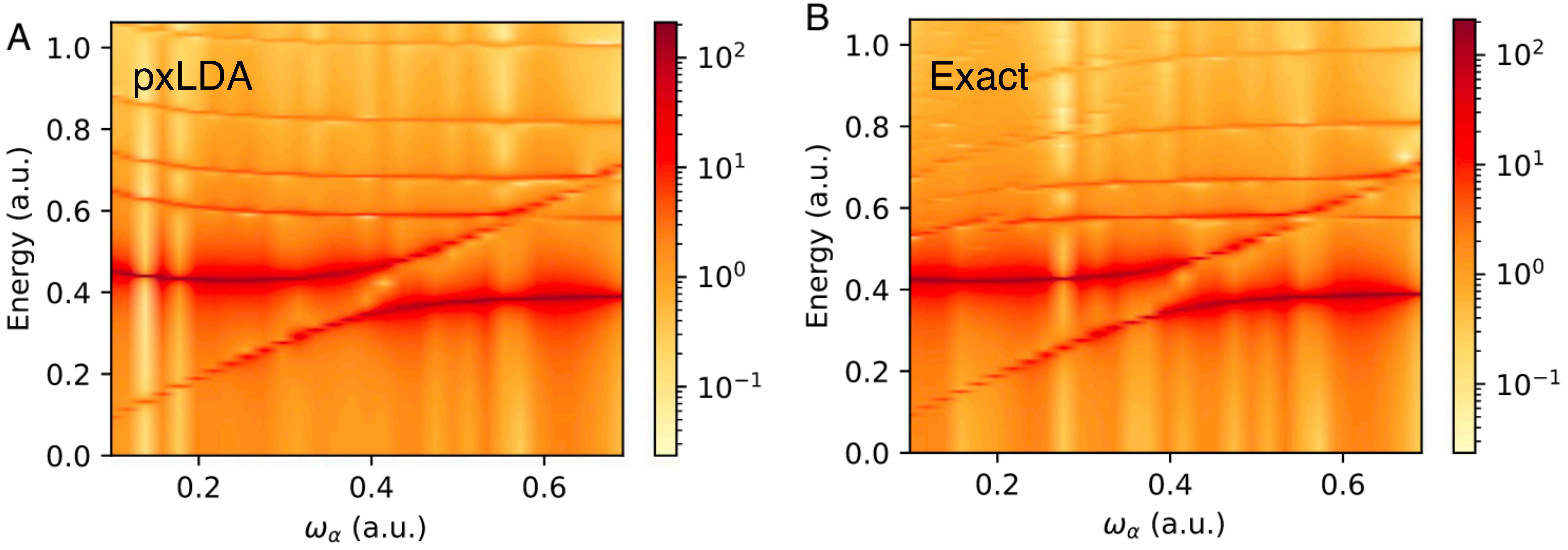


Searching functionals for electron-photon interactions: velocity gauges & force-balance approach

- Velocity gauge (suitable for **extended systems**)
- **Avoids** the differentiability issue for energy functionals, the causality issue for action functionals, the numerical costly OEP

C. Schäfer, F. Buchholz, M. Penz, M. Ruggenthaler, & A. Rubio, *PNAS*, 118 (41), e2110464118 (2021)

1D Hydrogen with soft Coulomb



I-T. Lu, M. Ruggenthaler, N. Tancogne-Dejean, S. Latini, M. Penz, & A. Rubio, *PRA*, 109, 052823 (2024)

The PF Hamiltonian within the long-wavelength approximation (LWA) for electron-photon coupled systems

Coulomb gauge and **long wavelength approximation** (**'effective' modes**)

$$\hat{H}_{\mathrm{PF}} = \frac{1}{2}\sum_{l=1}^{N_e}\left(-i\nabla_l + \frac{1}{c}\hat{\mathbf{A}}\right)^2 + \frac{1}{2}\sum_{l\neq k}^{N_e} w(\mathbf{r}_l, \mathbf{r}_k) + \sum_{l=1}^{N_e} v_{\mathrm{ext}}(\mathbf{r}_l) + \sum_{\alpha=1}^{M_p}\omega_\alpha\left(\hat{a}_\alpha^\dagger\hat{a}_\alpha + \frac{1}{2}\right)$$

where $\hat{\mathbf{A}} = \sum_{\alpha=1}^{M_p}\hat{A}_\alpha\boldsymbol{\varepsilon}_\alpha$ $\quad \hat{A}_\alpha = \frac{\lambda_\alpha}{\sqrt{2\omega_\alpha}}(\hat{a}_\alpha^\dagger + \hat{a}_\alpha)$

λ_α: vacuum field amplitude (mode strength, light-matter coupling) $\sim \frac{1}{\sqrt{\Omega_\alpha}}$

ω_α: photon frequency

M. K. Svendsen, M. Ruggenthaler, H. Hübener, C. Schäfer, M. Eckstein, A. Rubio, & S. Latini, arXiv:2312.17374 (2023)

Electron-electron and electron-photon exchange-correlation functionals from force-balance equation

From the **equations of motion** for the **paramagnetic current operator**

$$d\hat{\mathbf{j}}_{\mathrm{p}}(t)/dt = i\left[\hat{H}_{\mathrm{PF}}, \hat{\mathbf{j}}_{\mathrm{p}}(t)\right] \longrightarrow \rho(\mathbf{r})\nabla v_{\mathrm{ext}}(\mathbf{r}) = \langle \hat{\mathbf{F}}_T(\mathbf{r})\rangle_{\Psi} + \langle \hat{\mathbf{F}}_W(\mathbf{r})\rangle_{\Psi} - \frac{1}{c}\langle(\hat{\mathbf{A}}\cdot\nabla)\hat{\mathbf{j}}_{\mathrm{p}}(\mathbf{r})\rangle_{\Psi}$$

at equilibrium

$$d\hat{\mathbf{j}}_{\mathrm{p}}(t)/dt = i\left[\hat{H}_{\mathrm{KS}}, \hat{\mathbf{j}}_{\mathrm{p}}(t)\right] \longrightarrow \rho_s(\mathbf{r})\nabla v_{\mathrm{KS}}(\mathbf{r}) = \langle \hat{\mathbf{F}}_T(\mathbf{r})\rangle_{\Phi} - \frac{1}{c}(\tilde{\mathbf{A}}_{\mathrm{KS}}\cdot\nabla)\langle\hat{\mathbf{j}}_p(\mathbf{r})\rangle_{\Phi}$$

M.-L. M. Tchenkoue, M. Penz, I. Theophilou, M. Ruggenthaler, & A. Rubio, *J. Chem. Phys.* **151**, 154107 (2019)

N. Tancogne-Dejean. M. Penz, A. Laestadius, M. A. Csirik, M. Ruggenthaler, & A. Rubio, *J. Chem. Phys.* **160**, 024103 (2024)

Define mean-field **exchange-correlation** potential $v_{\mathrm{Mxc}}(\mathbf{r}) = v_{\mathrm{KS}}(\mathbf{r}) - v_{\mathrm{ext}}(\mathbf{r})$

$$\nabla^2 v_{\mathrm{Mxc}}(\mathbf{r}) = \nabla\cdot\frac{1}{\rho(\mathbf{r})}\left[\mathbf{F}_T([\Phi],\mathbf{r}) - \mathbf{F}_T([\Psi],\mathbf{r}) - \mathbf{F}_W([\Psi],\mathbf{r}) + \frac{1}{c}\langle(\hat{\mathbf{A}}\cdot\nabla)\hat{\mathbf{j}}_{\mathrm{p}}(\mathbf{r})\rangle_{\Psi} - \frac{1}{c}(\tilde{\mathbf{A}}_{\mathrm{KS}}\cdot\nabla)\langle\hat{\mathbf{j}}_p(\mathbf{r})\rangle_{\Phi}\right]$$

Electron-photon exchange approximation to capture the quantum fluctuations of transverse photon fields

Define electron-photon **exchange-correlation** (pxc) potential $\nabla^2 v_{\text{pxc}}(\mathbf{r}) = \frac{1}{c}\nabla \cdot \left[\frac{\langle(\hat{\mathbf{A}} \cdot \nabla)\hat{\mathbf{j}}_p(\mathbf{r})\rangle_\Psi}{\rho(\mathbf{r})}\right]$

Use $\hat{\mathbf{A}} = \langle\hat{\mathbf{A}}\rangle_\Psi + \Delta\hat{\mathbf{A}}$

Breit-type approximation $\Delta\hat{\tilde{A}}_\alpha \approx -c\frac{\tilde{\lambda}_\alpha^2}{\tilde{\omega}_\alpha^2}\tilde{\boldsymbol{\varepsilon}}_\alpha \cdot \Delta\hat{\mathbf{J}}_{\text{p}}$

Reduce the Hilbert space and keep photon quantum effect

Electron-photon **exchange** approximation

$$\nabla^2 v_{\text{px}}(\mathbf{r}) = -\nabla \cdot \left[\sum_{\alpha=1}^{M_p} \frac{\tilde{\lambda}_\alpha^2}{2\tilde{\omega}_\alpha^2} \frac{(\tilde{\boldsymbol{\varepsilon}}_\alpha \cdot \nabla)[\mathbf{f}_{\alpha,\text{px}}(\mathbf{r}) + \text{c.c.}]}{\rho(\mathbf{r})}\right]$$

where $\mathbf{f}_{\alpha,\text{px}}(\mathbf{r}) = \langle(\tilde{\boldsymbol{\varepsilon}}_\alpha \cdot \hat{\mathbf{J}}_{\text{p}})\hat{\mathbf{j}}_{\text{p}}(\mathbf{r})\rangle_\Phi$

I-T. Lu, M. Ruggenthaler, N. Tancogne-Dejean, S. Latini, M. Penz, & A. Rubio, *Phys. Rev. A*, 109, 052823 (2024)
C. Schäfer, F. Buchholz, M. Penz, M. Ruggenthaler, & A. Rubio, *PNAS*, 118 (41), e2110464118 (2021)

Electron-photon exchange (pxLDA) approximation for strongly light-matter coupled systems

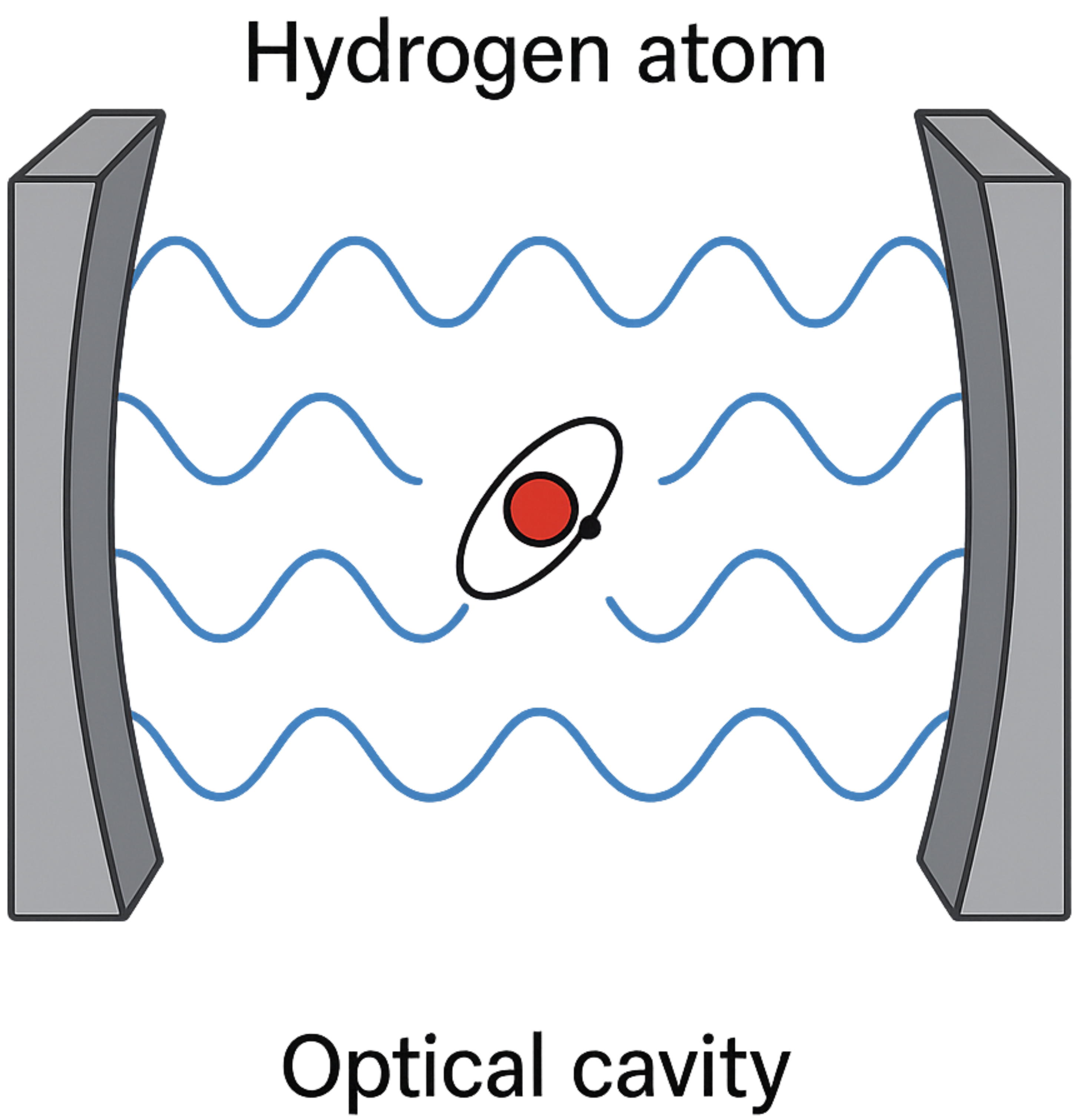
$\lambda_\alpha = 0.500$ $\omega_\alpha = 0.125$ resonates with the first excited state

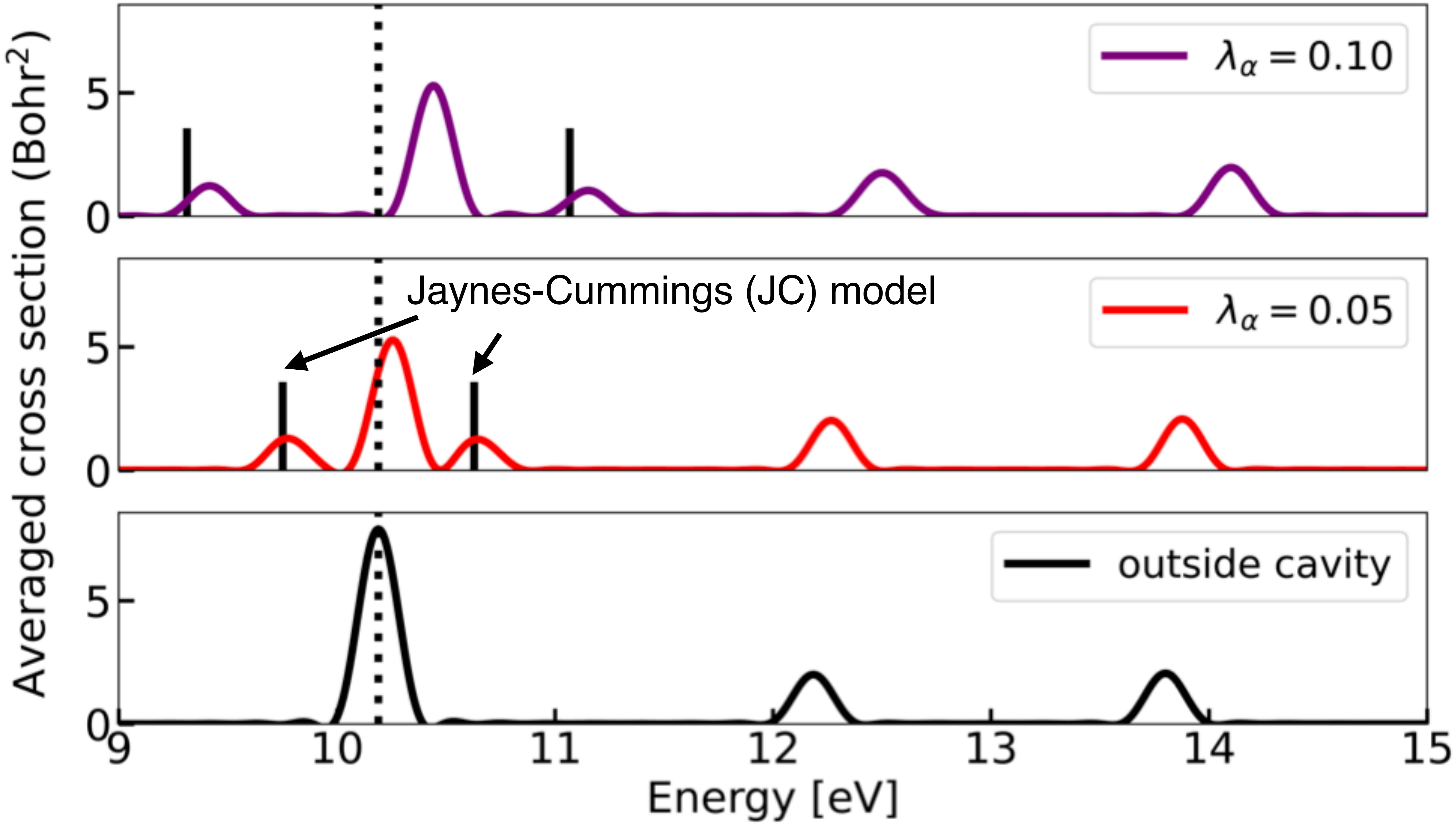
Electron-photon exchange functional **performs well at large light-matter coupling or photon frequency**

I-T. Lu, M. Ruggenthaler, N. Tancogne-Dejean, S. Latini, M. Penz, & A. Rubio, *Phys. Rev. A*, 109, 052823 (2024)

Time-dependent (adiabatic) QEDFT can reproduce vacuum Rabi splitting of a 3D hydrogen atom

Couple a hydrogen to a photon mode with **polarization along x direction** & frequency of 10.2 eV





I-T. Lu, M. Ruggenthaler, N. Tancogne-Dejean, S. Latini, M. Penz, & A. Rubio, *Phys. Rev. A*, 109, 052823 (2024)

Partition wave functions to separate systems at different time scales for light-matter coupled systems

Pauli-Fierz Hamiltonian $\hat{H}_{\mathrm{PF}}(\underline{\mathbf{r}}, \underline{\mathbf{R}}, \underline{\mathbf{A}})$ $\hat{H}_{\mathrm{PF}}(\underline{\mathbf{r}}, \underline{\mathbf{R}}, \underline{\mathbf{A}})\Psi_i(\underline{\mathbf{r}}, \underline{\mathbf{R}}, \underline{\mathbf{A}}) = E_i\Psi_i(\underline{\mathbf{r}}, \underline{\mathbf{R}}, \underline{\mathbf{A}})$

cavity Born-Oppenheimer (electronic) polaritonic surface

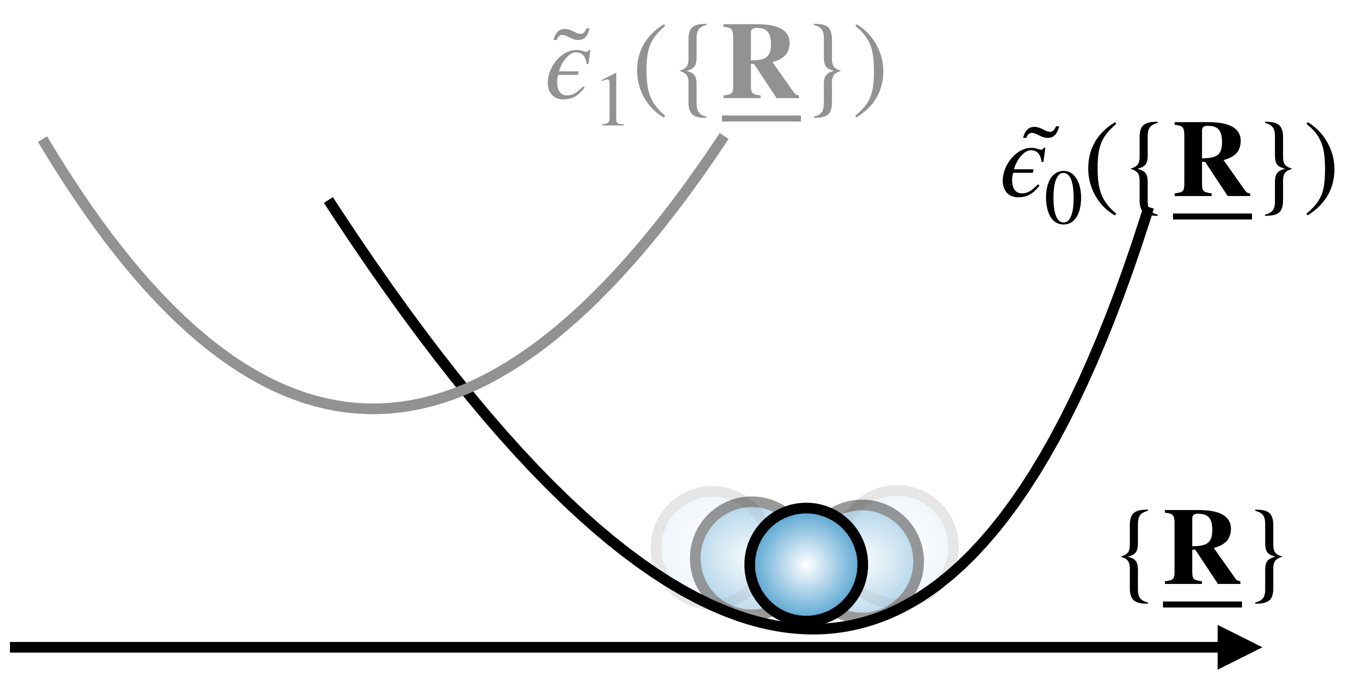
Separate '**slow**' and '**fast**' subsystems

$$\Psi_i(\underline{\mathbf{r}}, \underline{\mathbf{R}}, \underline{\mathbf{A}}) = \sum_{j=0}^{\infty} \chi_{ij}(\underline{\mathbf{R}}, \underline{\mathbf{A}})\psi_j(\underline{\mathbf{r}}; \{\underline{\mathbf{R}}\}, \{\underline{\mathbf{A}}\}) = \sum_{j=0}^{\infty} \tilde{\chi}_{ij}(\underline{\mathbf{R}})\tilde{\psi}_j(\underline{\mathbf{r}}, \underline{\mathbf{A}}; \{\underline{\mathbf{R}}\})$$

Assume that **photons** are coupled **only** to **electrons**

Born-Oppernheimer approximation (neglect non-adiabatic coupling)

$$\left[\sum_{I=1}^{N_n} \frac{\hat{\mathbf{P}}_I^2}{2M_I} + \tilde{\epsilon}_k(\{\underline{\mathbf{R}}\}) - E_i\right]\tilde{\chi}_{ik}(\underline{\mathbf{R}}) = 0$$



Minimal viable QEDFT toolbox for QED solid-state materials

Electron-photon systems

$$\left[-\frac{1}{2}\nabla^2 + v_{\mathrm{KS}}(\mathbf{r})\right]\psi_i(\mathbf{r}) = \varepsilon_i\psi_i(\mathbf{r})$$

$$v_{\mathrm{KS}}(\mathbf{r}) = v_{\mathrm{ext}}(\mathbf{r}) + v_{\mathrm{H}}(\mathbf{r}) + v_{\mathrm{xc}}(\mathbf{r}) + v_{\mathrm{pxc}}(\mathbf{r})$$

e-e interaction ($v_{\mathrm{H}}(\mathbf{r}) + v_{\mathrm{xc}}(\mathbf{r})$) e-$\gamma$ interaction ($v_{\mathrm{pxc}}(\mathbf{r})$)

I-T. Lu *et al.*, *PRA* 109, 052823 (2024)

Nuclear motion (classical ions)

$$M_I\frac{d^2\mathbf{R}_I}{dt^2} = \mathbf{F}_I + Z_I\mathbf{E}$$

Hellmann-Feynman forces $\mathbf{F}_I$

Dark cavity, i.e., $\mathbf{E} = 0$

Phonon properties (harmonic approximation)

Density functional perturbation theory (DFPT)

$$\partial_{\nu\mathbf{q}}v_{\mathrm{KS}}(\mathbf{r}) \leftrightarrow \partial_{\nu\mathbf{q}}\rho(\mathbf{r})$$

including $\partial_{\nu\mathbf{q}}v_{\mathrm{pxc}}(\mathbf{r})$

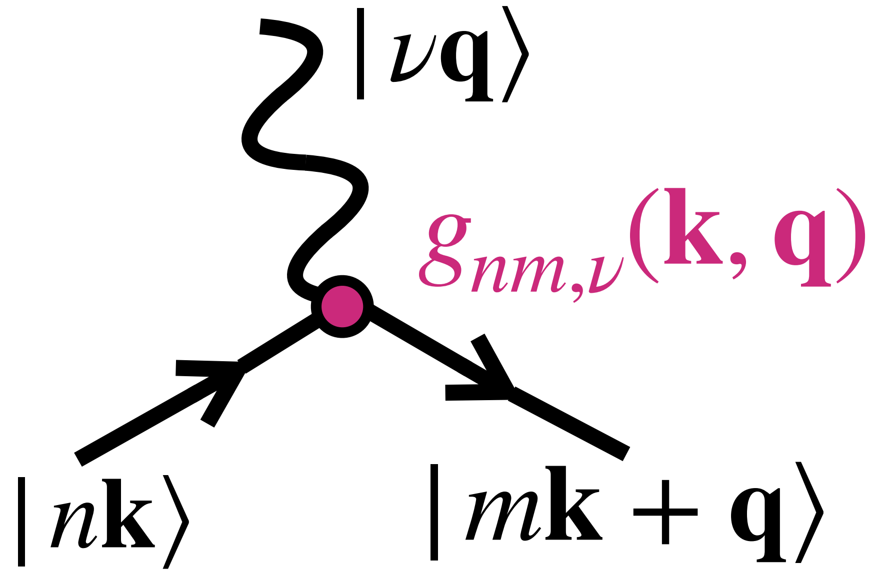
I-T. Lu *et al.*, PNAS 121, e2415061121 (2024)

Phonon dispersion

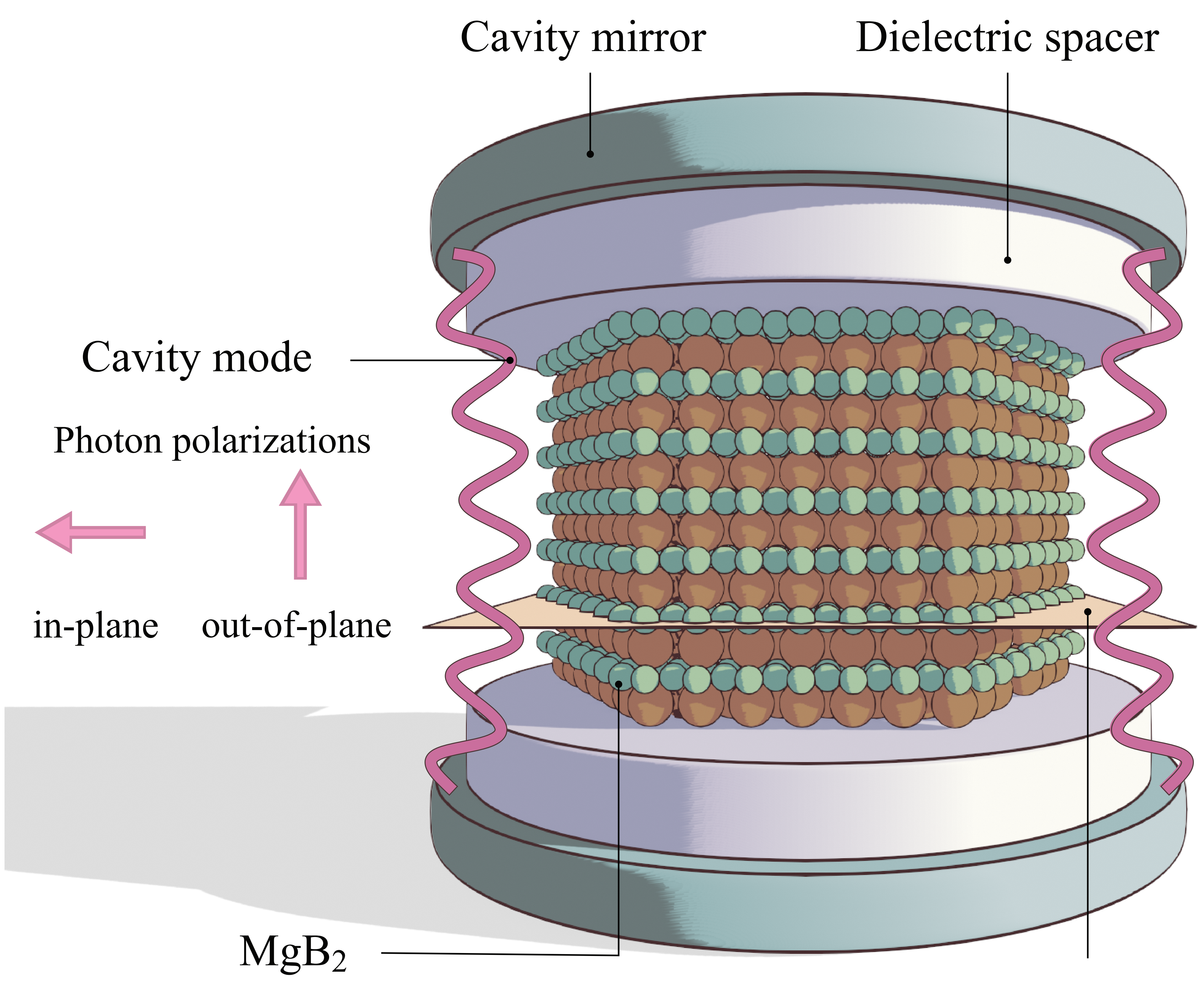
$\omega_{\nu\mathbf{q}}$ and $|\nu\mathbf{q}\rangle$

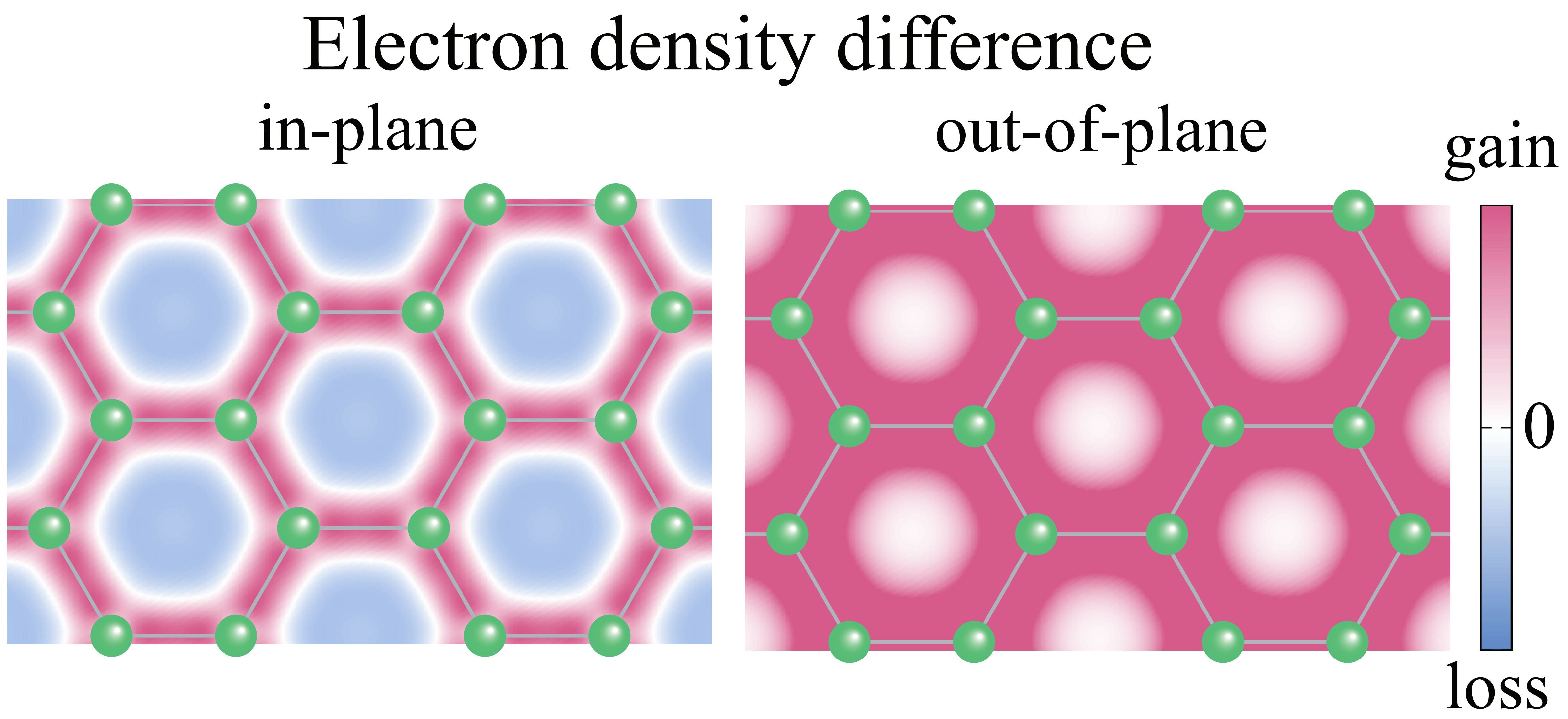
Electron-**phonon** coupling

$$g_{mn,\nu}(\mathbf{k},\mathbf{q}) = \langle m\mathbf{k}+\mathbf{q}|\partial_{\nu\mathbf{q}}v_{\mathrm{KS}}|n\mathbf{k}\rangle$$



Cavity-induced electron density redistribution (example: MgB_2)





The **physical mass of electron** is **modified** via the light-matter interaction, and electrons become heavier along the polarization direction; **electrons accumulate along B-B bonds**

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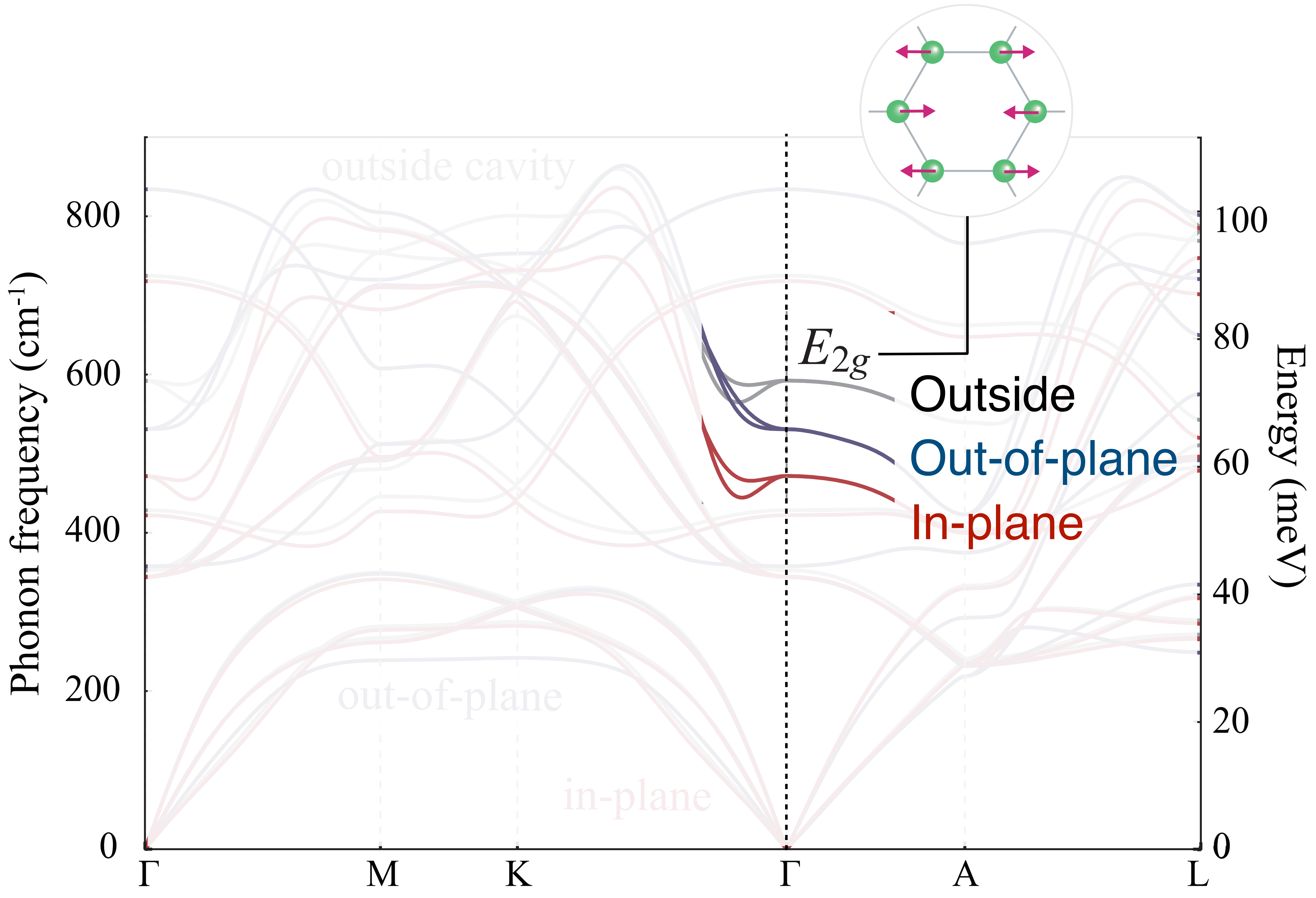
Cavity-modified phonon dispersion (example: MgB_2)

- Quantum vacuum fluctuations **affect phonons** beyond Γ and those that are **not necessarily IR-active**
- **Electron accumulation** around the boron-boron **screen the Coulomb repulsion** between boron-boron nuclei
- **Finite difference** method (from force) agree with **DFPT**, enabling calculations that do not rely on LDA functional for e-e interaction



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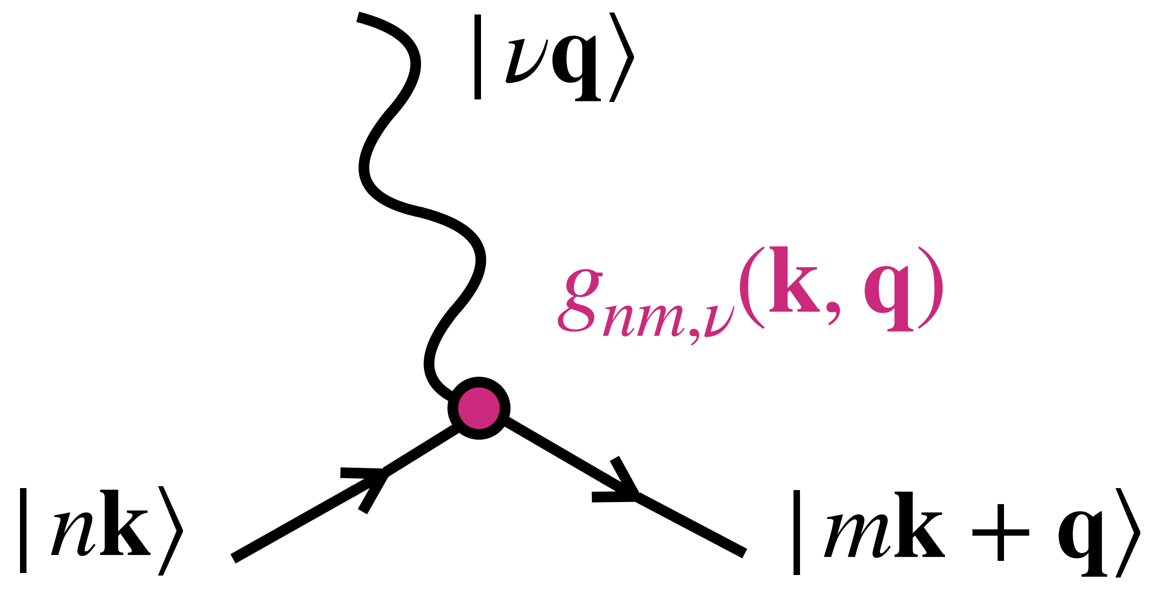
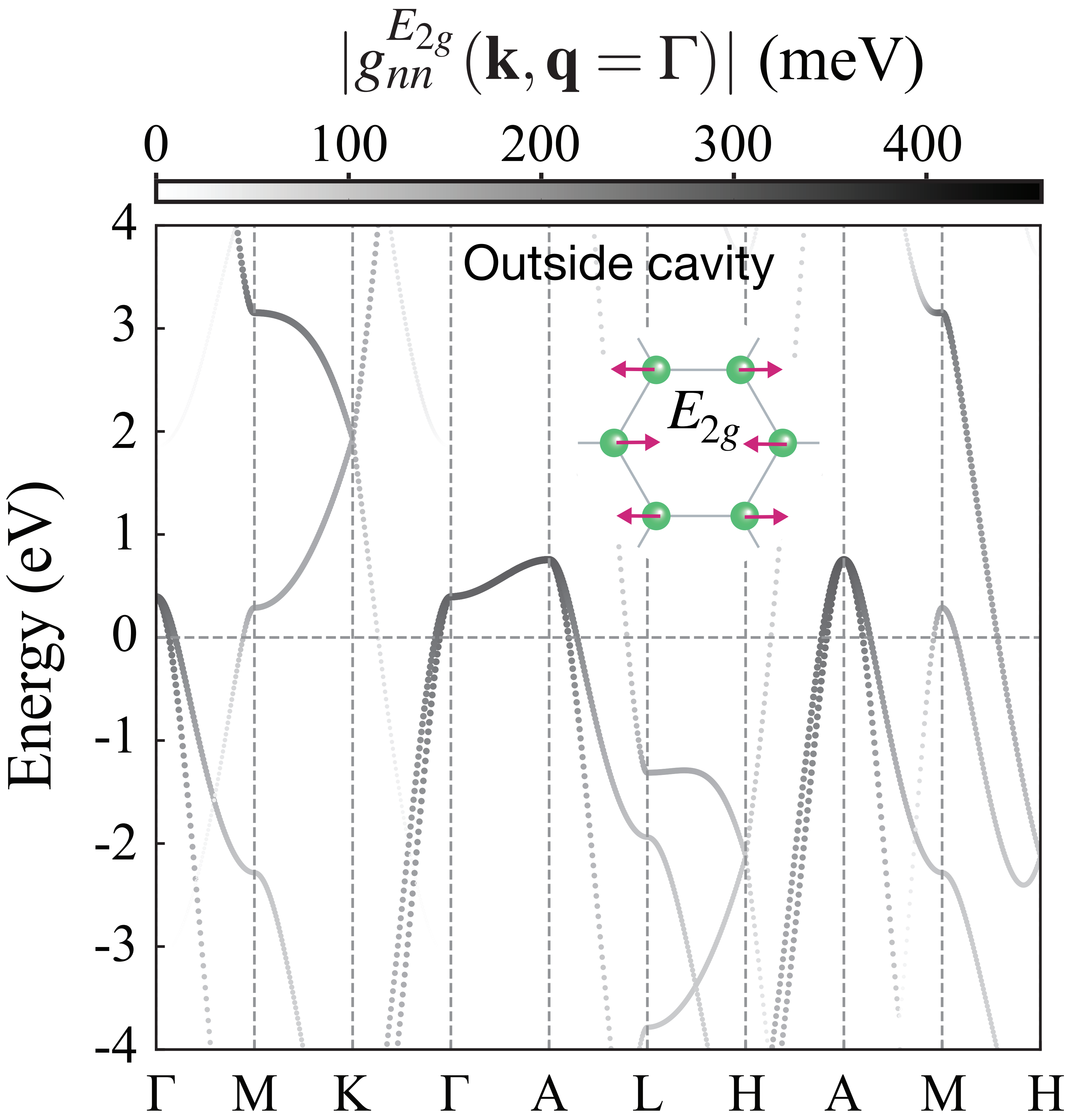
Cavity-modified electron-phonon coupling (example: MgB_2)

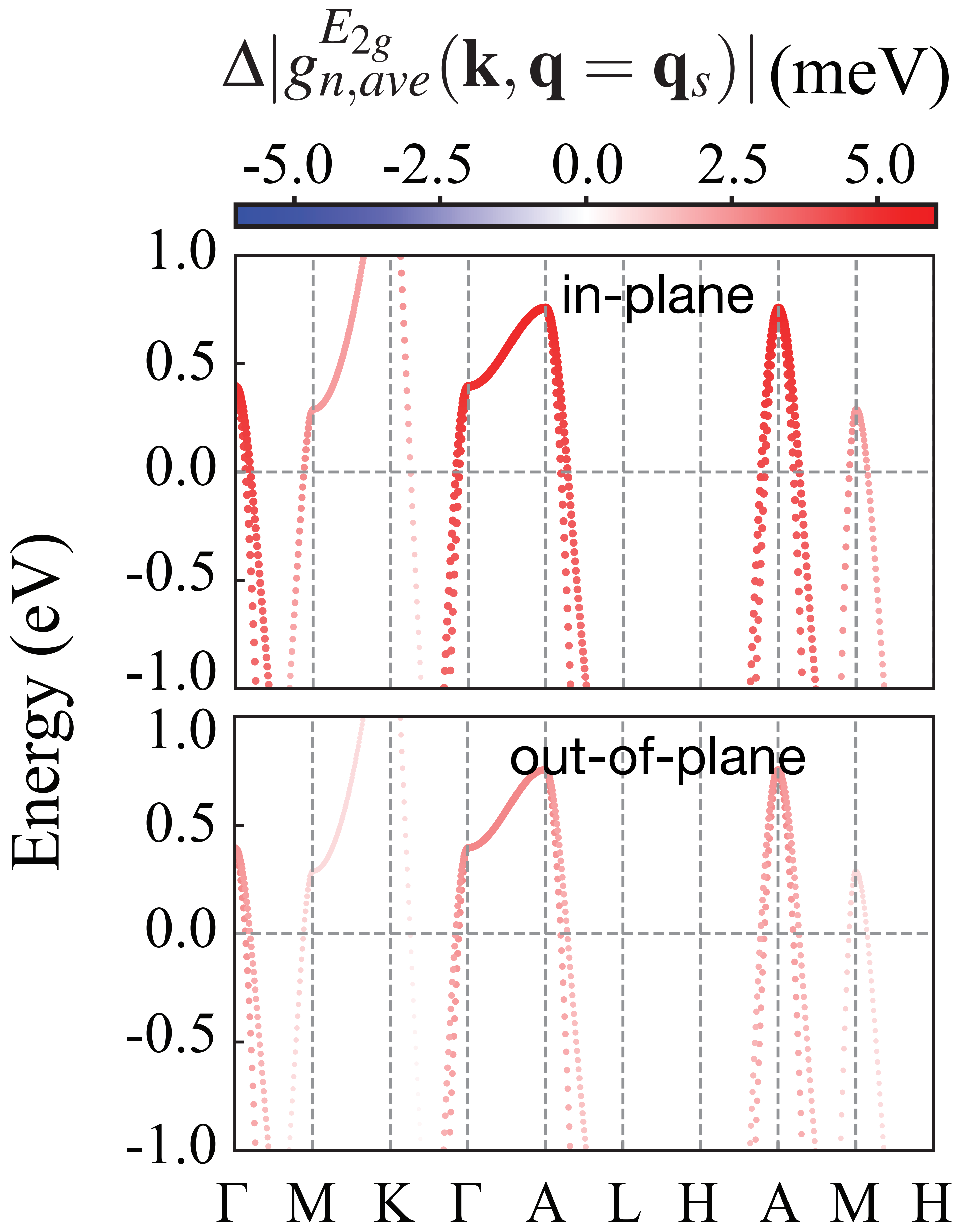
e-ph coupling matrix element

$$g_{mn,\nu}(\mathbf{k},\mathbf{q}) = \langle m\mathbf{k}+\mathbf{q}\,|\,\partial_{\nu\mathbf{q}} v_{\mathrm{KS}}\,|\,n\mathbf{k}\rangle$$



$$|g^{\nu}_{n,\mathrm{ave}}(\Gamma,\mathbf{q}_s)| = \sqrt{\sum_{m}^{N_b} |g_{nm,\nu}(\Gamma,\mathbf{q}_s)|^2/N_b}$$





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(Anisotropic) Eliashberg equations for (cavity-modified) phonon-mediated superconductors in nutshell

Eliashberg Eqs. requires **electronic band structure**, **phonon frequency**, **e-ph coupling** as inputs

$$Z(\mathbf{k}s, i\omega_n) = 1 + \frac{\pi k_B T}{\omega_n N(0)} \sum_{\mathbf{k}'s',n'} \frac{\omega_{n'}\delta(\epsilon_{\mathbf{k}'s'} - \epsilon_F)}{\sqrt{\omega_{n'}^2 + \Delta^2(\mathbf{k}'s', i\omega_{n'})}} \lambda(\mathbf{k}s, \mathbf{k}'s', n - n')$$

Mass renormalization function

e-ph matrix element

$$Z(\mathbf{k}s, i\omega_n)\, \Delta(\mathbf{k}s, i\omega_n) = \frac{\pi k_B T}{N(0)} \sum_{\mathbf{k}'s',n'} \frac{\Delta(\mathbf{k}'s', i\omega_{n'})\delta(\epsilon_{\mathbf{k}'s'} - \epsilon_F)}{\sqrt{\omega_{n'}^2 + \Delta^2(\mathbf{k}'s', i\omega_{n'})}} [\lambda(\mathbf{k}s, \mathbf{k}'s', n - n') - \mu^*]$$

Superconducting gaps

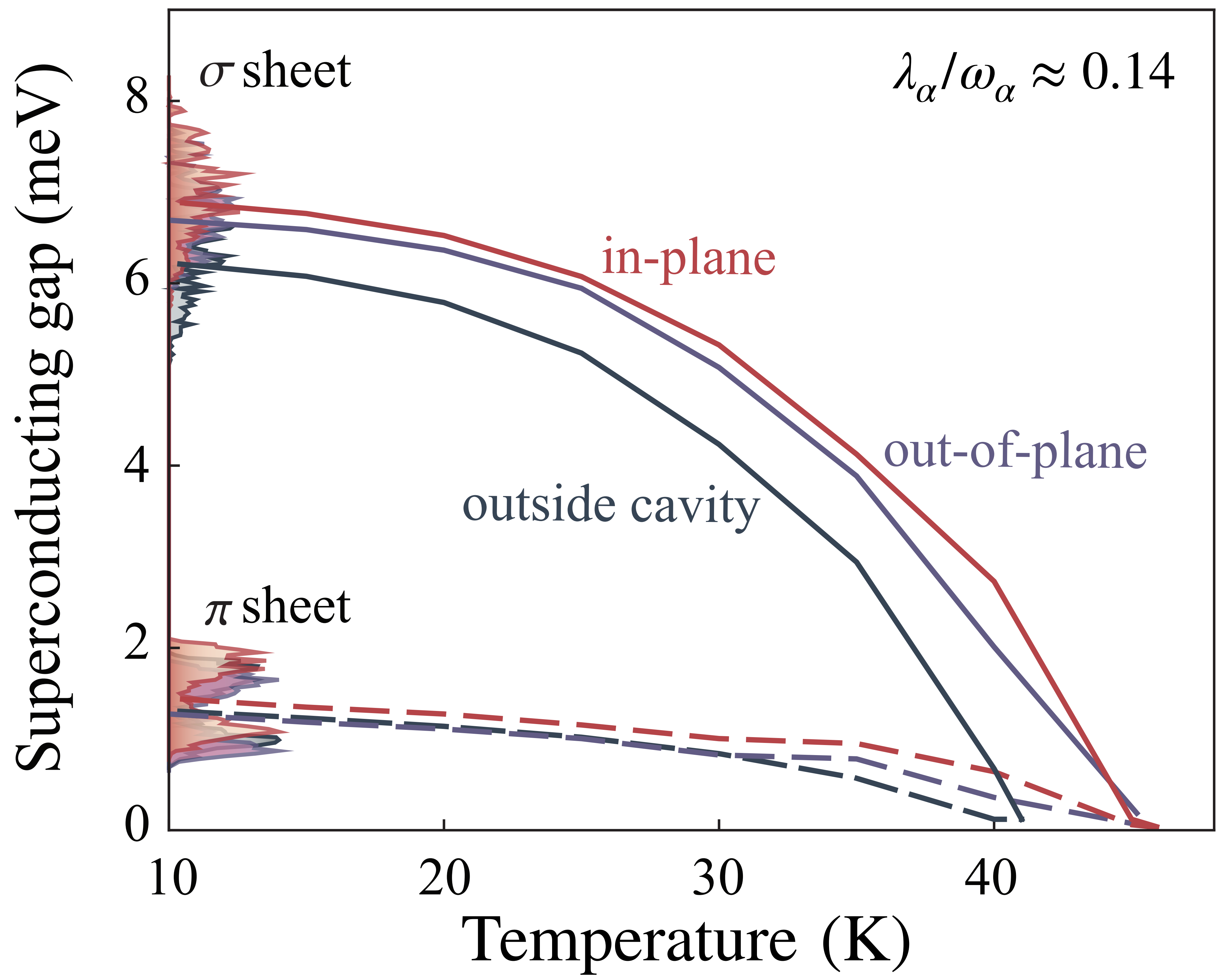
Coulomb screened parameter

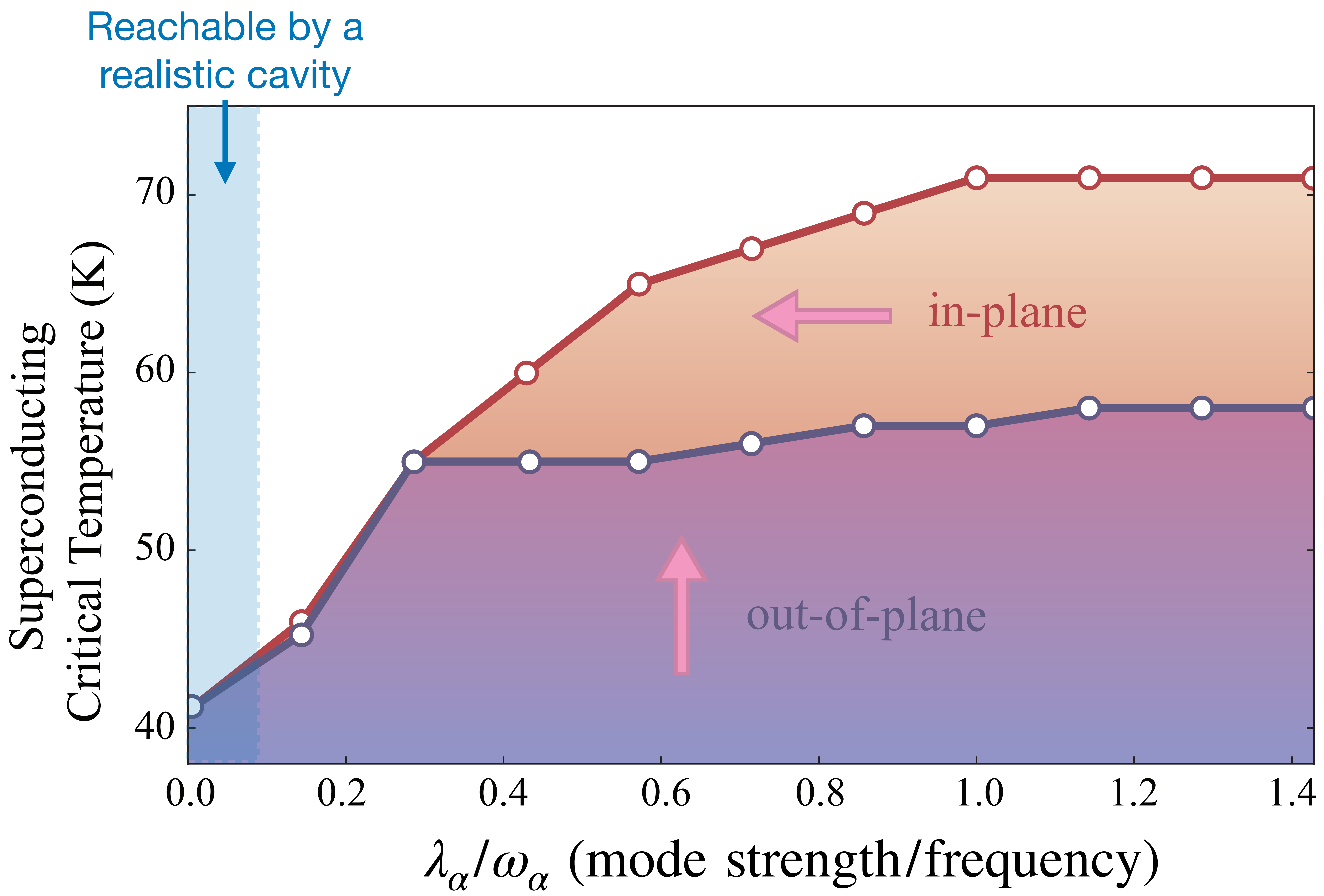
T_c can be found when the **superconducting gaps vanish**, i.e., $\Delta(\mathbf{k}s, 0) = 0$

e-ph matrix element

$$\lambda(n\mathbf{k}, m\mathbf{k}', l - l') = \int_0^\infty d\omega \frac{2\omega}{(\omega_l - \omega_{l'})^2 + \omega^2} \alpha^2 F(n\mathbf{k}, m\mathbf{k}', \omega)$$

Quantum vacuum fluctuation can modify superconducting gap and then superconducting transition temperature (example: MgB_2)





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Summary and future work

- Describe the Pauli-Fierz Hamiltonian as the starting point for light-matter coupled systems and QEDFT as the suitable first principle method (framework)
- Provide the electron-photon exchange functionals and related tools suitable for solid-state materials
- Demonstrate cavity-modified electronic structure, phonon dispersion, and electron-phonon couplings

- Recover photon fields from QEDFT (current-based density functional)
- Implement cavity-modified stress and search better functionals
- Explore cavity-engineered electrical and thermal transport properties

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