

Optical Properties of Two-dimensional Semiconductors: Excitonic and Polaritonic Effects

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22-01-2026

Secondment Host:

Prof. Juan José Palacios

Ph.D. Defense

- **P. Ninhos**, A. J. Uría-Álvarez, C. Tserkezis, N. Asger Mortensen and J. J. Palacios,
"Microscopic screening theory for excitons in two-dimensional materials: A bridge between effective model and ab initio descriptions", in preparations (2025)
- V. G. M. Duarte, **P. Ninhos**, C. Tserkezis, N. A. Mortensen, and N. M. R. Peres,
"Tunable exciton polaritons in biased bilayer graphene", *Phys. Rev. B* **111** 7, 075411 (2025)
- **P. Ninhos**, C. Tserkezis, N. A. Mortensen, and N. M. R. Peres,
"Tunable exciton polaritons in band-gap engineered hexagonal boron nitride", *ACS Nano* **18** 31, 20751 (2024)

List of Publications

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Outline

1 Introduction to Excitons in 2D Materials

- Context
- Motivation

2 Part I: Exciton-Polaritons in a 1D hBN Superlattice

- Setup
- Excitonic States
- Optical Response
- Exciton-Polaritons

3 Part II: Screening in 2D Materials with the Xatu Code

- 2D Dielectric Function: Theory
- 2D Dielectric Function and Excitons: Results
- Quasi-2D Approach for Screening

4 Conclusions

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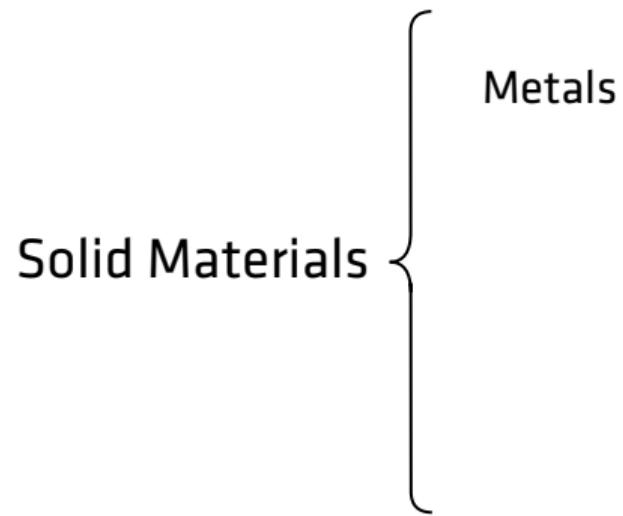
4 Conclusions

Solid Materials

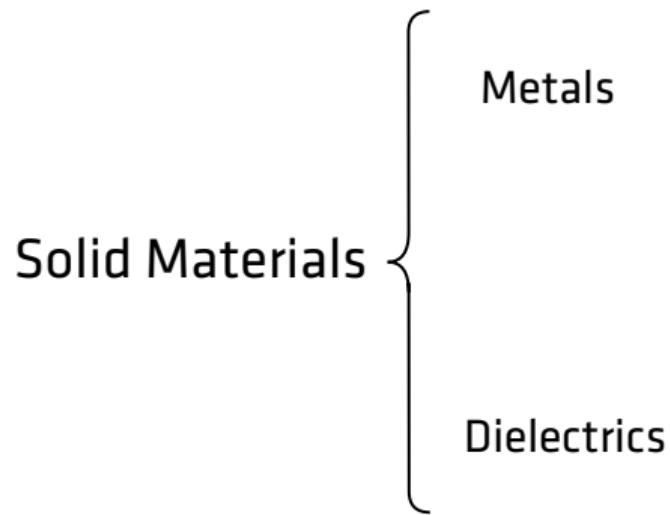
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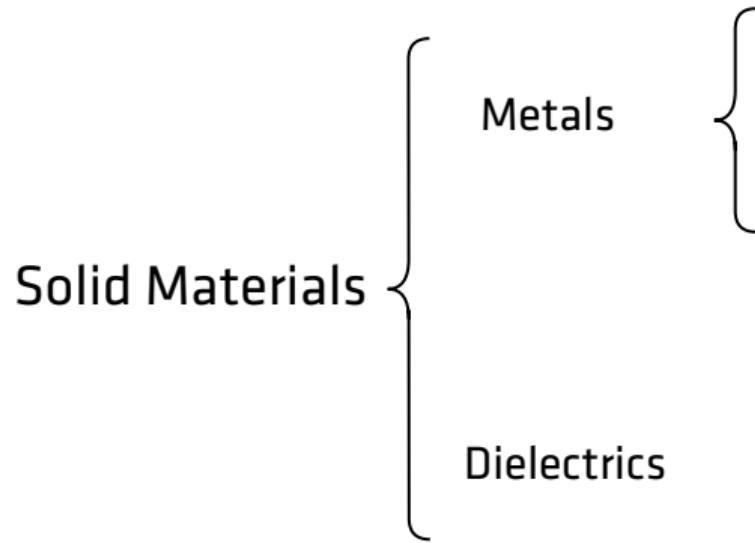
Optical Excitations in Matter



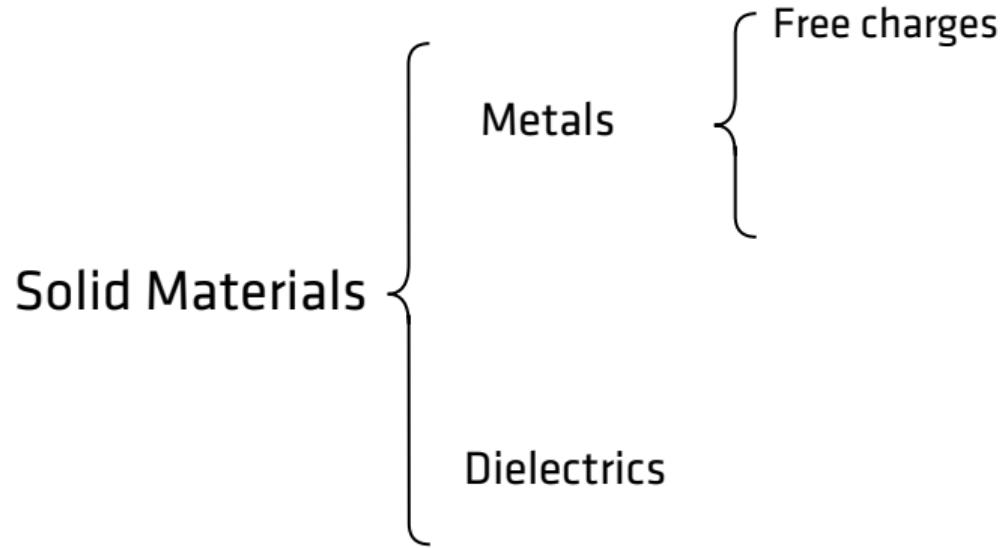
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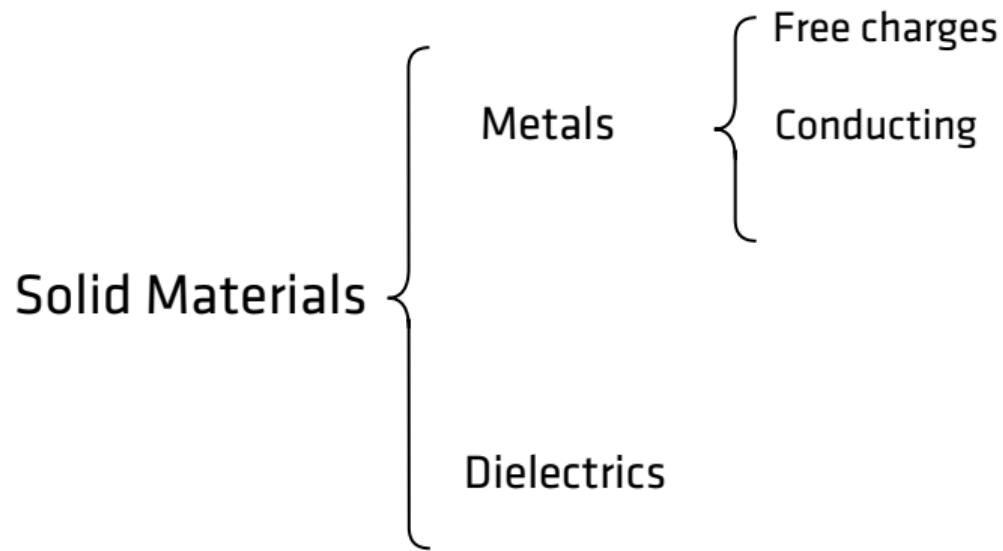
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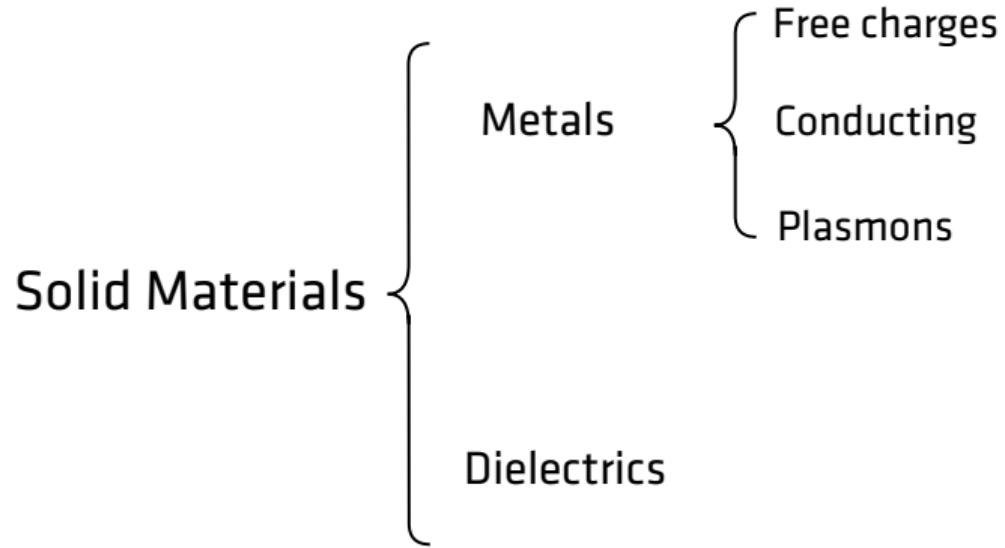
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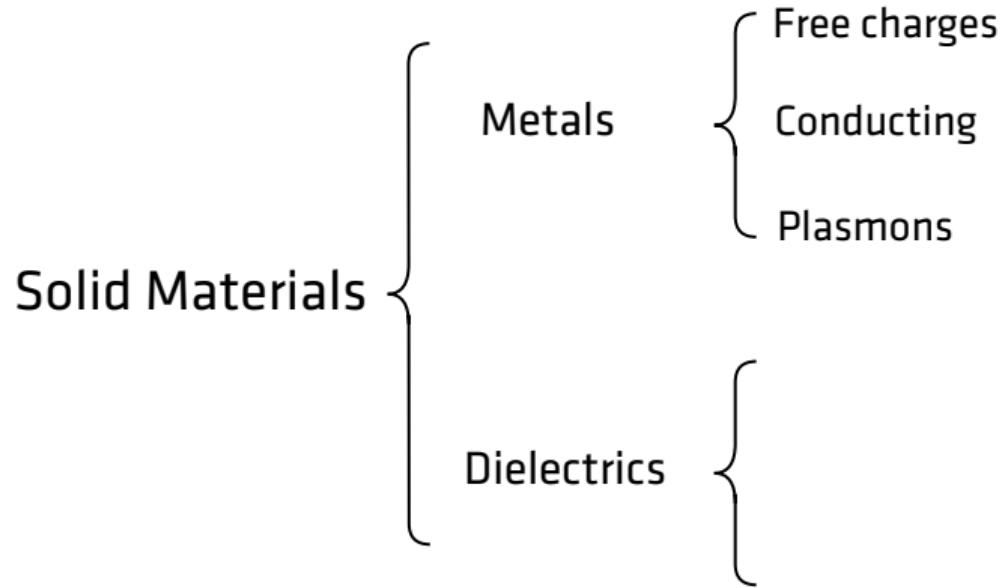


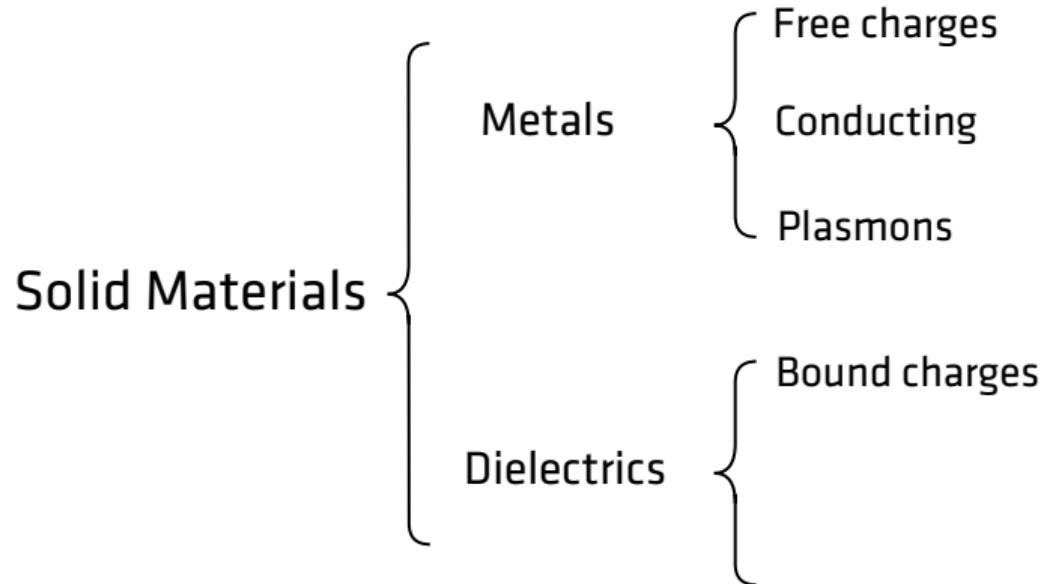
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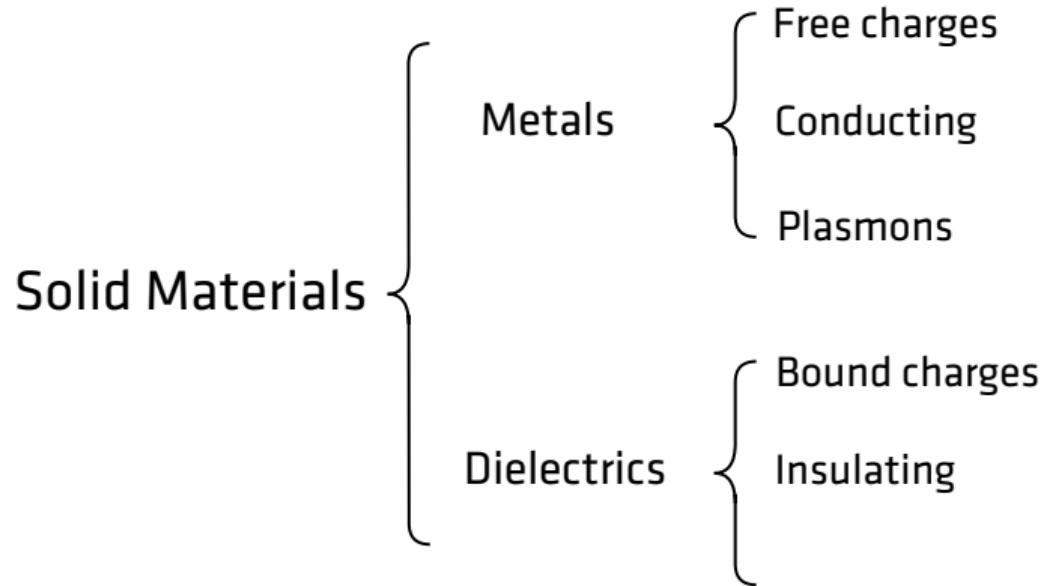


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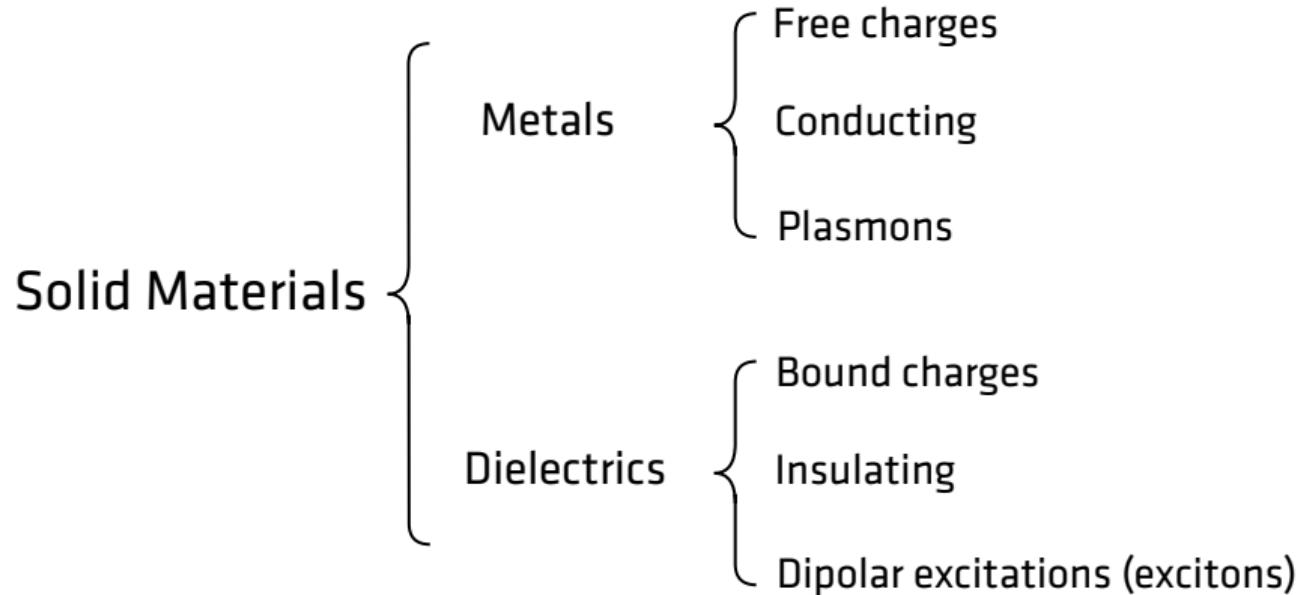








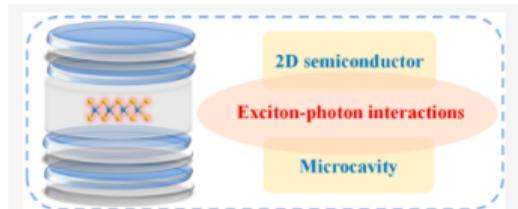
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Excitons in Photonics

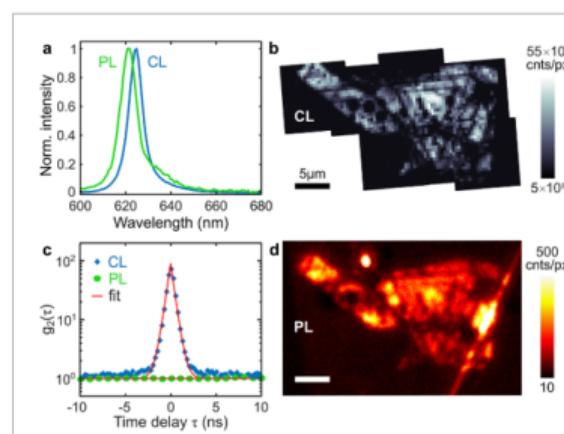
Relevant for:

Light-matter interactions



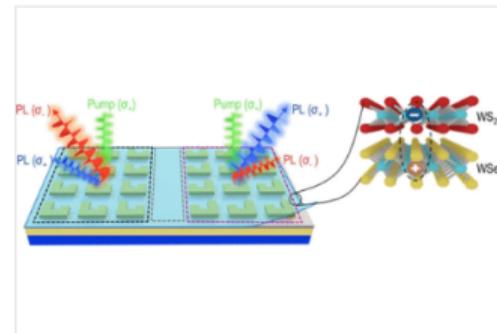
J. Shang et al. - *ACS Photonics*
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Quantum Light Sources



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Valleytronics

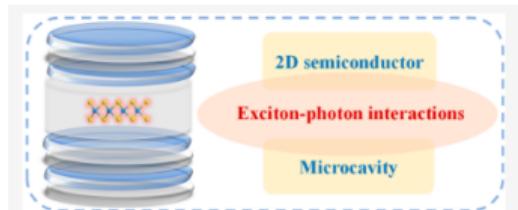


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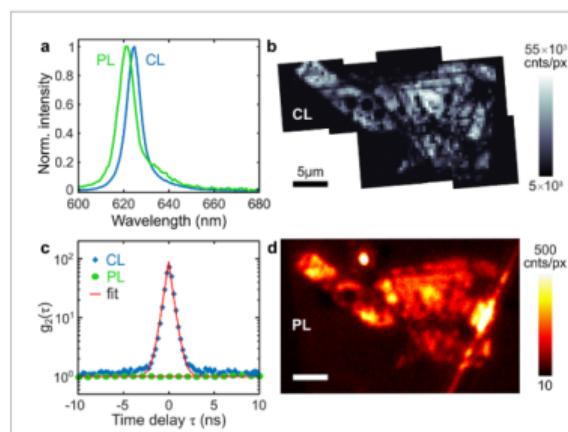
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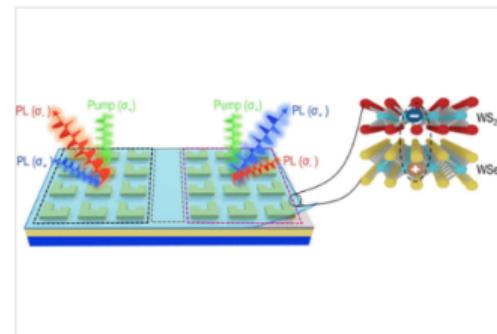
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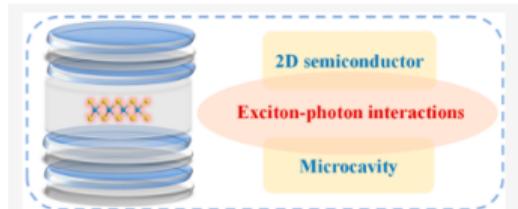


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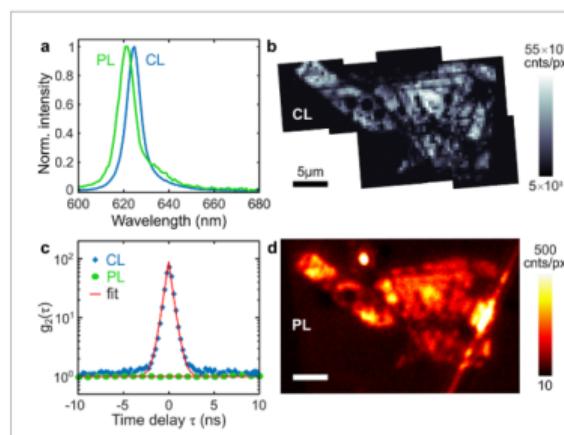
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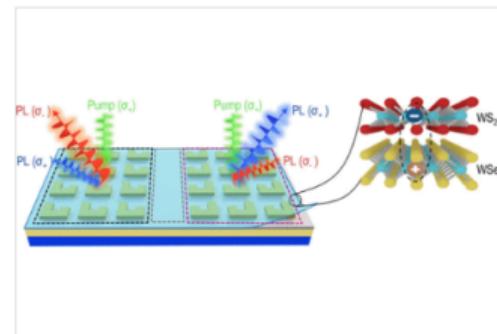
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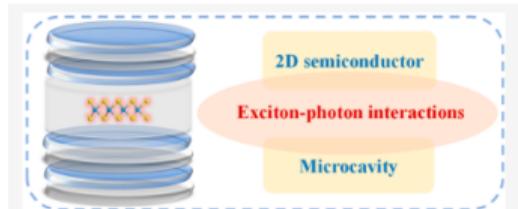


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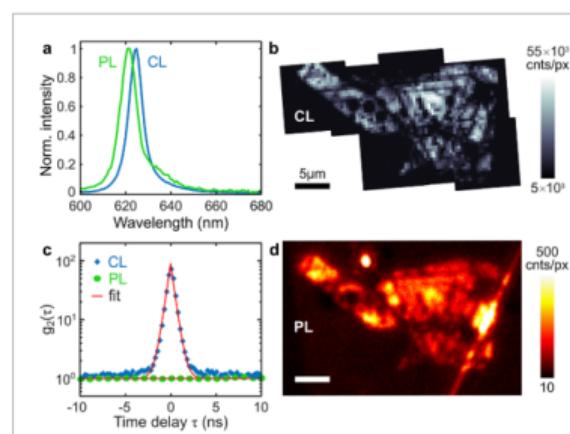
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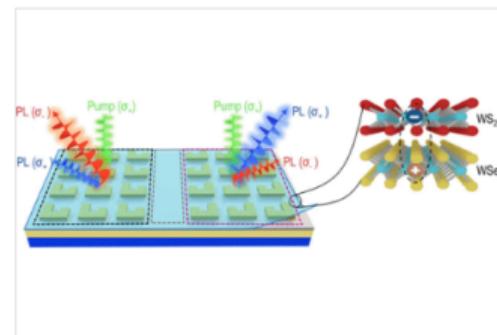
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Excitons in Two-Dimensional Materials

For a typical 3D material (e.g., GaAs)

$$E_{b,n} = -\frac{R^*}{n^2}$$

$$R^* = \frac{2\mu_{eh}^2 e^4}{\hbar^2 (8\pi\varepsilon\varepsilon_0)^2}$$

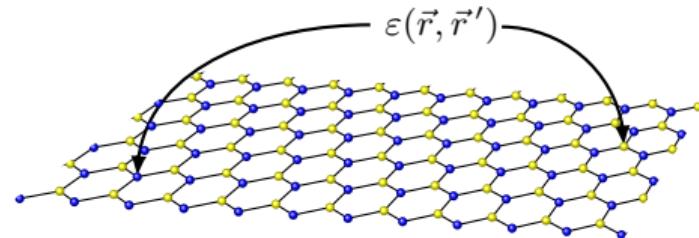
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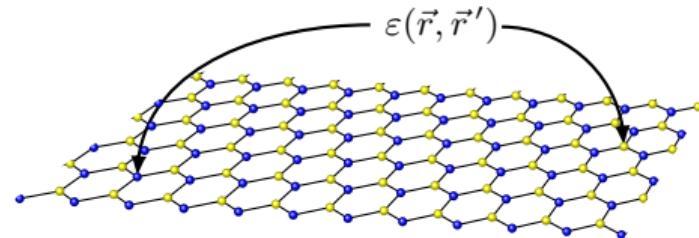
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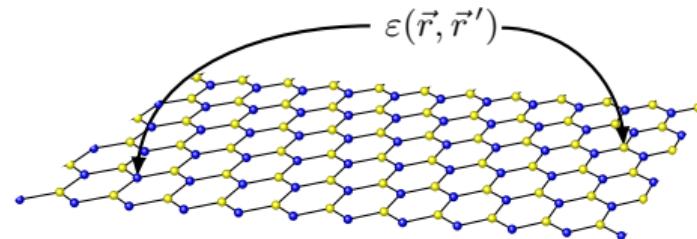
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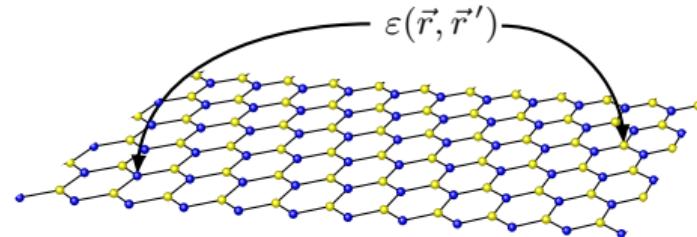
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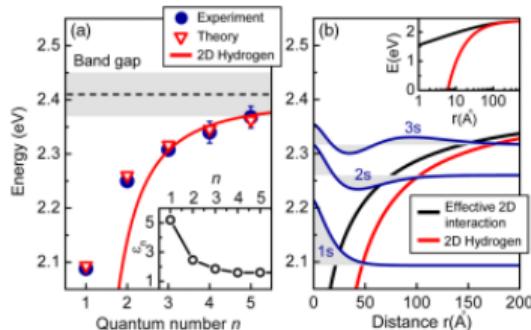


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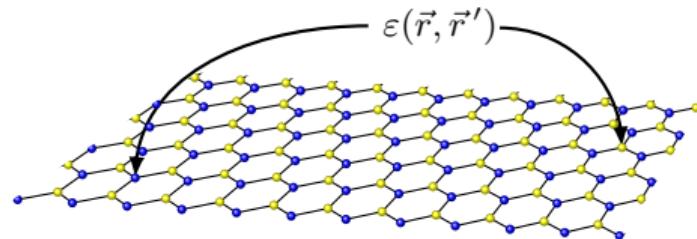
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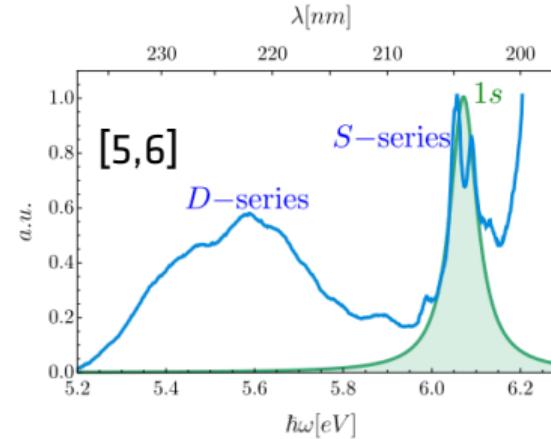
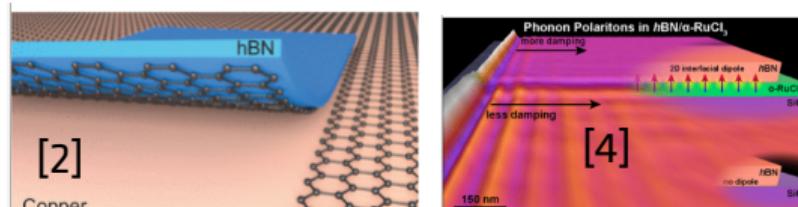
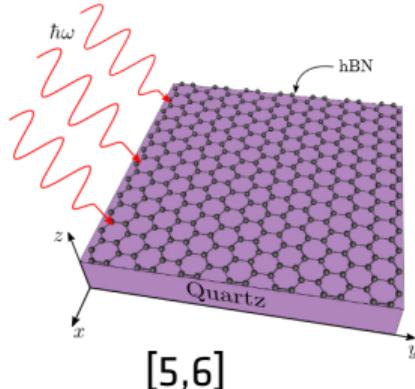


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A. Chernikov et al. - Phys. Rev. Lett. **113** 076802 (2014)

Hexagonal Boron Nitride in Photonics

- Low defects density [1]
- Ballistic transport in graphene [2]
- Hyperbolic material (MIR) [3]
- Polaritonics in the MIR [4]

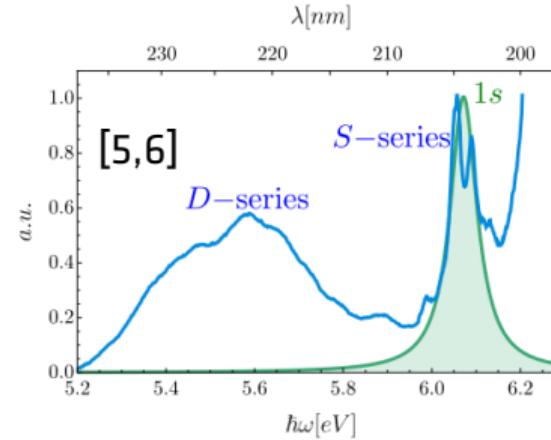
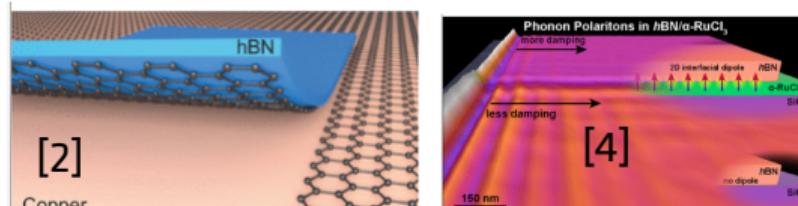
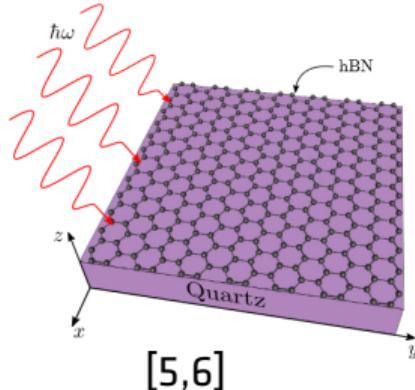


- [1] I. H. Abidi et al. - *Adv. Opt. Mater.* **7** 1900397 (2019)
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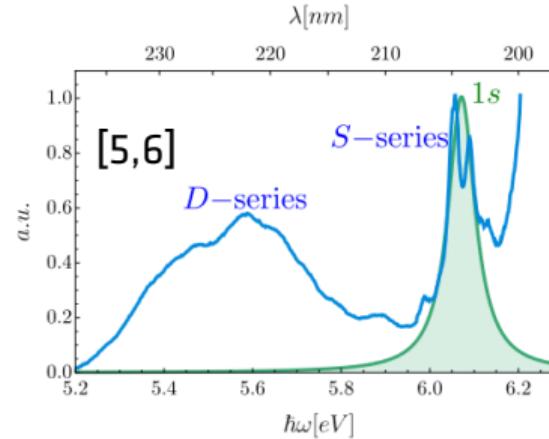
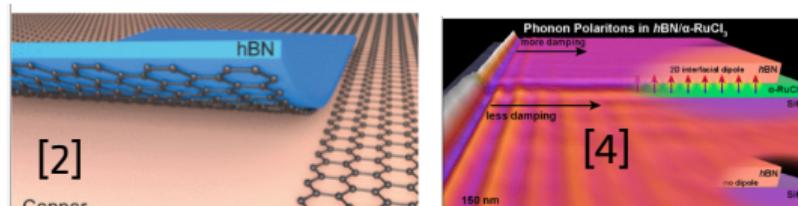
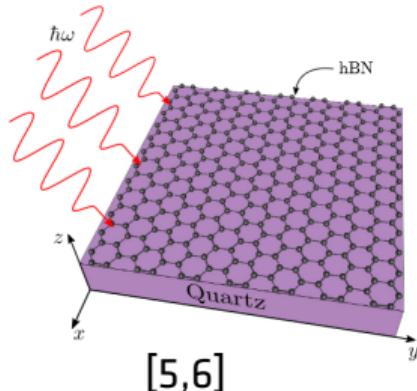


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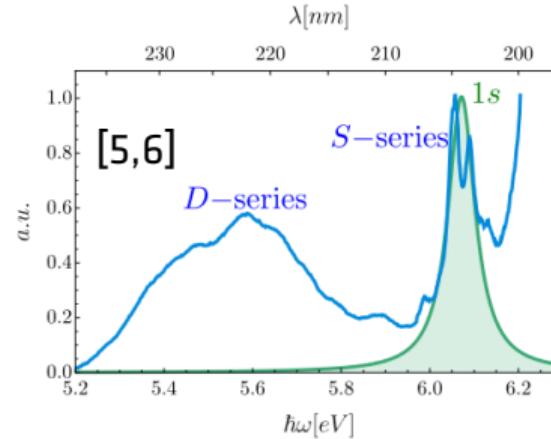
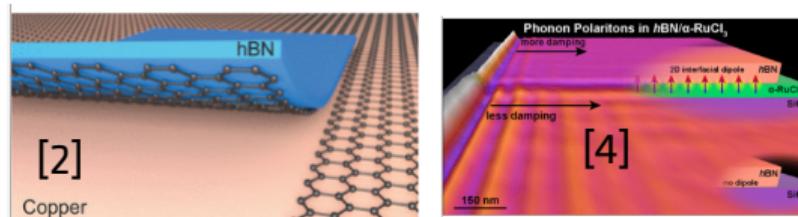
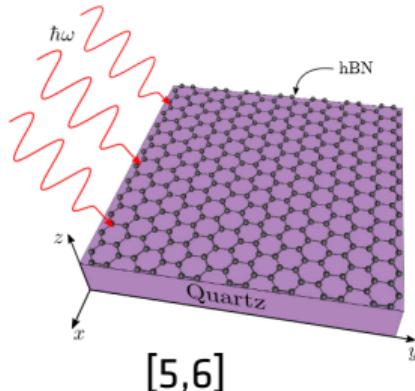


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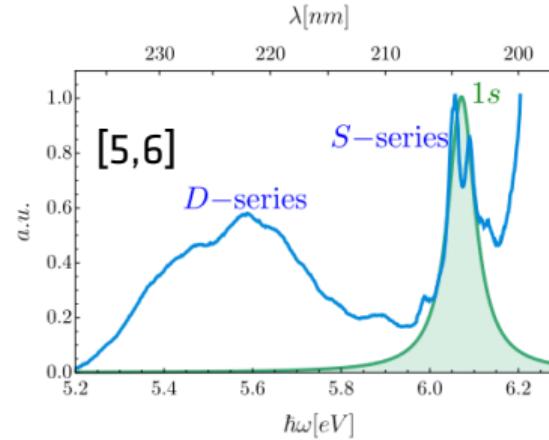
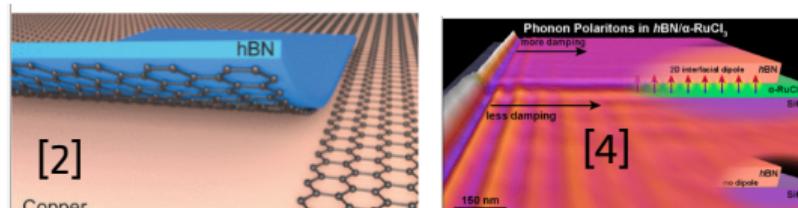
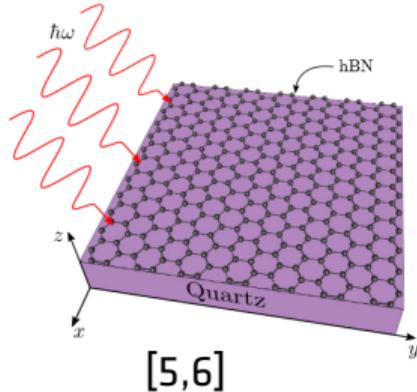


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Rytova-Keldysh model

$$\varepsilon_{\text{RK}}(q) = 1 + r_0 q , V_{\text{RK}}(q) = \frac{e^2}{2\varepsilon_0 q \varepsilon_{\text{RK}}(q)}$$

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- Excitons are determined numerically
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- Captures screening in its q entirety
- Computationally heavy
- Physics harder to grasp
- Codes are designed for 3D systems

Motivation

Rytova-Keldysh model What can we do with it?

$$\varepsilon_{\text{RK}}(q) = 1 + r_0 q, V_{\text{RK}}(q) = \frac{e^2}{2\varepsilon_0 q \varepsilon_{\text{RK}}(q)}$$

$$V_{\text{RK}}(r) = \frac{e^2}{4\pi\varepsilon_0} \frac{\pi}{2r_0} \left[\mathbf{H}_0\left(\frac{r}{r_0}\right) - Y_0\left(\frac{r}{r_0}\right) \right]$$

- Intuitive
- Analytical expression
- Excitons are determined numerically
- Questionable for layered systems
- Screening parameter r_0 obtained from *ab initio* methods either way

Full numerical *ab initio*

$$\varepsilon_{GG'}(\mathbf{q}) = \delta_{GG'} - v_c(\mathbf{q} + \mathbf{G}) \chi_{GG'}^0(\mathbf{q})$$

- Works for any kind of system
- Several packages available (BerkeleyGW, Yambo, VESPA, etc...)
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Full numerical *ab initio* Can we optimize?

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Outline

1 Introduction to Excitons in 2D Materials

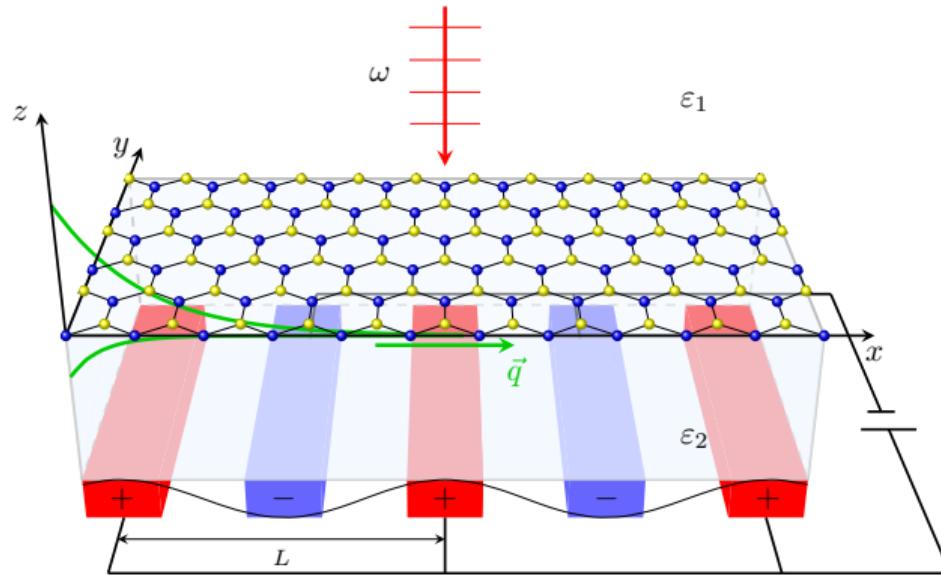
2 Part I: Exciton-Polaritons in a 1D hBN Superlattice

- Setup
- Excitonic States
- Optical Response
- Exciton-Polaritons

3 Part II: Screening in 2D Materials with the Xatu Code

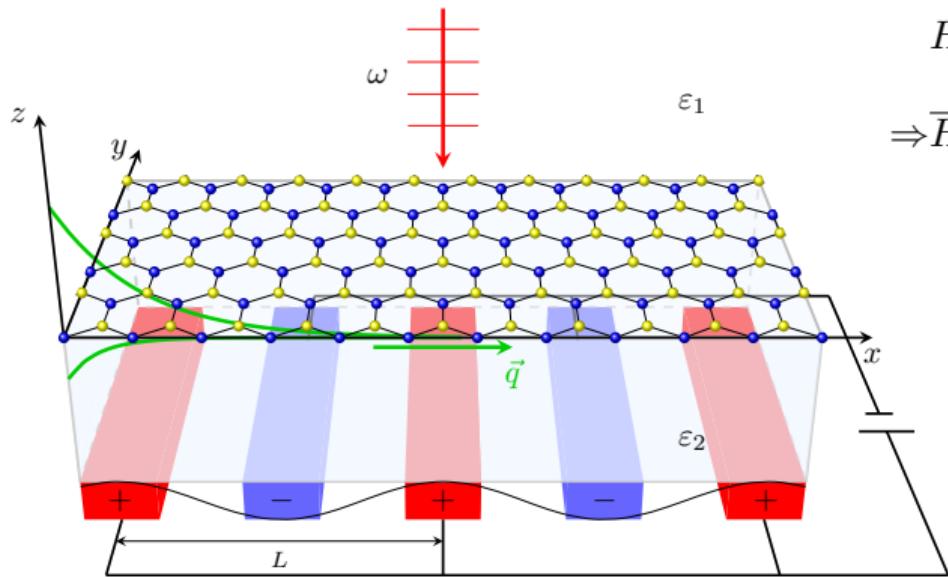
4 Conclusions

hBN under an external periodic potential



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hBN under an external periodic potential



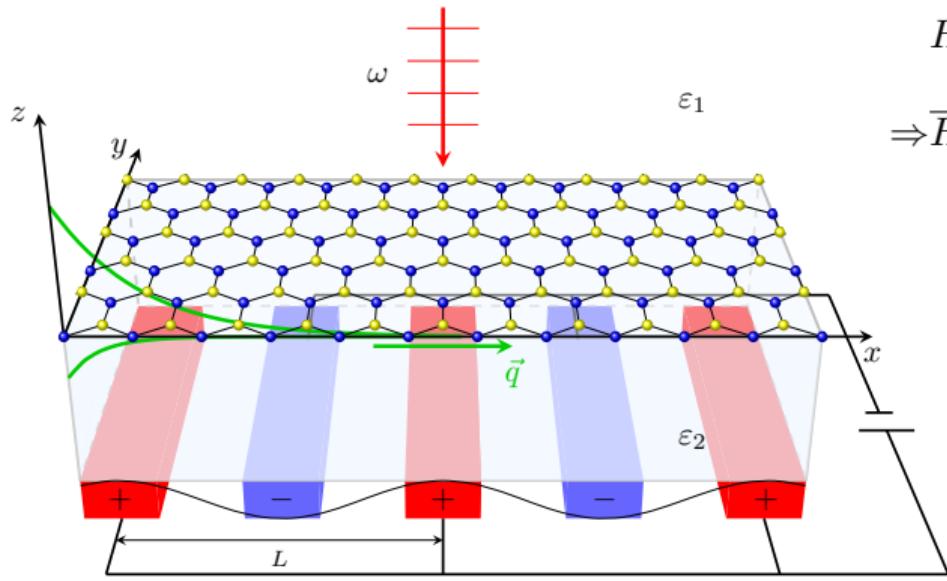
$$H_0 = H_{\text{Dirac}} + V_0 \cos(G_0 x), \quad G_0 = \frac{2\pi}{L} \hat{\mathbf{x}}$$

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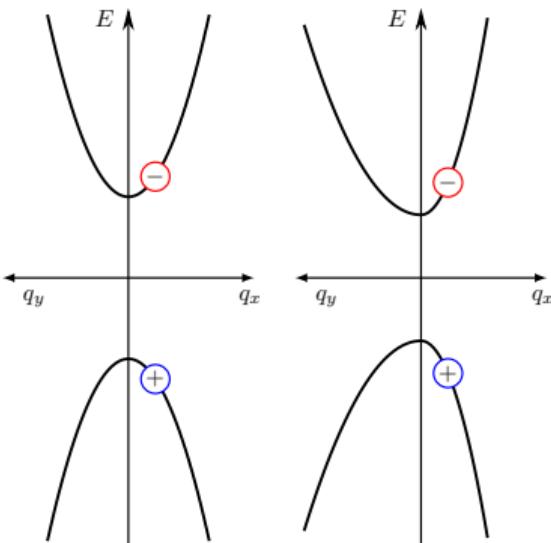
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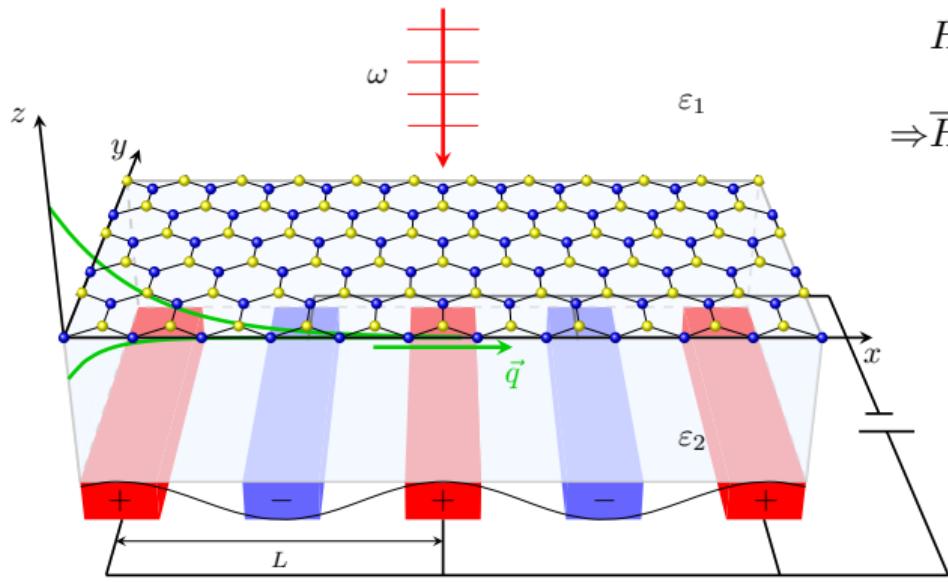
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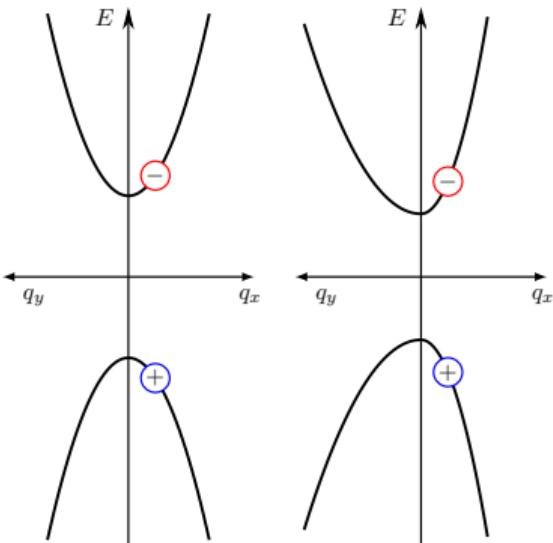
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For $\beta \sim 1$, and $V_0 \sim 40$ meV, $L \sim 40$ nm

Wannier Equation and Variational Method

Wannier equation [1]

$$E_{bind.,\nu}\psi_\nu(\mathbf{r}) = \left(\frac{p_x^2}{2\mu_x} + \frac{p_y^2}{2\mu_y} \right) \psi_\nu(\mathbf{r}) - V_{\text{RK}}(\mathbf{r})\psi_\nu(\mathbf{r})$$

[1] M. Vasilevskiy et al. - *J. Phys.: Condens. Matter* **34** 045702 (2022)

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Trial wavefunctions:

$$\Psi_{1s} = C_{1s} e^{-\rho_{1s}}$$

$$\Psi_{2x} = C_{2x} x e^{-\rho_{2x}}$$

$$\Psi_{2y} = C_{2y} y e^{-\rho_{2y}}$$

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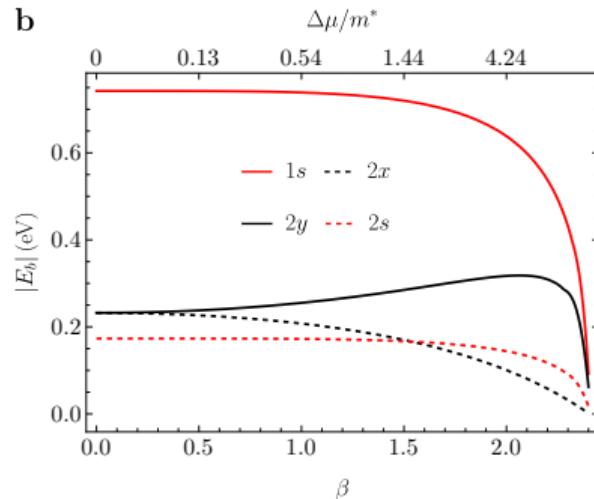
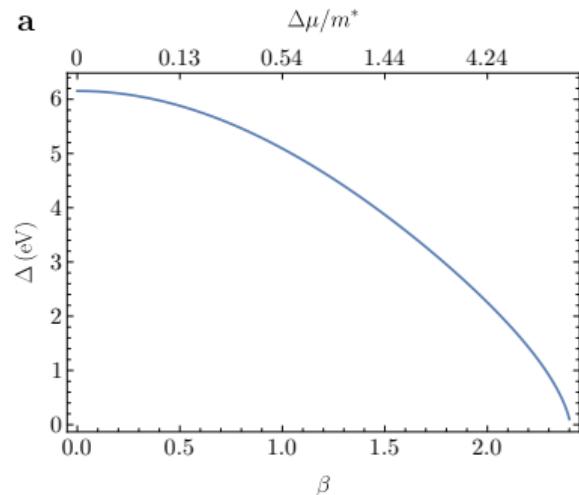
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Optical Conductivity

According to Pedersen [1]

$$\sigma_{jj}(\omega) = -i\sigma_0 \sum_{\nu=1s,2s} \frac{E_\nu |\Omega_\nu^j|^2}{E_\nu - (\hbar\omega + i\Gamma)}$$

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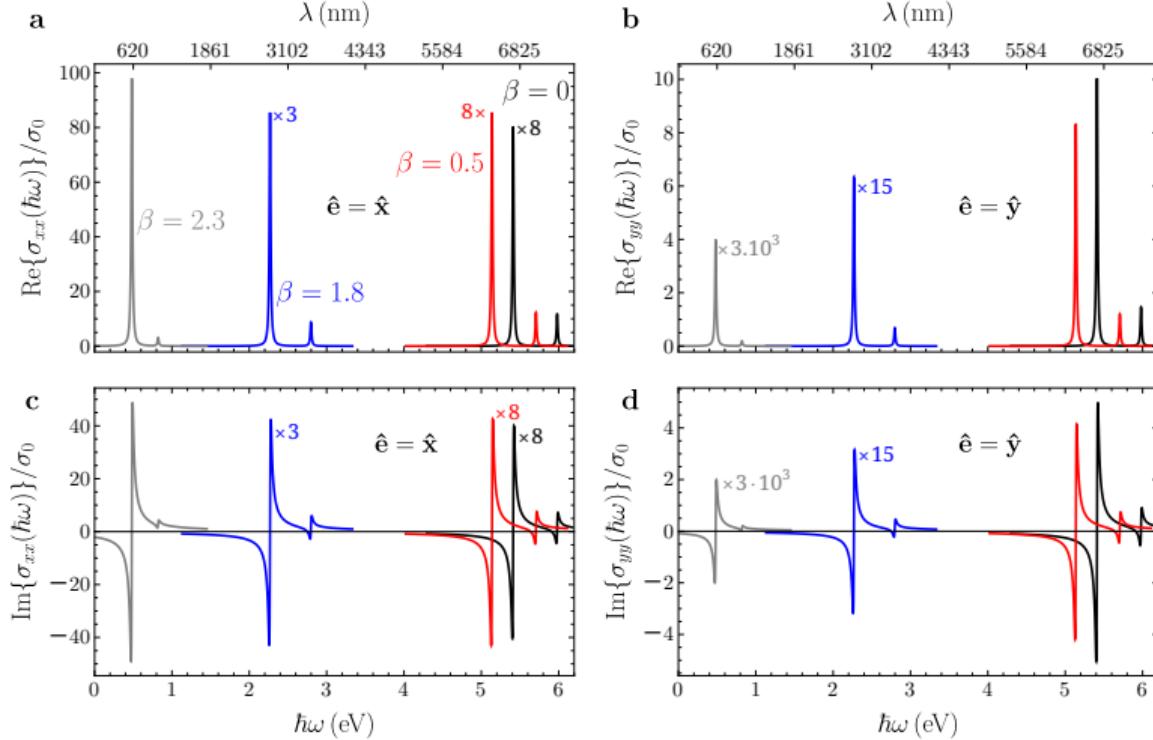
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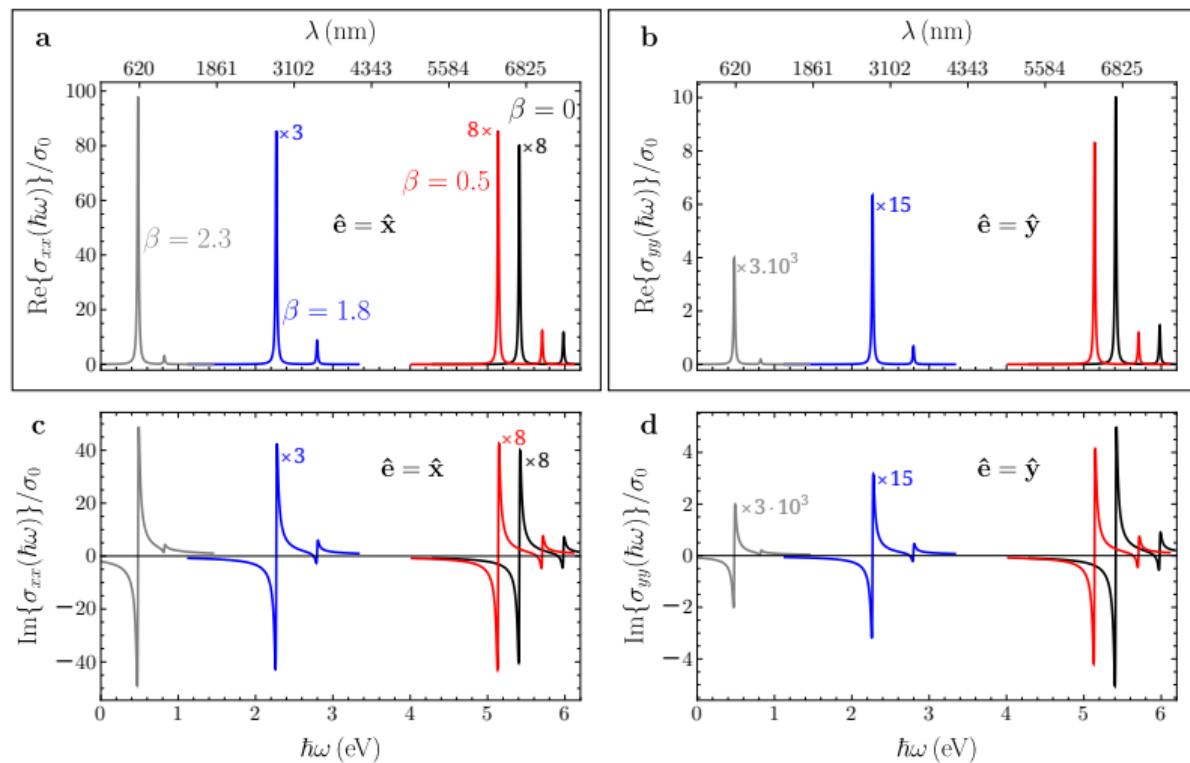
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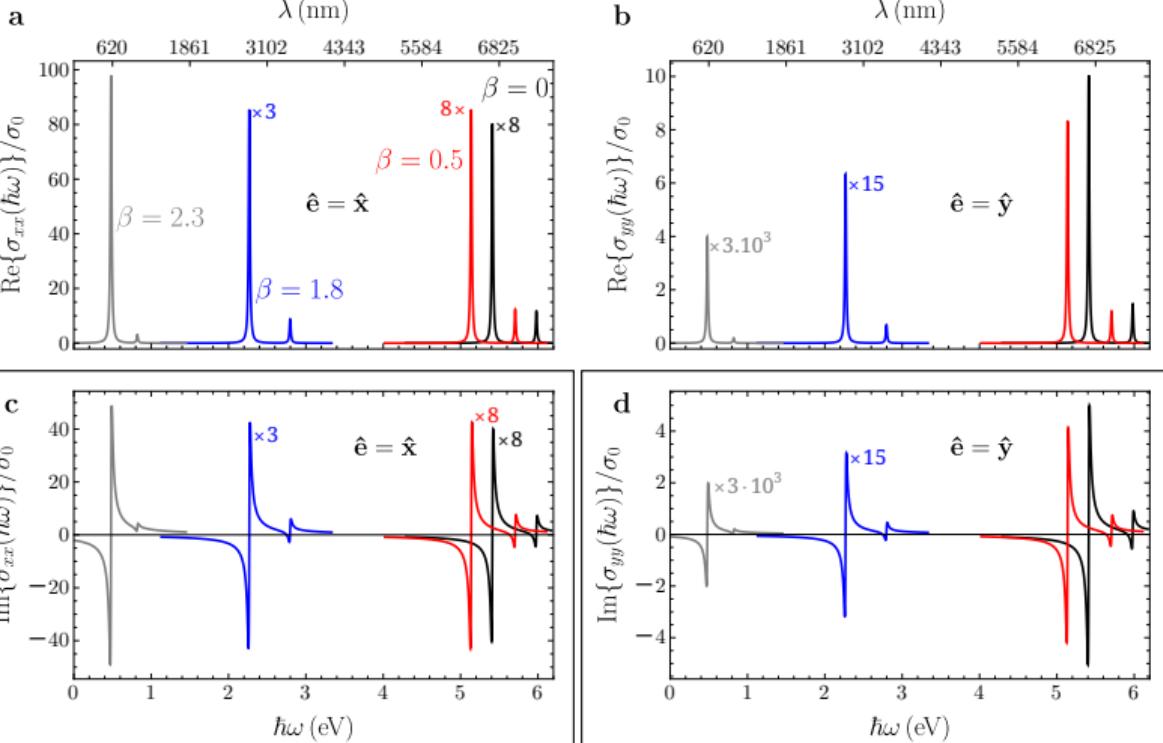
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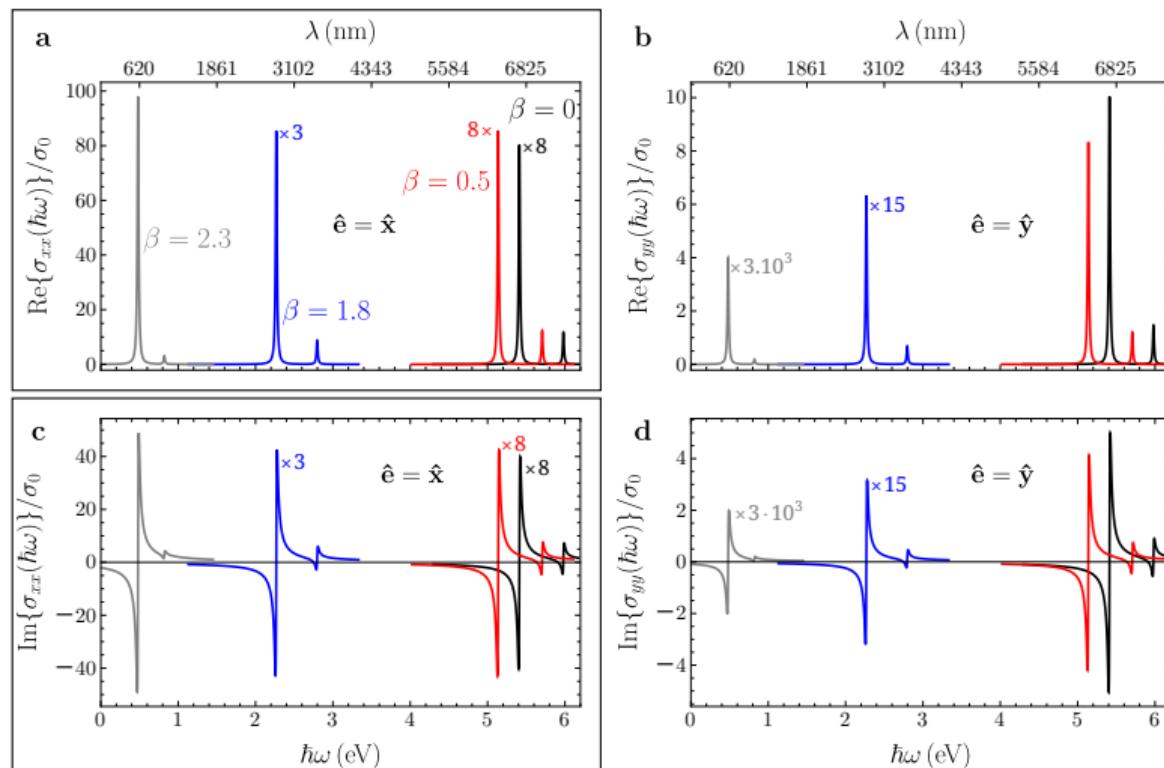
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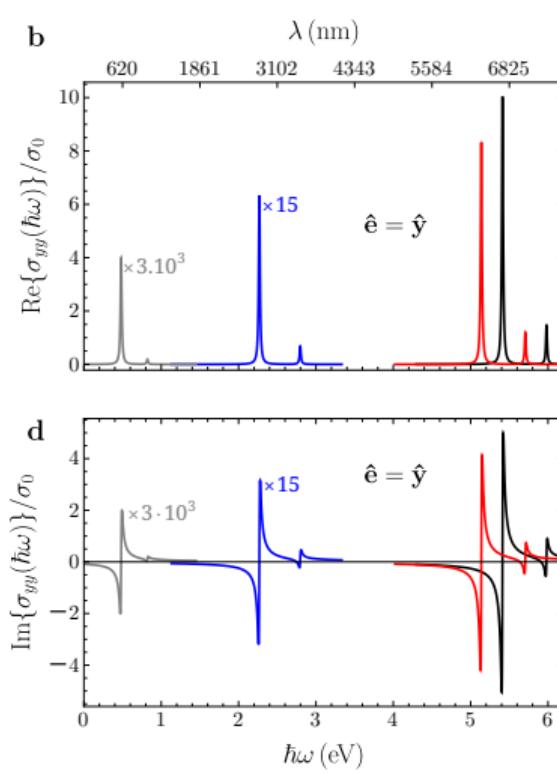
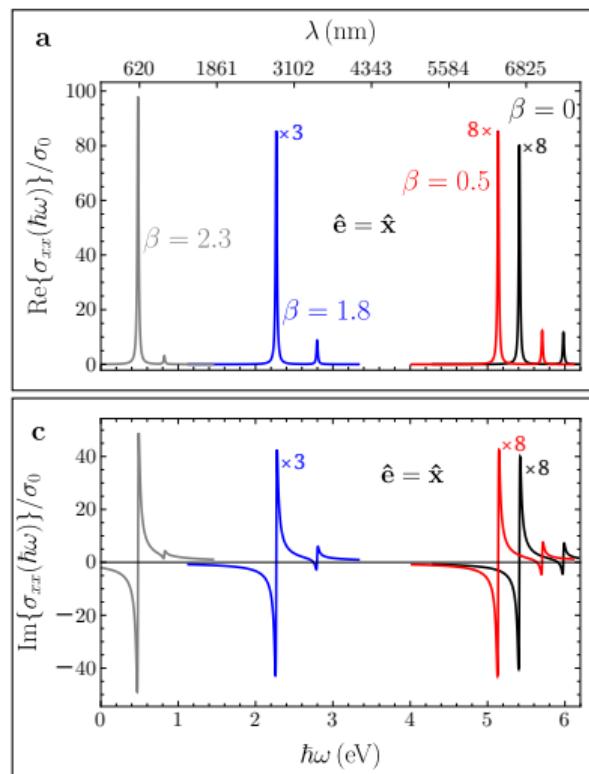
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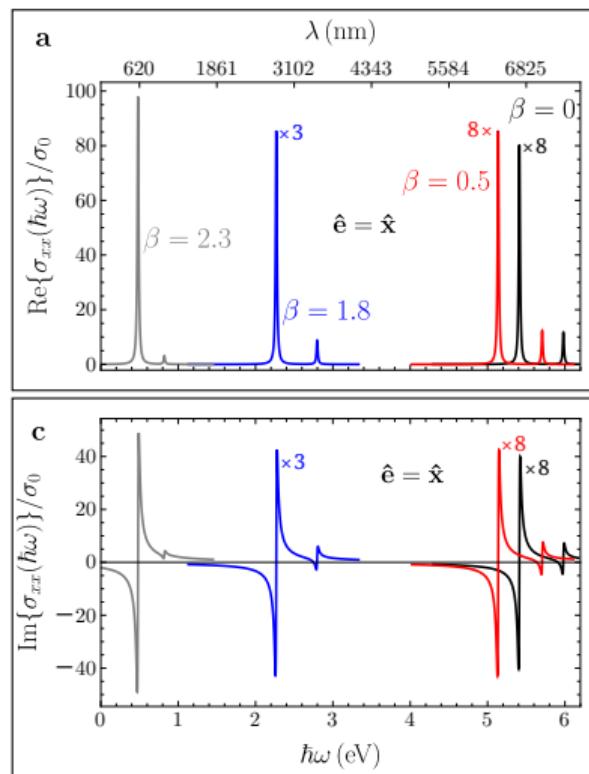
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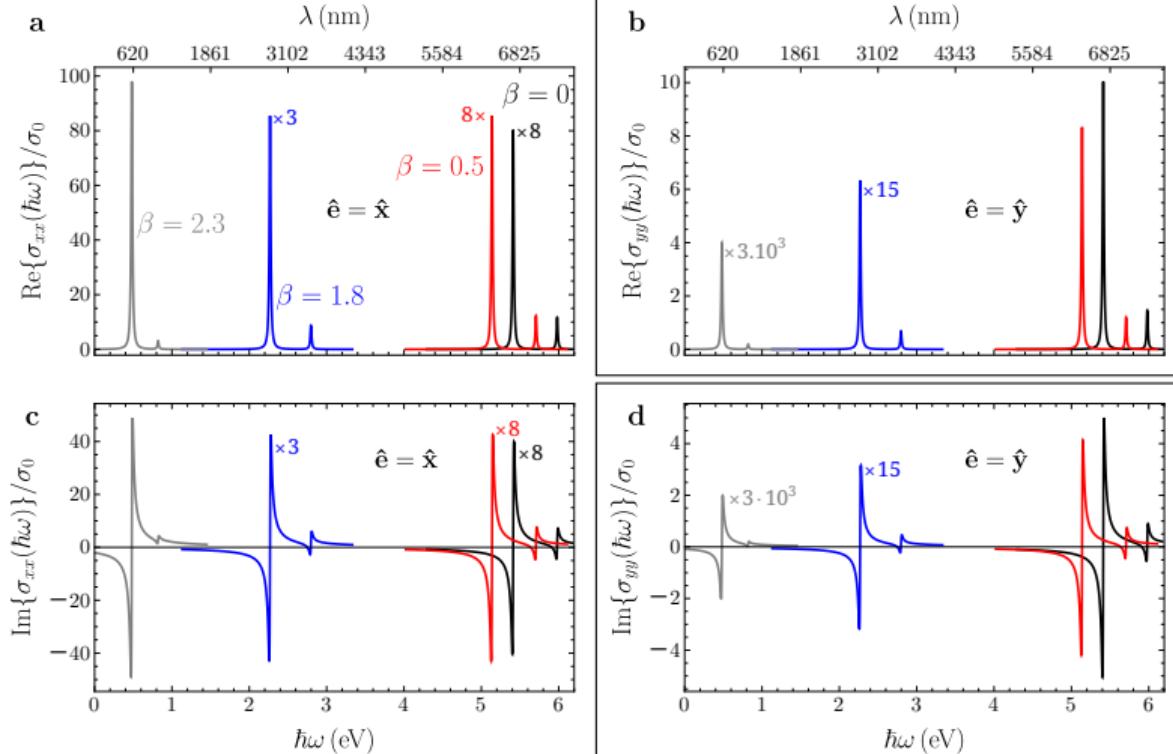
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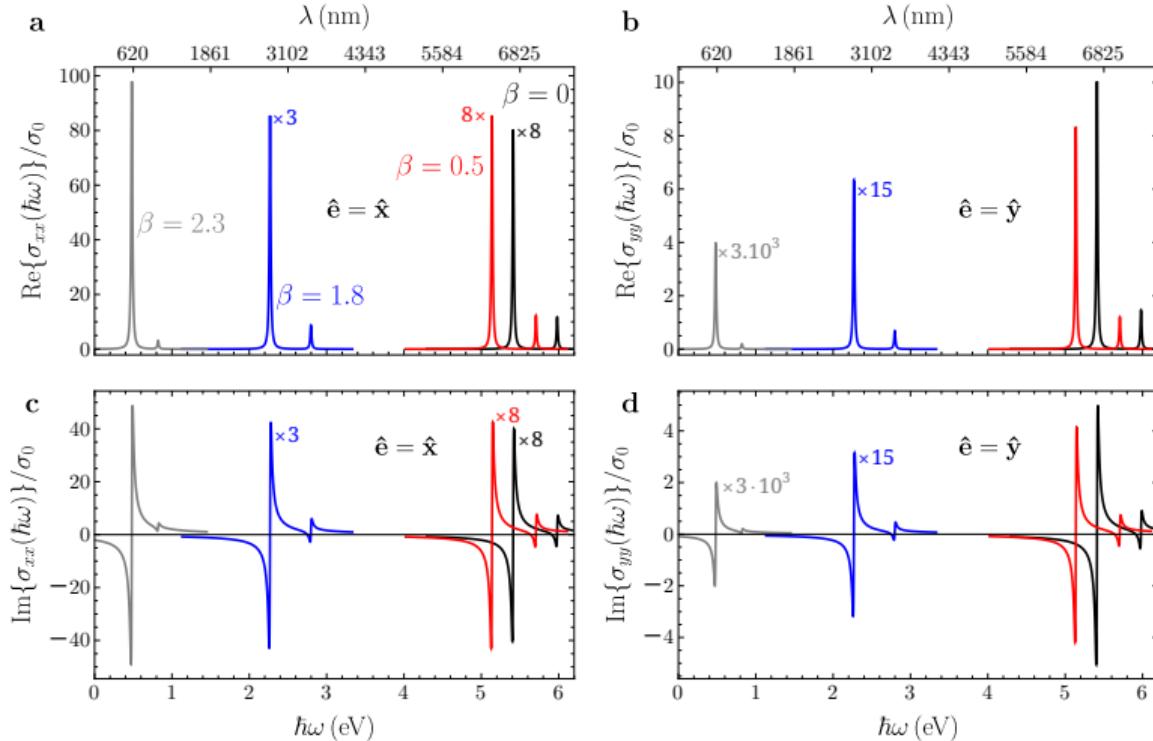
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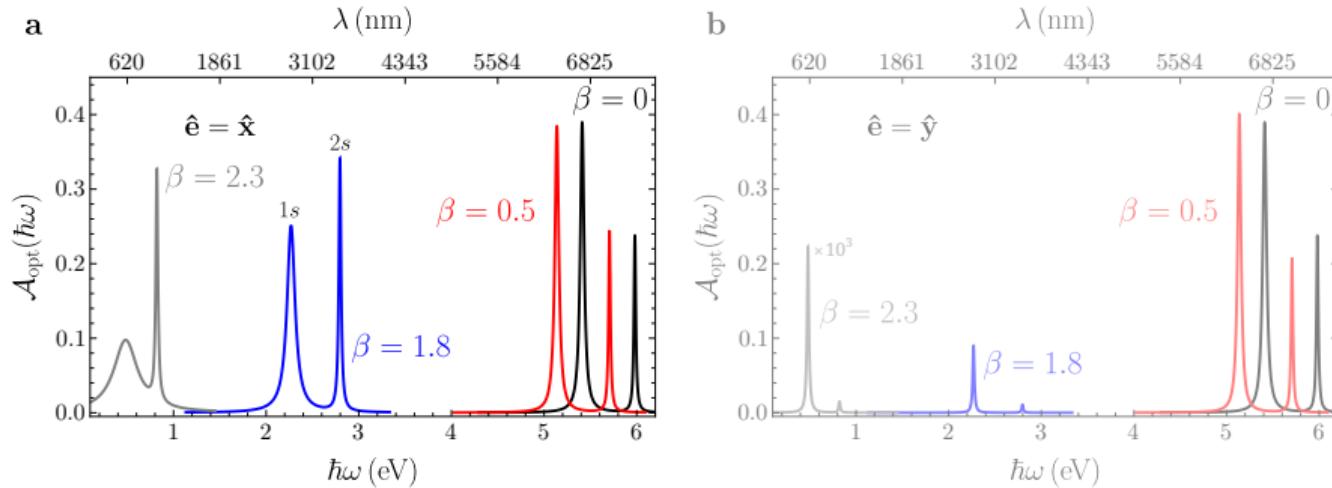
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$$\mathcal{A}_{\text{opt}} = 1 - \mathcal{R} - \frac{\text{Re}\{\sqrt{\varepsilon_2}\}}{\text{Re}\{\sqrt{\varepsilon_1}\}} \mathcal{T}, \quad \mathcal{R} = \left| \frac{\sqrt{\varepsilon_2} - \sqrt{\varepsilon_1} + \frac{\sigma}{\varepsilon_0 c}}{\sqrt{\varepsilon_2} + \sqrt{\varepsilon_1} + \frac{\sigma}{\varepsilon_0 c}} \right|^2, \quad \mathcal{T} = \left| \frac{2\sqrt{\varepsilon_1}}{\sqrt{\varepsilon_2} + \sqrt{\varepsilon_1} + \frac{\sigma}{\varepsilon_0 c}} \right|^2$$

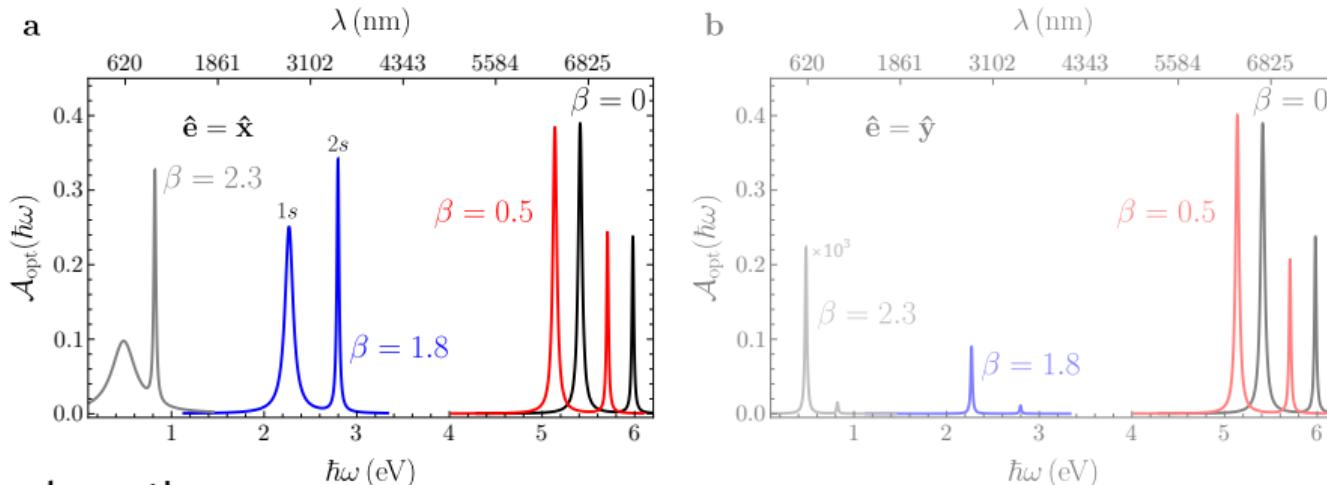
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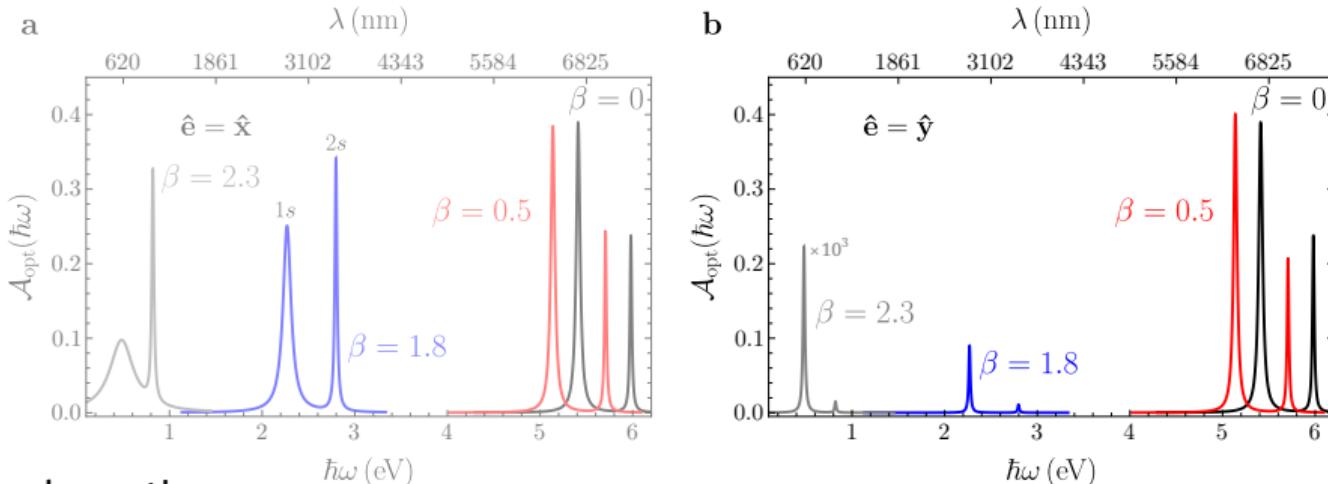
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- Tunable absorption
- Non-monotonic behaviour of the absorption
- 2s peak higher than 1s peak

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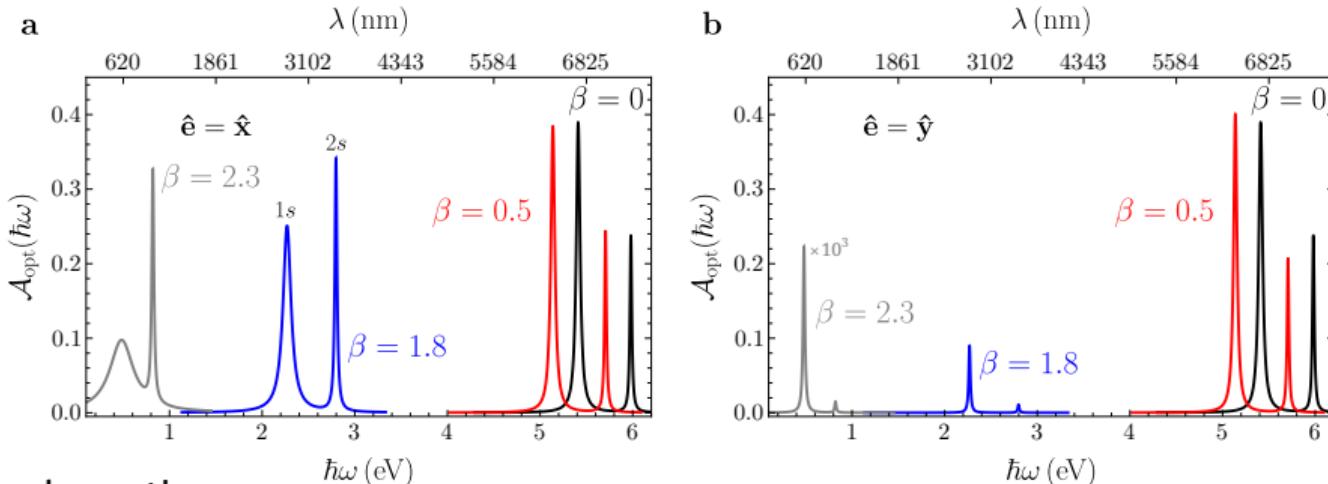
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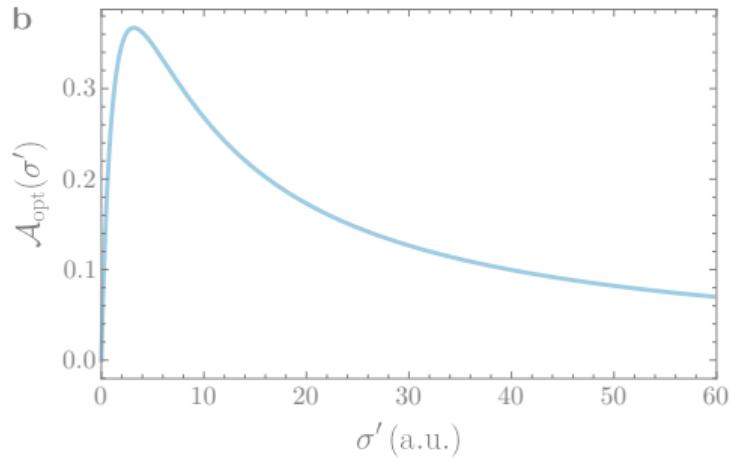
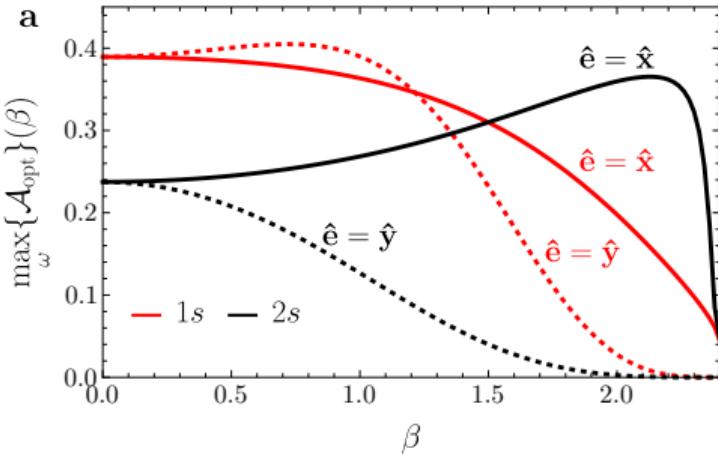
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Absorption Peaks

$$\max_{\omega} \mathcal{A}_{\text{opt}} = \frac{4\sqrt{\varepsilon_1}\sigma'}{(\sqrt{\varepsilon_2} + \sqrt{\varepsilon_1} + \sigma')^2}, \omega = E_{\nu}/\hbar, \nu = 1s, 2s$$

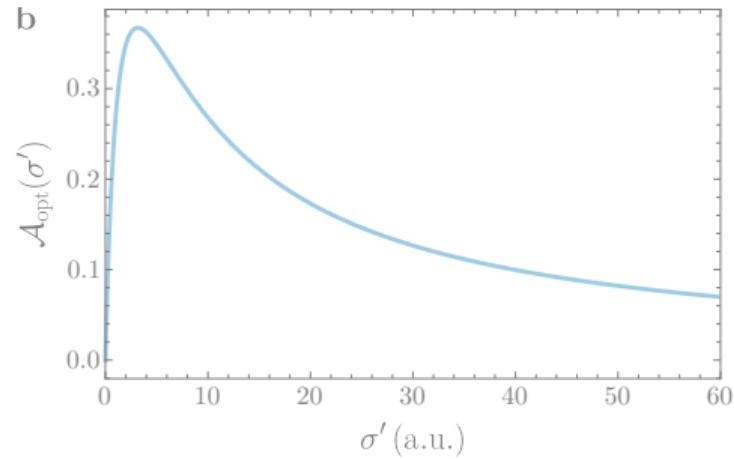
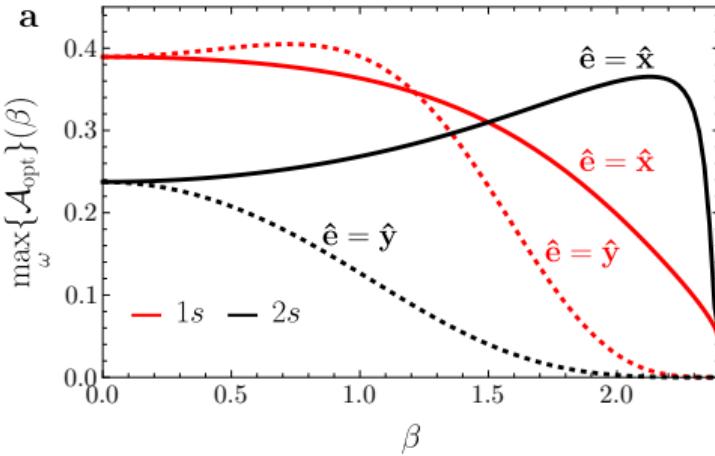
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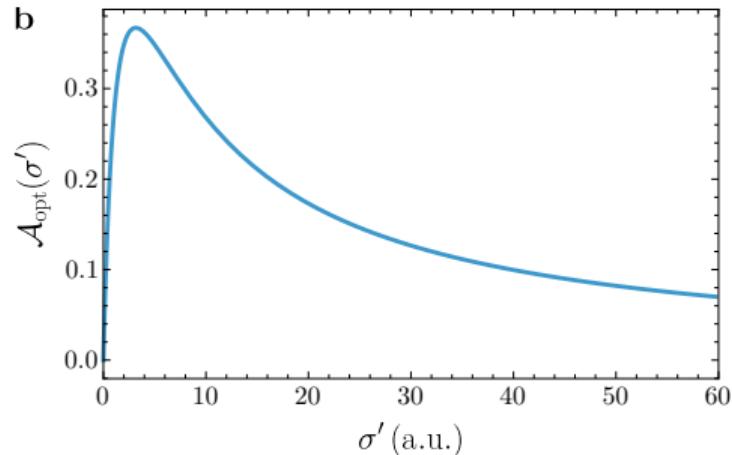
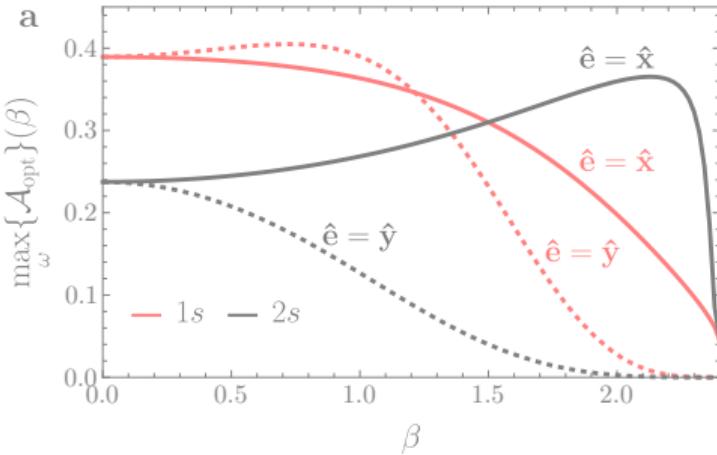
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- Tunable absorption
- Different response for different polarizations \Rightarrow grid polarizer

Absorption Peaks

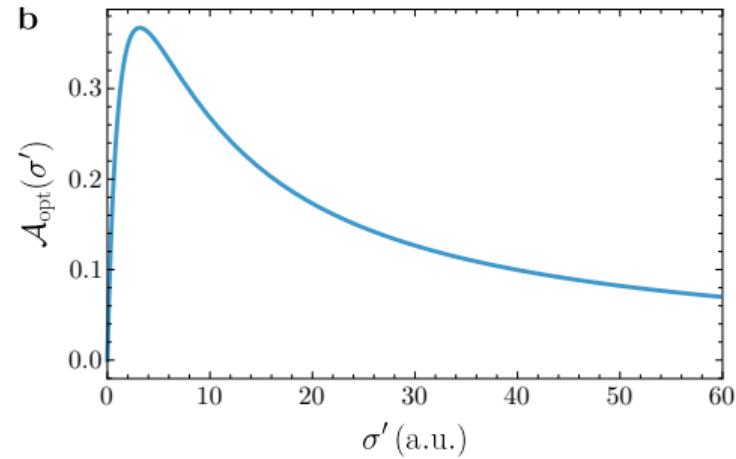
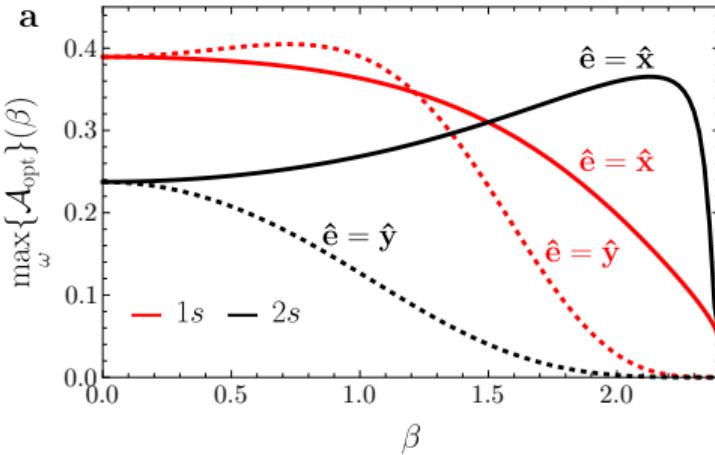
$$\max_{\omega} \mathcal{A}_{\text{opt}} = \frac{4\sqrt{\varepsilon_1}\sigma'}{(\sqrt{\varepsilon_2} + \sqrt{\varepsilon_1} + \sigma')^2}, \quad \omega = E_{\nu}/\hbar, \nu = 1s, 2s$$



- Tunable absorption
- Different response for different polarizations \Rightarrow grid polarizer
- Non-monotonic behaviour of the absorption peak

Absorption Peaks

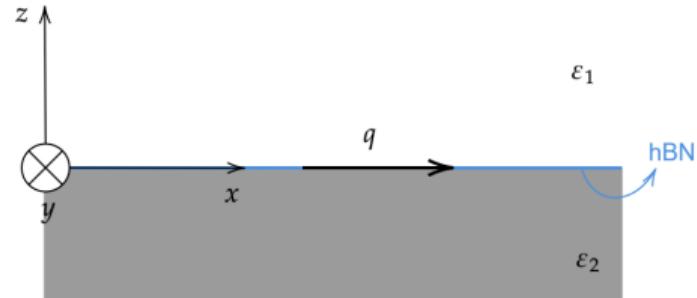
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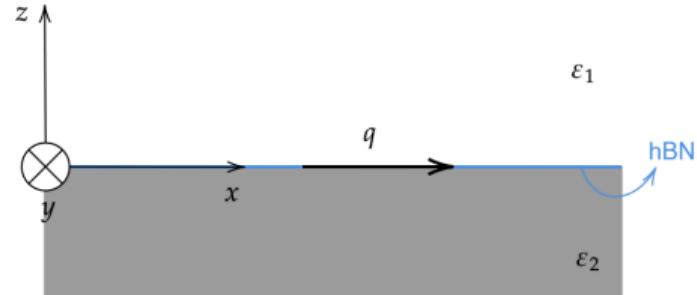
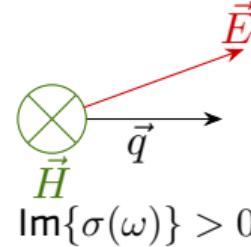
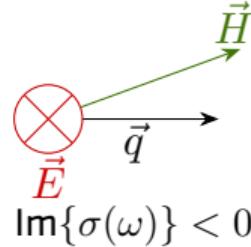
Exciton-Polaritons

Transverse Electric (TE) Transverse Magnetic (TM)



Exciton-Polaritons

Transverse Electric (TE) Transverse Magnetic (TM)



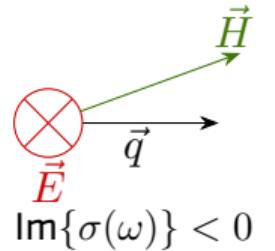
$$\kappa_1 + \kappa_2 - i\omega\mu_0\sigma_{yy}(\omega) = 0$$

$$\frac{\varepsilon_1}{\kappa_1} + \frac{\varepsilon_2}{\kappa_2} + i\frac{\sigma_{xx}(\omega)}{\varepsilon_0\omega} = 0$$

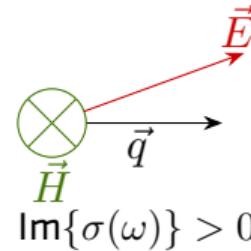
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Exciton-Polaritons

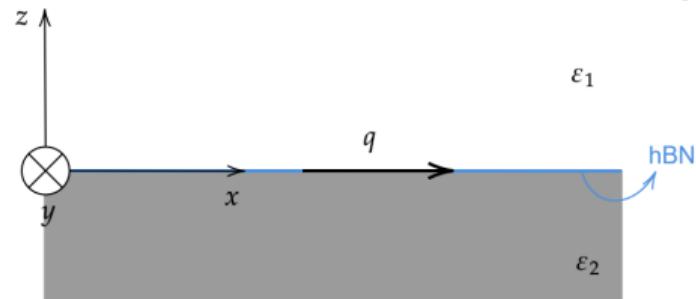
Transverse Electric (TE) Transverse Magnetic (TM)



$$\text{Im}\{\sigma(\omega)\} < 0$$



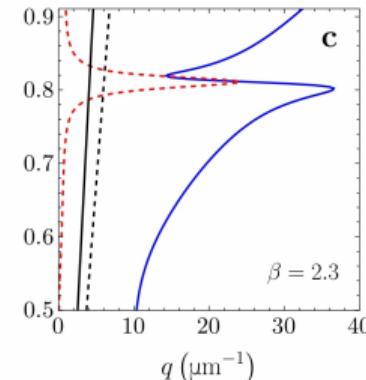
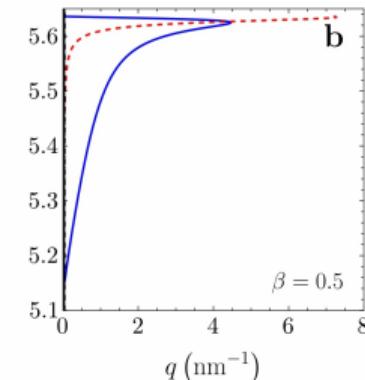
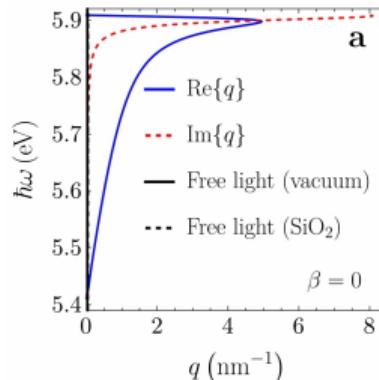
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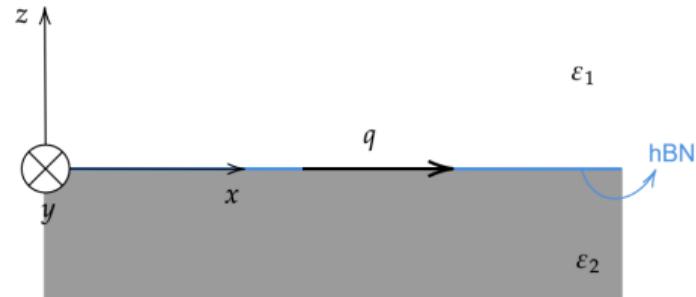
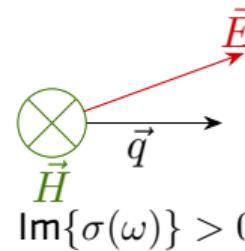
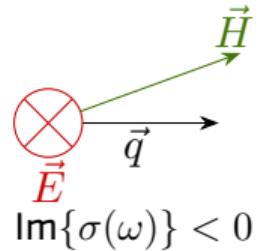
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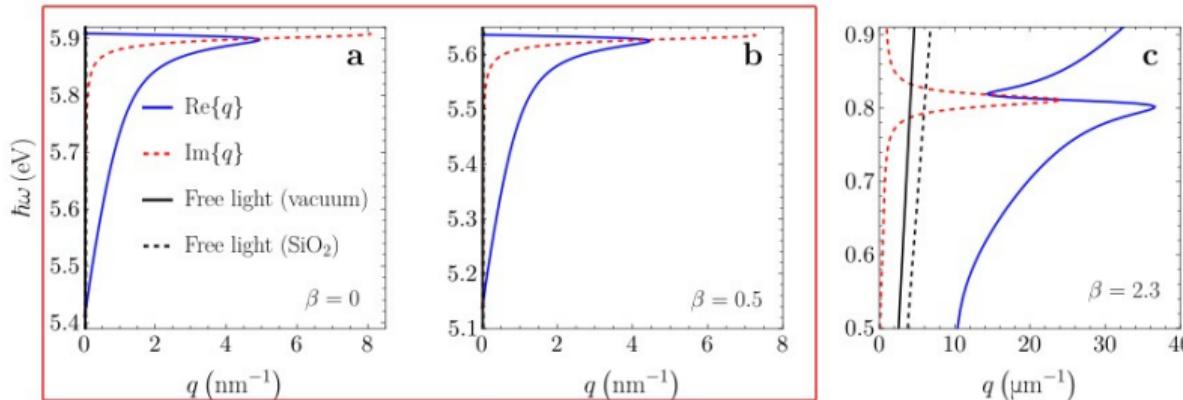


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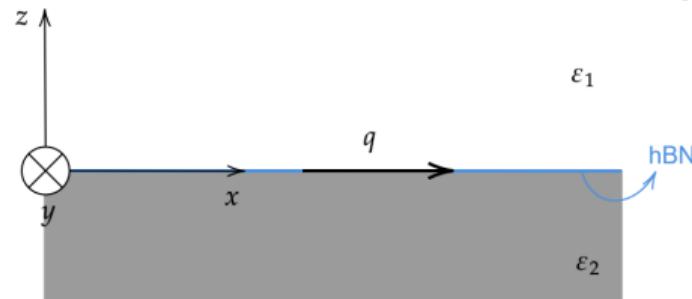
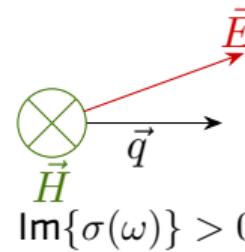
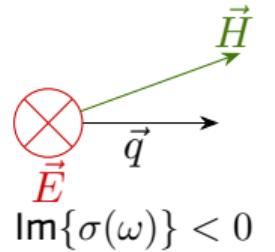


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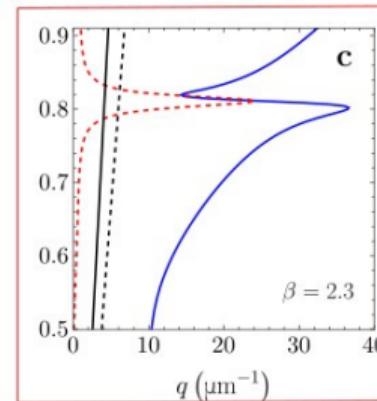
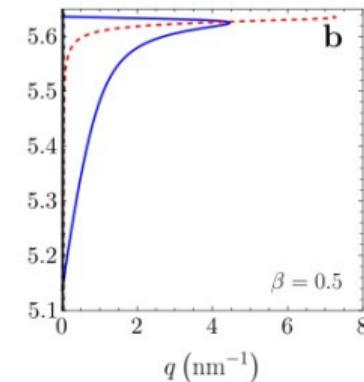
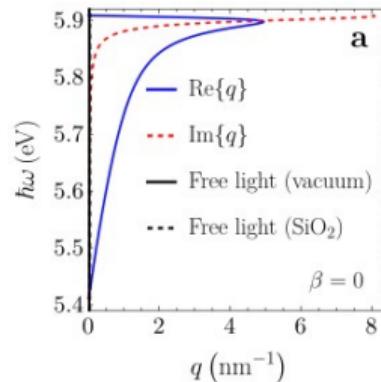


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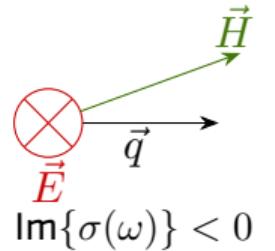


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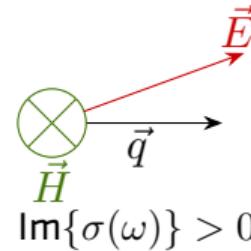


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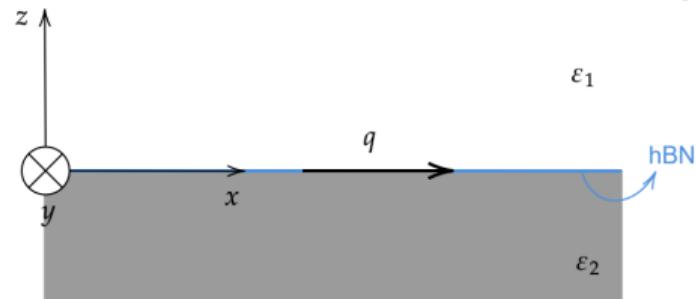
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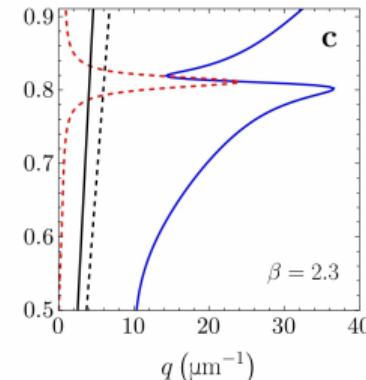
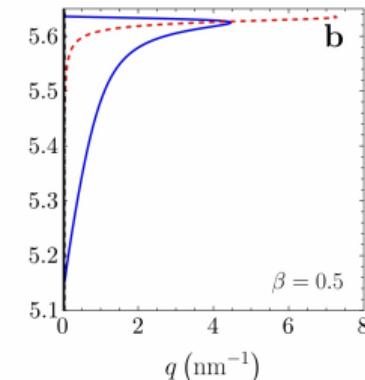
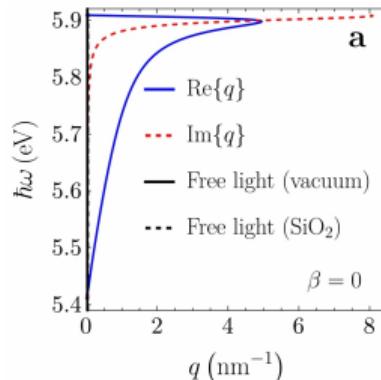
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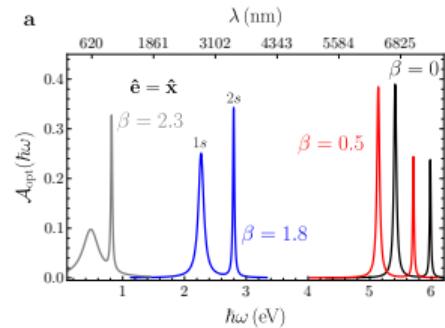
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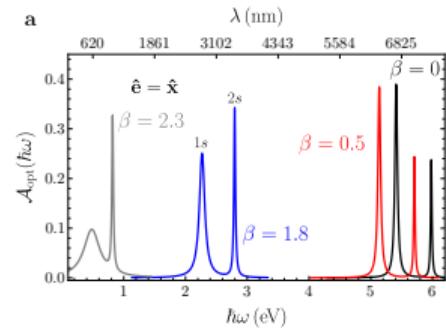
Summary

- Tune the frequency of the optical resonances

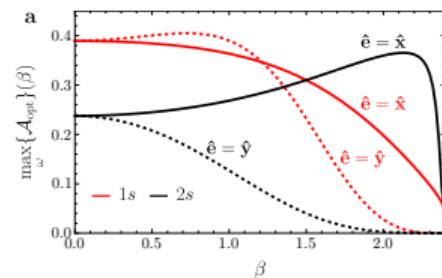


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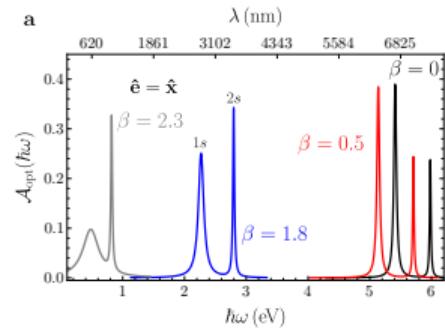


- Tunable absorption by changing the polarization



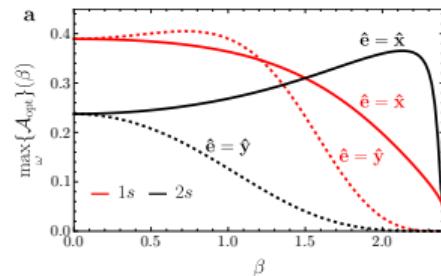
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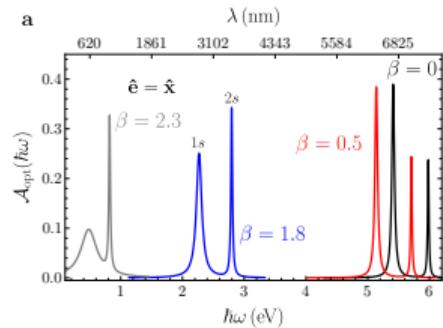
Of experimental relevance

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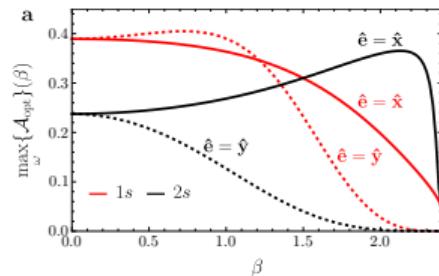


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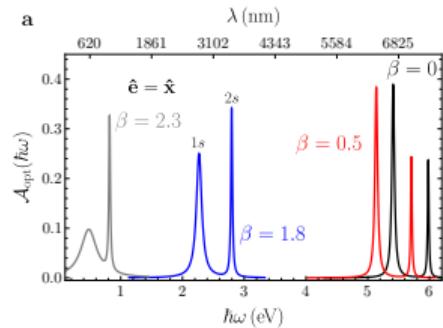


Of experimental relevance

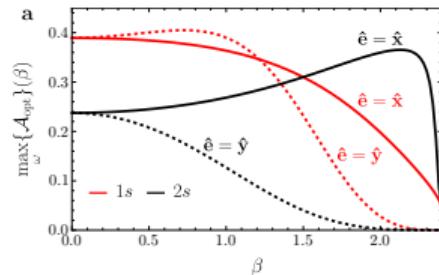
► $L \sim 40$ nm, $V_0 \sim 40$ meV feasible

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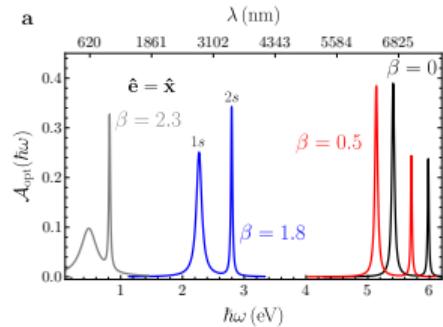


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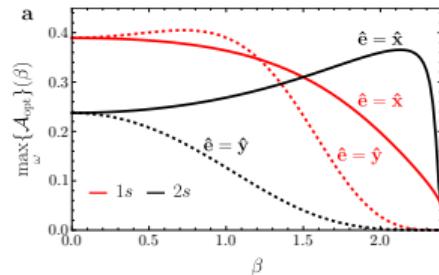
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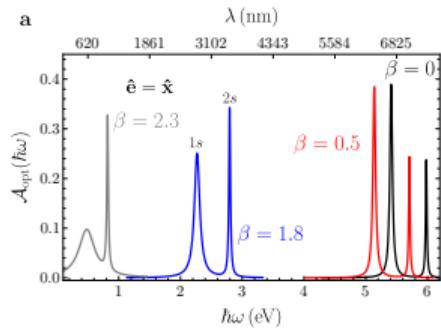


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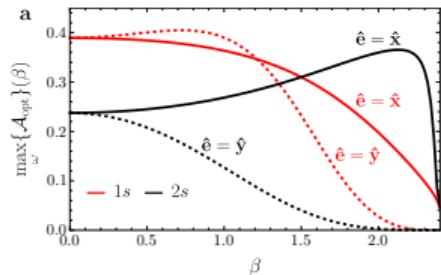
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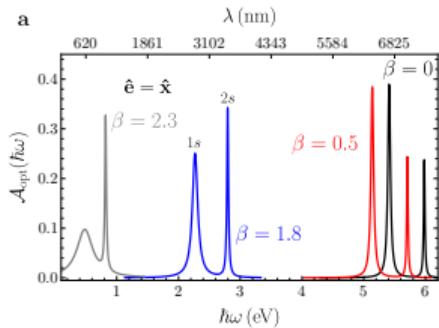
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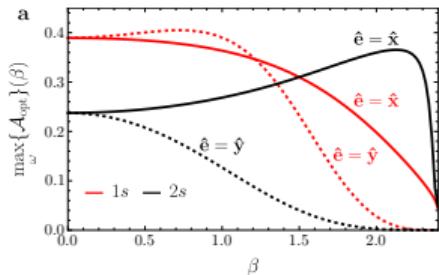
However....

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Of experimental relevance

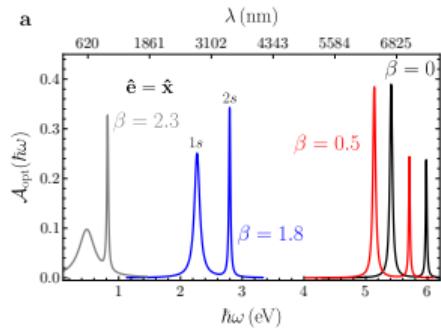
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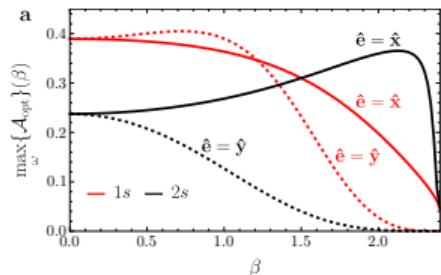
- Where does $\varepsilon_{\text{RK}}(q)$ come from?

Summary

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- Tunable absorption by changing the polarization



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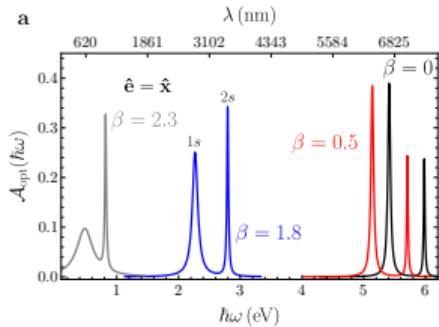
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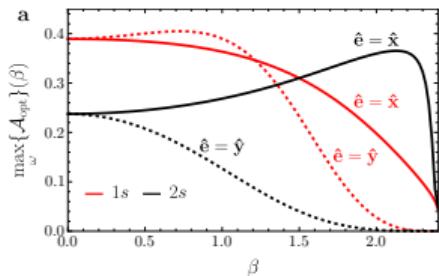
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However....

- Where does $\varepsilon_{\text{RK}}(q)$ come from?
- How to determine r_0 ?
- $\varepsilon_{2D}(q)$ for higher q ?

Outline

- 1 Introduction to Excitons in 2D Materials
- 2 Part I: Exciton–Polaritons in a 1D hBN Superlattice
- 3 Part II: Screening in 2D Materials with the Xatu Code
 - 2D Dielectric Function: Theory
 - 2D Dielectric Function and Excitons: Results
 - Quasi-2D Approach for Screening
- 4 Conclusions

2D (RPA) Dielectric Function

$$\varepsilon^{\text{RPA}}(\mathbf{r}, \mathbf{r}'; t, t') = \delta(\mathbf{r} - \mathbf{r}')\delta(t - t') - \int v_c(\mathbf{r} - \mathbf{r}'')\chi^0(\mathbf{r}'', \mathbf{r}'; t - t'') \, d\mathbf{r}''$$

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$\Downarrow \mathcal{F}$ and $\omega \rightarrow 0$

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$\Downarrow \mathcal{F}$ and $\omega \rightarrow 0$

$$\varepsilon_{\mathbf{G}\mathbf{G}'}(\mathbf{q}) = \delta_{\mathbf{G}\mathbf{G}'} - \sqrt{v_c(\mathbf{q} + \mathbf{G})}\chi^0_{\mathbf{G}\mathbf{G}'}(\mathbf{q})\sqrt{v_c(\mathbf{q} + \mathbf{G}')}\begin{cases} v_c(\mathbf{q}) = \frac{e^2}{2\varepsilon_0|\mathbf{q}|} & \text{in 2D} \\ v_c(\mathbf{q}) = \frac{e^2}{\varepsilon_0|\mathbf{q}|^2} & \text{in 3D} \end{cases}$$

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$\Downarrow \mathcal{F}$ and $\omega \rightarrow 0$

$$\epsilon_{GG'}(\mathbf{q}) = \delta_{GG'} - \sqrt{v_c(\mathbf{q} + \mathbf{G})}\chi^0_{GG'}(\mathbf{q})\sqrt{v_c(\mathbf{q} + \mathbf{G}')}\begin{cases} v_c(\mathbf{q}) = \frac{e^2}{2\varepsilon_0|\mathbf{q}|} & \text{in 2D} \\ v_c(\mathbf{q}) = \frac{e^2}{\varepsilon_0|\mathbf{q}|^2} & \text{in 3D} \end{cases}$$

For an insulator/semiconductor

$$\boxed{\chi^0_{GG'}(\mathbf{q}) = \frac{2}{A} \sum_{vc} \sum_{\mathbf{k}\sigma} \frac{\langle c, \mathbf{k} | e^{-i(\mathbf{q}+\mathbf{G}) \cdot \mathbf{r}} | v, \mathbf{k} + \mathbf{q} \rangle \langle v, \mathbf{k} + \mathbf{q} | e^{i(\mathbf{q}+\mathbf{G}') \cdot \mathbf{r}} | c, \mathbf{k} \rangle}{\epsilon_{v\mathbf{k}+\mathbf{q}} - \epsilon_{c\mathbf{k}}}}$$

Jack Deslippe et al. - *Comp. Phys. Comm.* **183** 6 (2012) ← BerkeleyGW

Macroscopic Dielectric Function

- Screened Coulomb potential in a crystal:

$$W(\mathbf{r}, \mathbf{r}') = \int d\mathbf{r}'' \varepsilon^{-1}(\mathbf{r}, \mathbf{r}'') v_c(\mathbf{r}'' - \mathbf{r}') \xrightarrow{\mathcal{F}} W_{\mathbf{G}\mathbf{G}'}(\mathbf{q}) = \sqrt{v_c(\mathbf{q} + \mathbf{G})} \varepsilon_{\mathbf{G}\mathbf{G}'}^{-1}(\mathbf{q}) \sqrt{v_c(\mathbf{q} + \mathbf{G}')}$$

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- Defining the macroscopic screened potential as:

$$W(\mathbf{q}) \equiv W_{\mathbf{0}\mathbf{0}}(\mathbf{q}) = \varepsilon_{\mathbf{0}\mathbf{0}}^{-1}(\mathbf{q}) v_c(\mathbf{q}) = \frac{v_c(\mathbf{q})}{\varepsilon_M(\mathbf{q})}$$

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- where the macroscopic dielectric function is $\varepsilon_M(\mathbf{q}) \equiv \frac{1}{\varepsilon_{00}^{-1}(\mathbf{q})}$

Note: $\varepsilon_{00}^{-1}(\mathbf{q})$ is the **00** element of the inverse \neq inverse of the **00** element

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Note: $\varepsilon_{00}^{-1}(\mathbf{q})$ is the **00** element of the inverse \neq inverse of the **00** element

For a 2D semiconductor/insulator, where $v_c(\mathbf{q}) \sim 1/q$, we have

$$\varepsilon_{2D}(\mathbf{q}) \equiv \varepsilon_M(\mathbf{q}) \xrightarrow{q \rightarrow 0} 1 + r_0 q \equiv \varepsilon_{RK}(\mathbf{q})$$

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$$W(\mathbf{r}, \mathbf{r}') = \int d\mathbf{r}'' \varepsilon^{-1}(\mathbf{r}, \mathbf{r}'') v_c(\mathbf{r}'' - \mathbf{r}') \xrightarrow{\mathcal{F}} W_{GG'}(\mathbf{q}) = \sqrt{v_c(\mathbf{q} + \mathbf{G})} \varepsilon_{GG'}^{-1}(\mathbf{q}) \sqrt{v_c(\mathbf{q} + \mathbf{G}')}}$$

- Defining the macroscopic screened potential as:

$$W(\mathbf{q}) \equiv W_{00}(\mathbf{q}) = \varepsilon_{00}^{-1}(\mathbf{q}) v_c(\mathbf{q}) = \frac{v_c(\mathbf{q})}{\varepsilon_M(\mathbf{q})}$$

- where the macroscopic dielectric function is $\varepsilon_M(\mathbf{q}) \equiv \frac{1}{\varepsilon_{00}^{-1}(\mathbf{q})}$

Note: $\varepsilon_{00}^{-1}(\mathbf{q})$ is the **00** element of the inverse \neq inverse of the **00** element

For a 2D semiconductor/insulator, where $v_c(\mathbf{q}) \sim 1/q$, we have

$$\varepsilon_{2D}(\mathbf{q}) \equiv \varepsilon_M(\mathbf{q}) \xrightarrow{q \rightarrow 0} 1 + r_0 q \equiv \varepsilon_{RK}(\mathbf{q}) \Rightarrow V_{RK}(q) = \frac{v_c(q)}{\varepsilon_{RK}(q)} = \frac{e^2}{2\varepsilon_0(1 + r_0 q)q}$$

Bloch States in the Tight-Binding Approximation

Linear combination of atomic orbitals (LCAO) method

$$\psi_{n,\mathbf{k}}(\mathbf{r}) = \frac{1}{\sqrt{N}} \sum_{\mathbf{R}} e^{i\mathbf{k}\cdot\mathbf{R}} \sum_{i\alpha} C_{i\alpha}^{n\mathbf{k}} \phi_{\alpha}(\mathbf{r} - \mathbf{R} - \mathbf{t}_i)$$

$$H\psi_{n,\mathbf{k}}(\mathbf{r}) = \epsilon_{n\mathbf{k}}\psi_{n,\mathbf{k}}(\mathbf{r})$$

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$$H(\mathbf{k}) \mathbf{C}^{n\mathbf{k}} = \epsilon_{n\mathbf{k}} \mathbf{C}^{n\mathbf{k}}$$

$$H(\mathbf{k}) \begin{bmatrix} C_{1,1}^{n\mathbf{k}} \\ C_{1,2}^{n\mathbf{k}} \\ \vdots \\ C_{1,N_o^1}^{n\mathbf{k}} \\ C_{2,1}^{n\mathbf{k}} \\ \vdots \\ C_{2,N_o^2}^{n\mathbf{k}} \\ \vdots \\ C_{N_a,N_o^{(N_a)}-1}^{n\mathbf{k}} \\ C_{N_a,N_o^{(N_a)}}^{n\mathbf{k}} \end{bmatrix} = \epsilon_{n\mathbf{k}} \begin{bmatrix} C_{1,1}^{n\mathbf{k}} \\ C_{1,2}^{n\mathbf{k}} \\ \vdots \\ C_{1,N_o^1}^{n\mathbf{k}} \\ C_{2,1}^{n\mathbf{k}} \\ \vdots \\ C_{2,N_o^2}^{n\mathbf{k}} \\ \vdots \\ C_{N_a,N_o^{(N_a)}-1}^{n\mathbf{k}} \\ C_{N_a,N_o^{(N_a)}}^{n\mathbf{k}} \end{bmatrix}$$

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$$(\mathbf{C}^{n\mathbf{k}})_{i\alpha} = C_{i\alpha}^{n\mathbf{k}} \rightarrow \text{Tight-binding (TB) coefficients}$$

$$H(\mathbf{k}) \begin{bmatrix} C_{1,1}^{n\mathbf{k}} \\ C_{1,2}^{n\mathbf{k}} \\ \vdots \\ C_{1,N_o^1}^{n\mathbf{k}} \\ C_{2,1}^{n\mathbf{k}} \\ \vdots \\ C_{2,N_o^2}^{n\mathbf{k}} \\ \vdots \\ C_{N_a,N_o^{(N_a)}-1}^{n\mathbf{k}} \\ C_{N_a,N_o^{(N_a)}}^{n\mathbf{k}} \end{bmatrix} = \epsilon_{n\mathbf{k}} \begin{bmatrix} C_{1,1}^{n\mathbf{k}} \\ C_{1,2}^{n\mathbf{k}} \\ \vdots \\ C_{1,N_o^1}^{n\mathbf{k}} \\ C_{2,1}^{n\mathbf{k}} \\ \vdots \\ C_{2,N_o^2}^{n\mathbf{k}} \\ \vdots \\ C_{N_a,N_o^{(N_a)}-1}^{n\mathbf{k}} \\ C_{N_a,N_o^{(N_a)}}^{n\mathbf{k}} \end{bmatrix}$$

Polarizability in the TB Approximation



Polarizability in the TB Approximation

Recalling that $H(\mathbf{k})\mathbf{C}^{nk} = \epsilon_{nk}\mathbf{C}^{nk}$ and the expression for the polarizability

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Auxiliary calculation:

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Auxiliary calculation:

In the point-like orbital approximation

$$\phi_\alpha^*(\mathbf{r} - \mathbf{R} - \mathbf{t}_i) \phi_\beta(\mathbf{r} - \mathbf{R}' - \mathbf{t}_j) \approx \delta_{ij} \delta_{\alpha\beta} \delta_{\mathbf{R}\mathbf{R}'} \delta(\mathbf{r} - \mathbf{R} - \mathbf{t}_i) \Rightarrow$$

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$$\langle n, \mathbf{k} | e^{-i(\mathbf{q}+\mathbf{G}) \cdot \mathbf{r}} | n', \mathbf{k} + \mathbf{q} \rangle = \int_A d\mathbf{r} \psi_{n,\mathbf{k}}^*(\mathbf{r}) e^{-i(\mathbf{q}+\mathbf{G}) \cdot \mathbf{r}} \psi_{n',\mathbf{k}+\mathbf{q}}(\mathbf{r}) =$$

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Exciton Computation Scheme with the Xatu Code

- ➊ Diagonalize $H(\mathbf{k} + \mathbf{q})$ and store all $\{\epsilon_{n\mathbf{k}+\mathbf{q}}\}, \{\mathbf{C}^{n\mathbf{k}+\mathbf{q}}\}$ $\forall \mathbf{q} \in \text{BZ}, \forall \mathbf{k} \in \text{BZ}', \text{BZ} \neq \text{BZ}'$
- ➋ Compute dielectric matrix $\varepsilon_{GG'}(\mathbf{q}) \forall \mathbf{q} \in \text{BZ}$
- ➌ Invert $\varepsilon_{GG'}(\mathbf{q}) \forall \mathbf{q} \in \text{BZ}$
- ➍ Compute the exciton (following slides)

A. J. Uría-Alvárez et al. - *Comp. Phys. Comm.* **295** 109001 (2024) ← 1st version of Xatu

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Example: Monolayer hBN

Model Hamiltonian from CRYSTAL [1]: DFT calculations in a Gaussian basis using the HSE06 functional

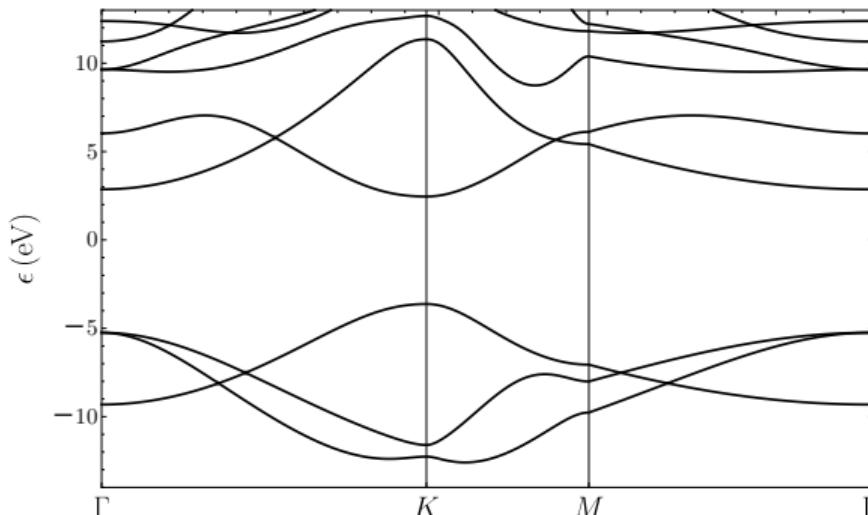


Figure: Band structure of monolayer hBN

- [1] A Erba et al. - *J. Chem. Theory Comput.* **13** 10 (2017)

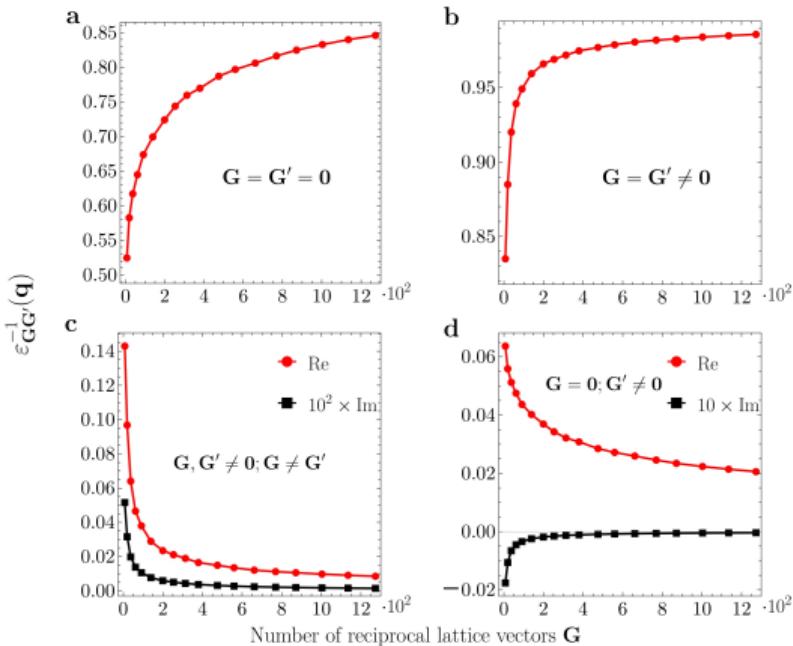
Macroscopic Dielectric Function: Results



Does $\varepsilon_{GG'}^{-1}(q)$ converge?

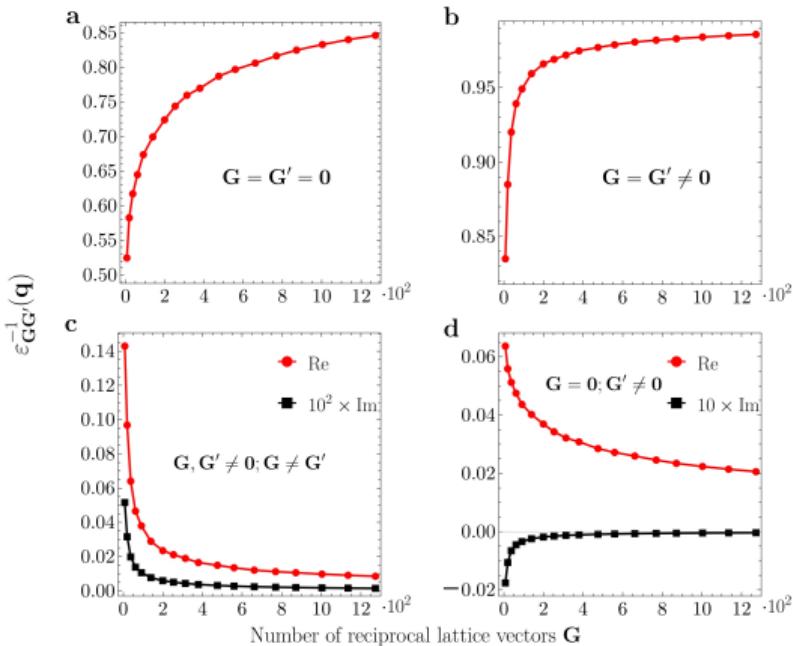
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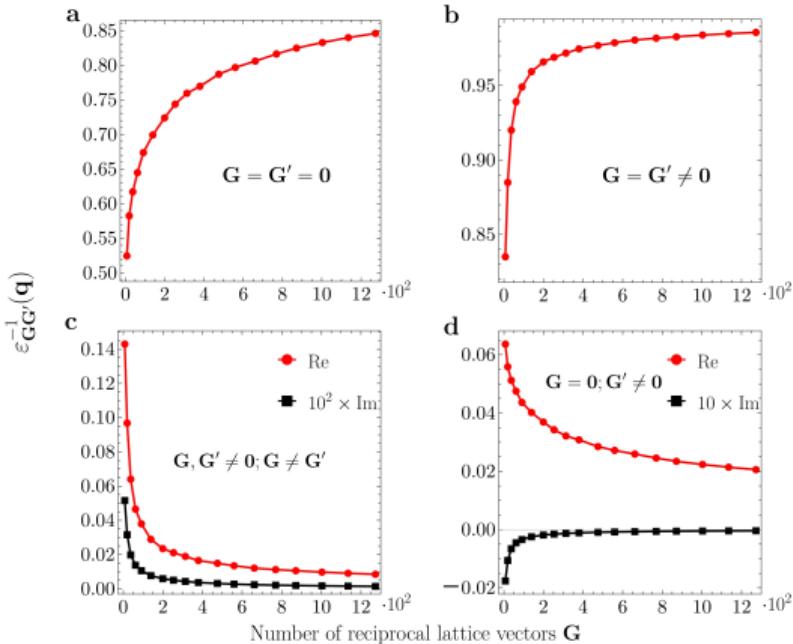
Does $\varepsilon_{GG'}^{-1}(q)$ converge? No!



Macroscopic Dielectric Function: Results

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But still,

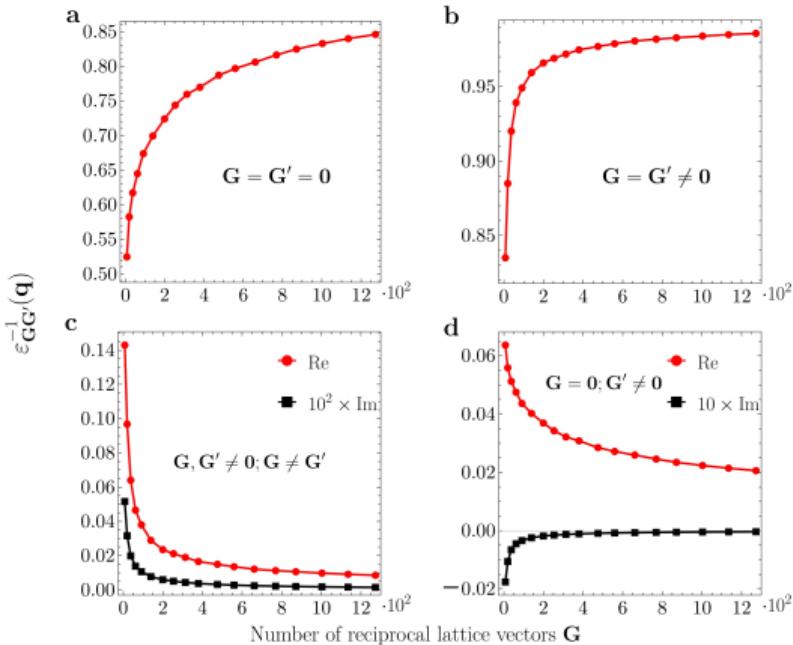


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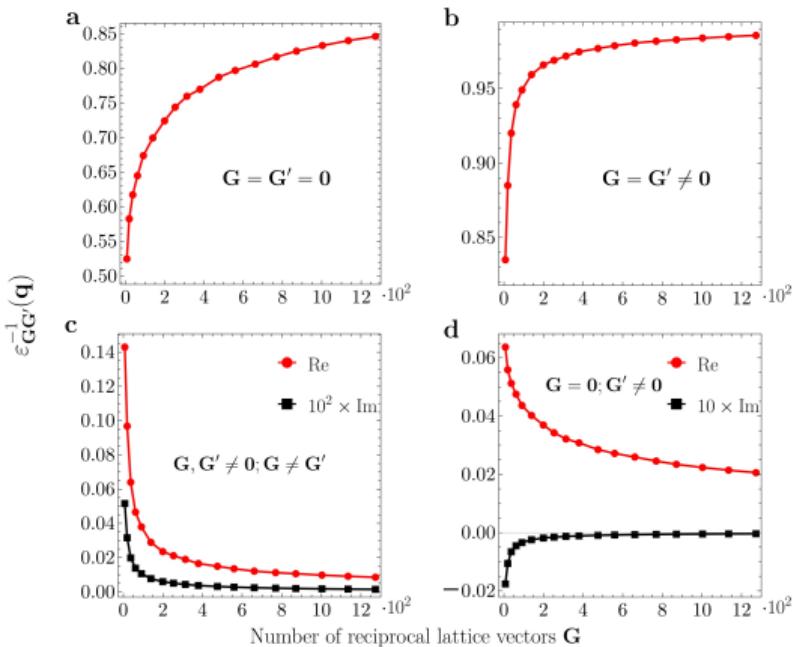
But still,

- How close can we get to the *ab initio* result?



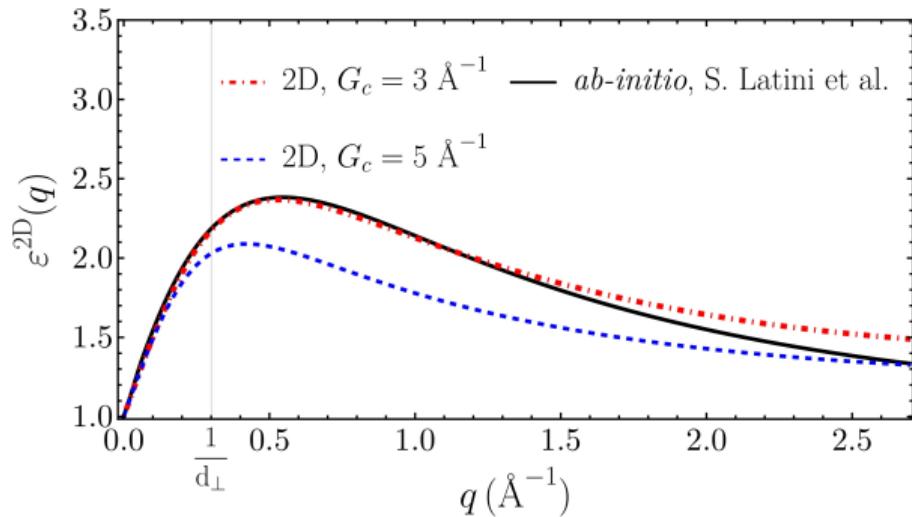
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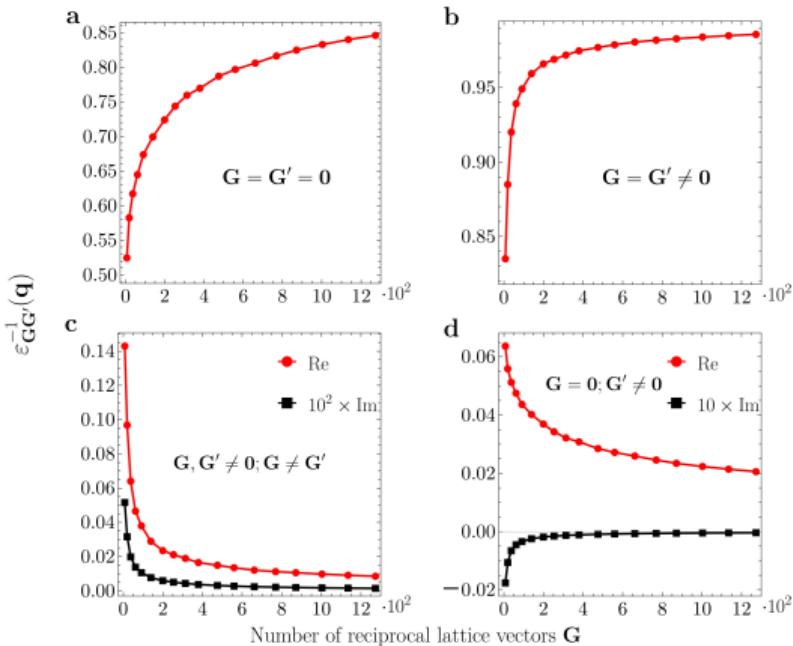
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S. Latini, T. Olsen, K. S. Thygesen - *Phys. Rev. B* **92** 245123
(2015)

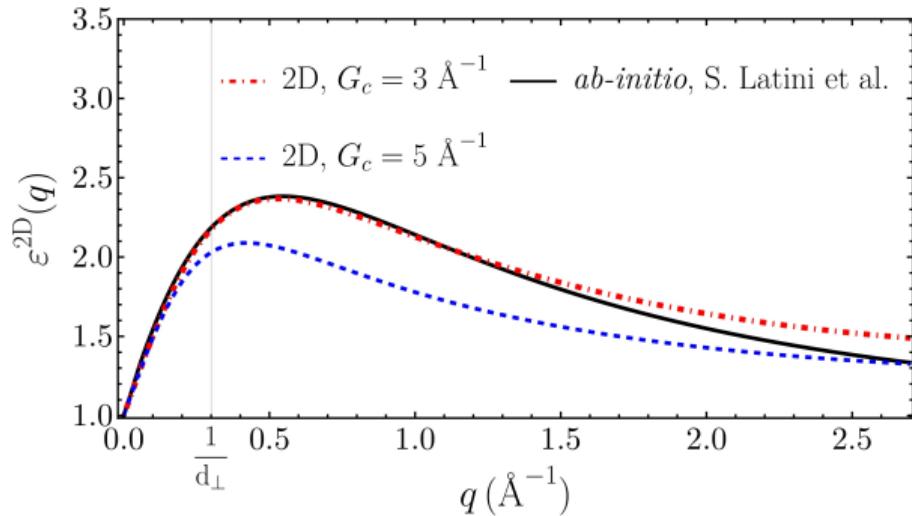
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Does $\varepsilon_{GG'}^{-1}(q)$ converge? No!



But still,

- How close can we get to the *ab initio* result?
- Does the exciton binding energy converge?



S. Latini, T. Olsen, K. S. Thygesen - *Phys. Rev. B* **92** 245123
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Macroscopic Dielectric Function: 2D vs. *Ab initio*

2D approach

- ① $\varepsilon_{GG'}(\mathbf{q}) = \delta_{GG'} - \frac{e^2}{2|\mathbf{q}+\mathbf{G}|\varepsilon_0} \chi_{GG'}^0(\mathbf{q})$
w/ $\langle n, \mathbf{k} | e^{-i(\mathbf{q}+\mathbf{G}) \cdot \mathbf{r}} | n', \mathbf{k}' \rangle$ computed on the fly
- ② invert $\varepsilon_{GG'}(\mathbf{q})$
- ③ pick the head element $\varepsilon^{2D}(\mathbf{q}) = \frac{1}{\varepsilon_{00}^{-1}(\mathbf{q})}$

Ab initio

- ④ $\varepsilon_{GG'}(\mathbf{q}) = \delta_{GG'} - \frac{e^2}{|\mathbf{q}+\mathbf{G}|^2 \varepsilon_0} \chi_{GG'}^0(\mathbf{q})$ w/
 $\langle n, \mathbf{k} | e^{-i(\mathbf{q}+\mathbf{G}) \cdot \mathbf{r}} | n', \mathbf{k}' \rangle$ via FFT
- ⑤ invert $\varepsilon_{GG'}(\mathbf{q})$
- ⑥ $\varepsilon_{00}^{-1}(\mathbf{q}, z, z') = \frac{1}{L_z} \sum_{G_x, G_z} e^{iG_x z} \varepsilon_{G_x, G_z, z}^{-1}(\mathbf{q}) e^{-iG_x z'}$
- ⑦ $\varepsilon^{2D}(\mathbf{q}) = 1 / \langle \varepsilon_{00}^{-1}(\mathbf{q}, z, z') \rangle_{\text{off-plane}}$

Also, the Coulomb potential is truncated as

$$u_c(r) = \frac{\Theta(R_c - r)}{r}, \text{ with } R_c \rightarrow \infty$$

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Exact diagonalization of the Bethe-Salpeter Equation (BSE)

$$(\epsilon_{c\mathbf{k}+\mathbf{Q}} - \epsilon_{v\mathbf{k}}) A_{vc}^{\mathbf{Q}}(\mathbf{k}) + \sum_{v'c',\mathbf{k}'} K_{vc,v'c'}(\mathbf{k}, \mathbf{k}', \mathbf{Q}) A_{v'c'}^{\mathbf{Q}}(\mathbf{k}') = E_X A_{vc}^{\mathbf{Q}}(\mathbf{k})$$

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Excitons in hBN: Numerical Results

Table: $N_k = 60^2$, $N_c = N_v = 1$, All values are in eV.

		G_c^ε					
		0	3	5.1	6	8	9
G_c^X	0	4.14935	5.5566	5.75416	6.011076	$E_b > \text{gap}$	
	3	2.503138	4.380231	3.803146	3.811565	4.326392	
	5.1		2.797365	2.99418	3.888089	4.630105	
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- Quite remarkably, E_b converges!

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where $\chi^0_{GG'}(\mathbf{q}, z, z') = \int_{\mathcal{A}} d\mathbf{r}_{||} \int_{\mathcal{A}} d\mathbf{r}'_{||} e^{-i(\mathbf{q} + \mathbf{G}) \cdot \mathbf{r}} \chi^0(\mathbf{r}, \mathbf{r}') e^{i(\mathbf{q}' + \mathbf{G}') \cdot \mathbf{r}'}$

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Defining an effective 2D macroscopic dielectric function by averaging over d_{\perp}

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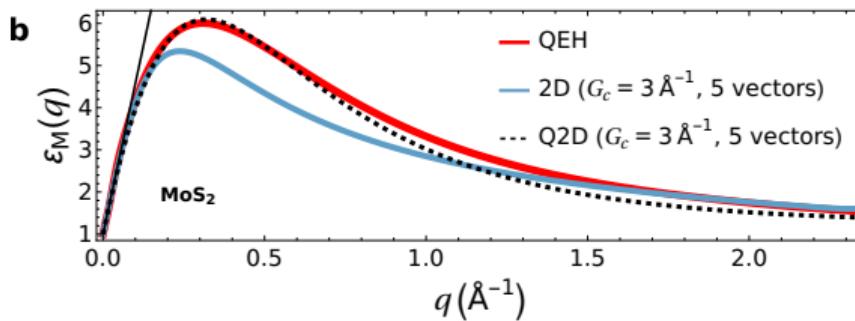
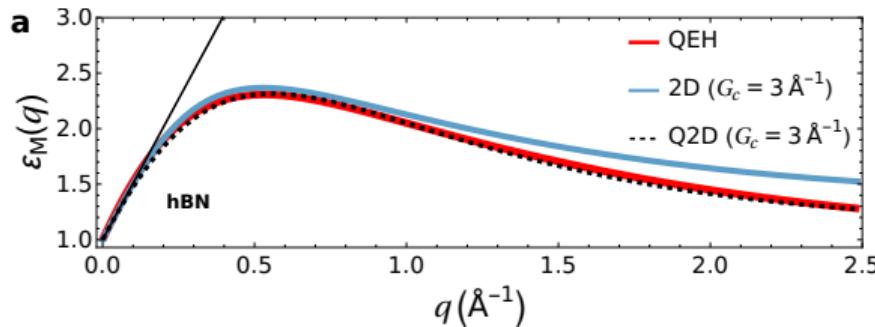
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But does $\bar{\varepsilon}_{GG'}(\mathbf{q})$ improve our dielectric function?

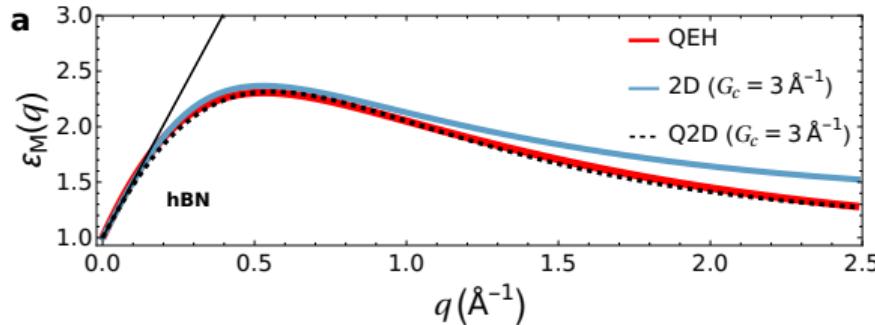
Q2D Dielectric Function: Results



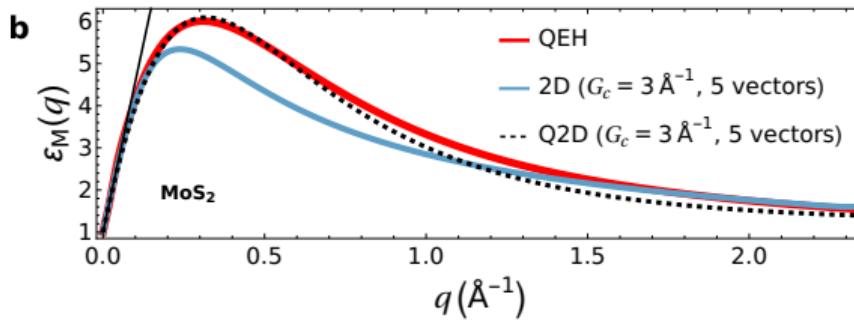
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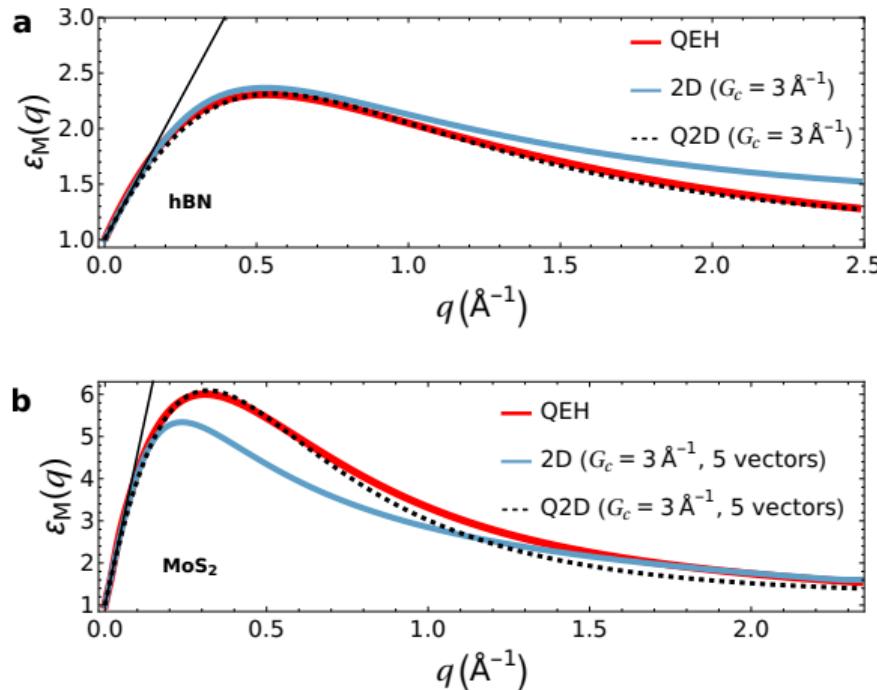


QE_H → Python package for $\varepsilon(q)$ of van der Waals heterostructures [1]



[1] K. Andersen et al. - *Nano Lett.* **15** 7 (2015)

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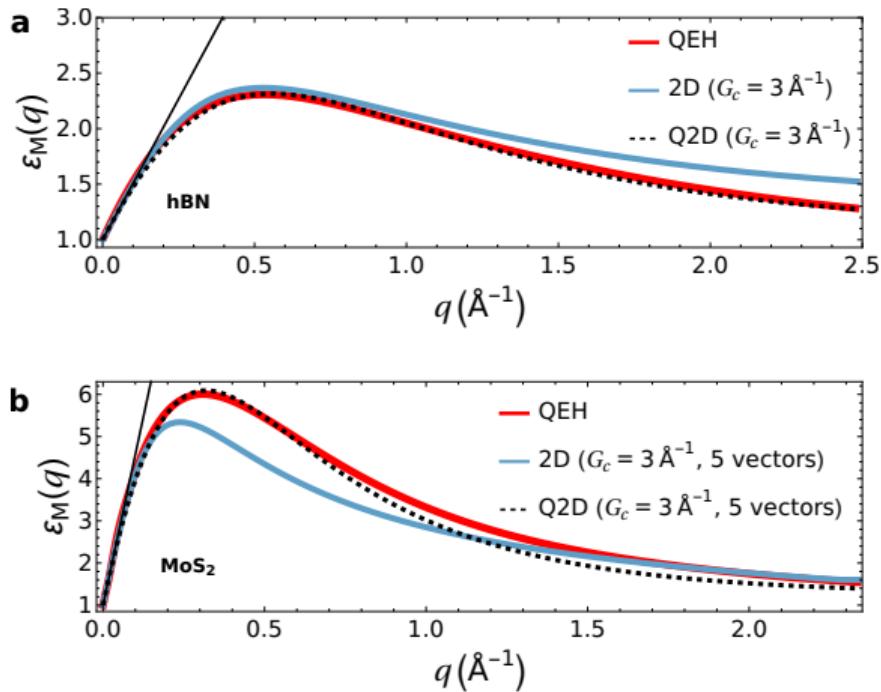


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- Better agreement overall

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Q2D Dielectric Function: Results

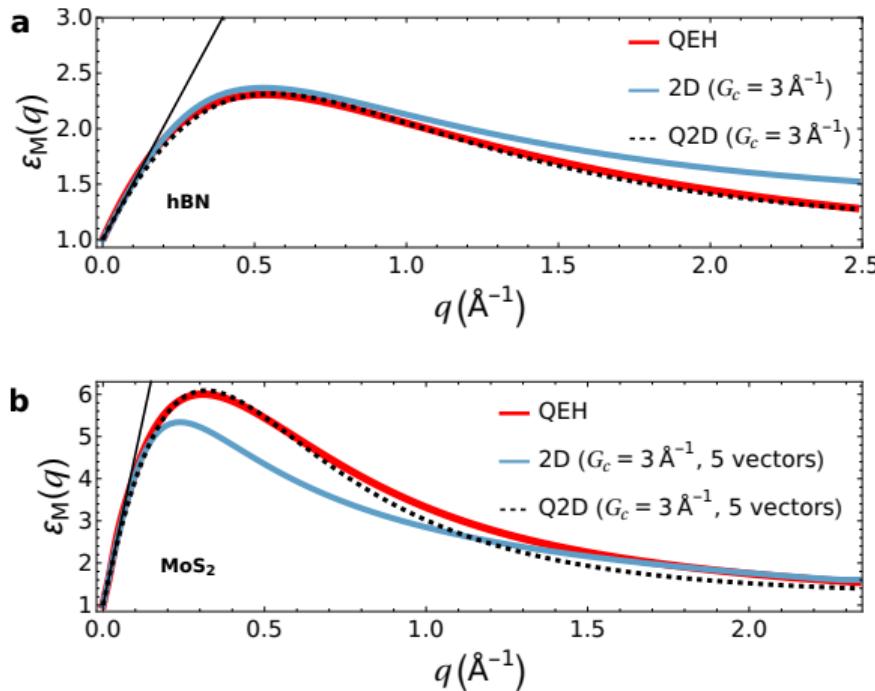


QEHD → Python package for $\varepsilon(q)$ of van der Waals heterostructures [1]

- Better agreement overall
- *Ab initio*, 2D and Q2D approaches all agree in the small- q limit!

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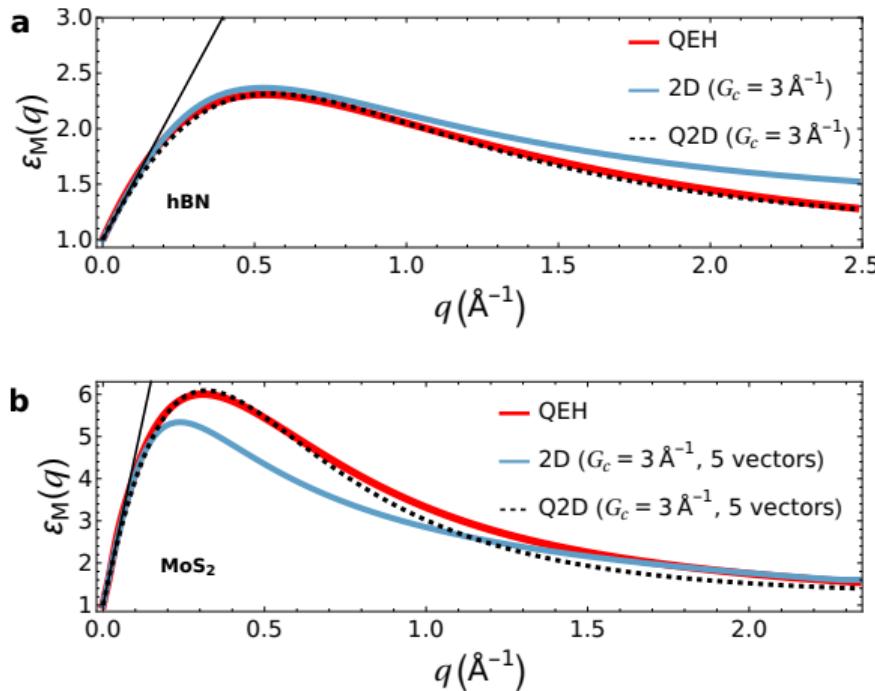


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- Better agreement overall
- *Ab initio*, 2D and Q2D approaches all agree in the small- q limit!
- r_0 can be very well estimated with vanishing computational cost!
- Very good agreement with the literature!
For MoS₂ $r_0 \approx 32 \text{ \AA}$; for GeS $r_0 \approx 20 \text{ \AA}$

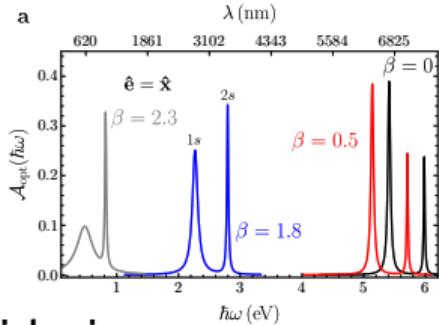
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Outline

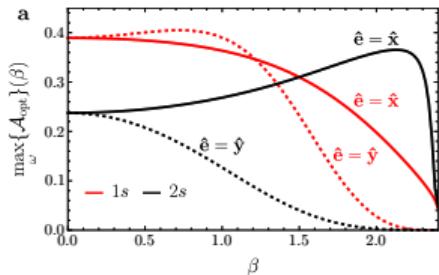
- 1 Introduction to Excitons in 2D Materials
- 2 Part I: Exciton–Polaritons in a 1D hBN Superlattice
- 3 Part II: Screening in 2D Materials with the Xatu Code
- 4 Conclusions

Conclusions: Part I

- hBN as a promising material for mid IR-UV polaritonics
- Tune the frequency of the optical resonances



■ Linear dichroism

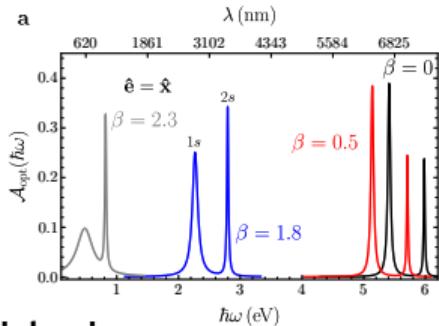


Of experimental relevance (recalling)

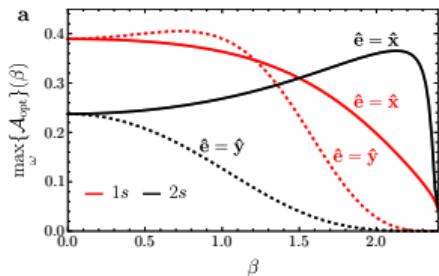
- ▶ D. R. Danielsen et al. - *ACS Nano* **19** 22 (2025) ← experiment with WS₂
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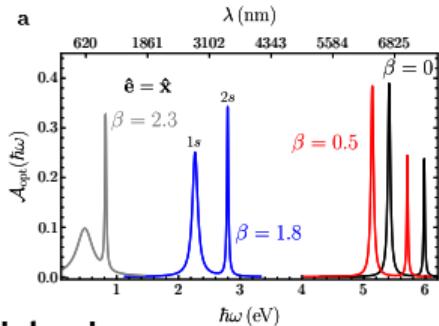


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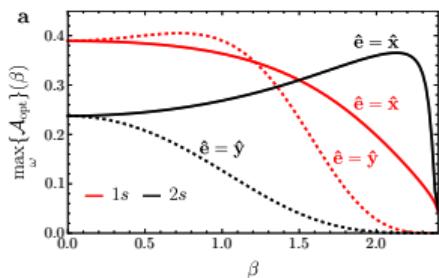
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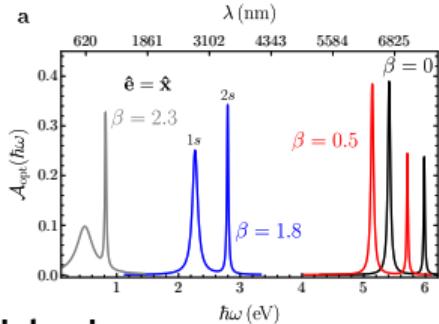


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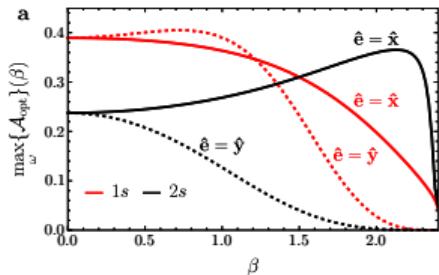
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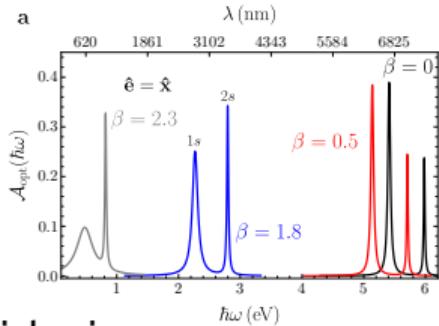


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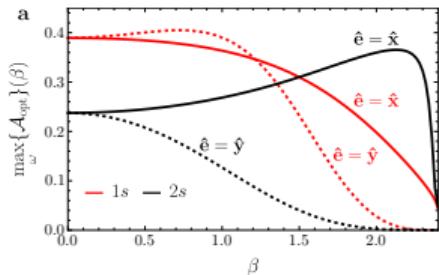
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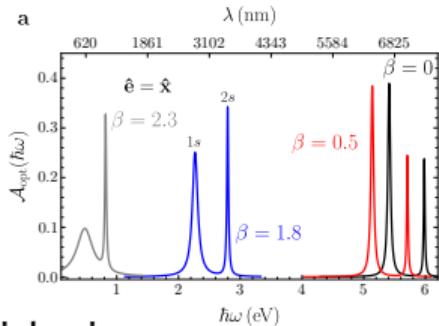


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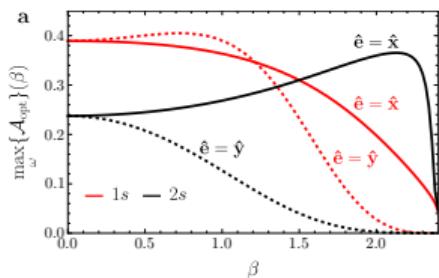
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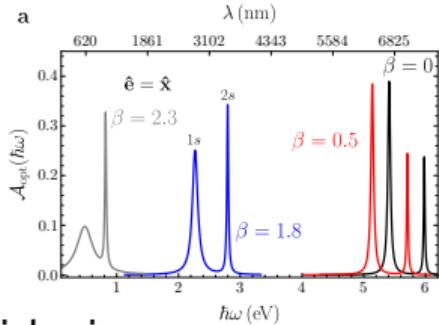


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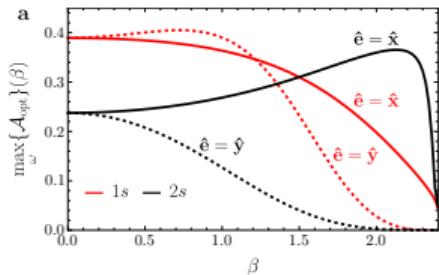
- ▶ D. R. Danielsen et al. - *ACS Nano* **19** 22 (2025) ← experiment with WS_2
- ▶ G. Ermolaev et al. - *Arxiv* **2509** 18866 (2024) ← experiment with CrSBr
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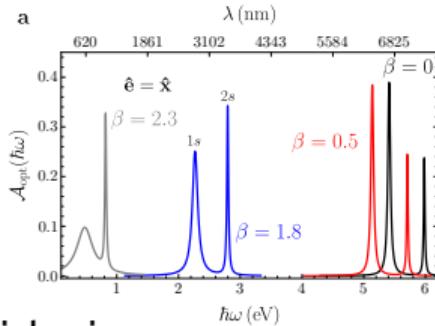


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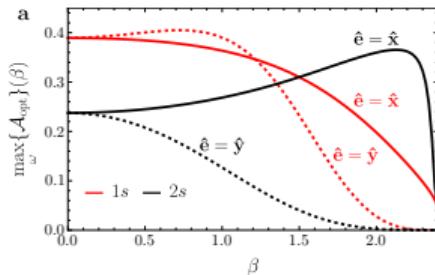
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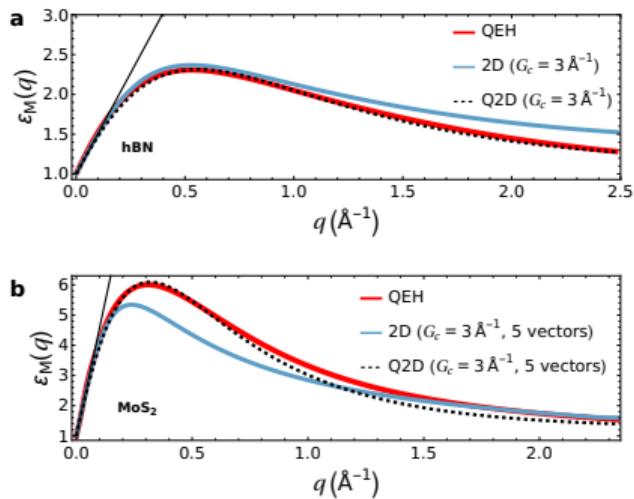
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Conclusions: Part II

- ① Point-like orbital approximation 

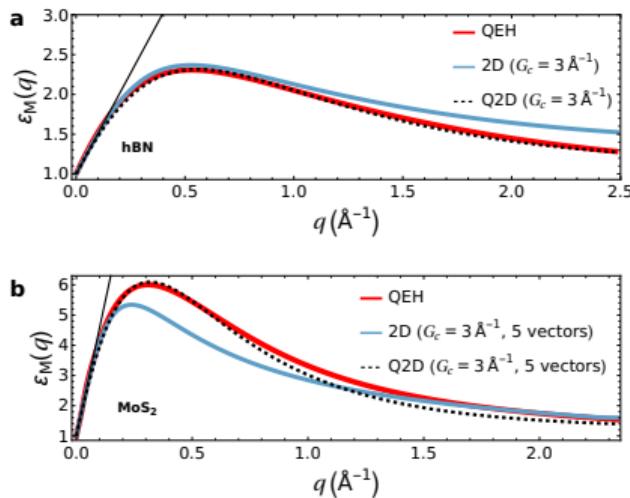
Conclusions: Part II

- ➊ Point-like orbital approximation 
- ➋ $\varepsilon^{2D}(q)$ by direct inversion of $\varepsilon_{GG'}(q)$ 



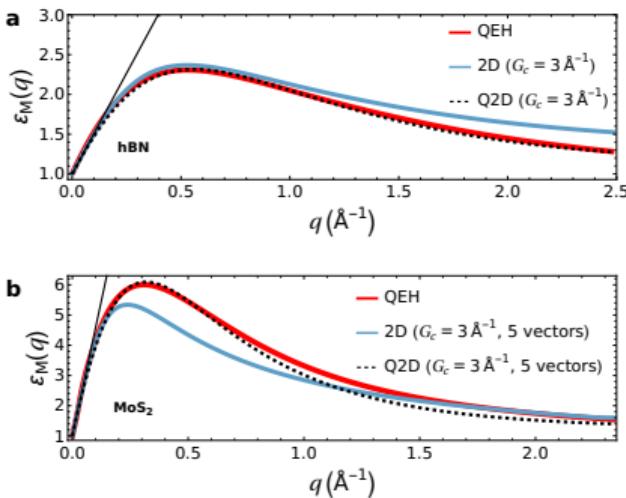
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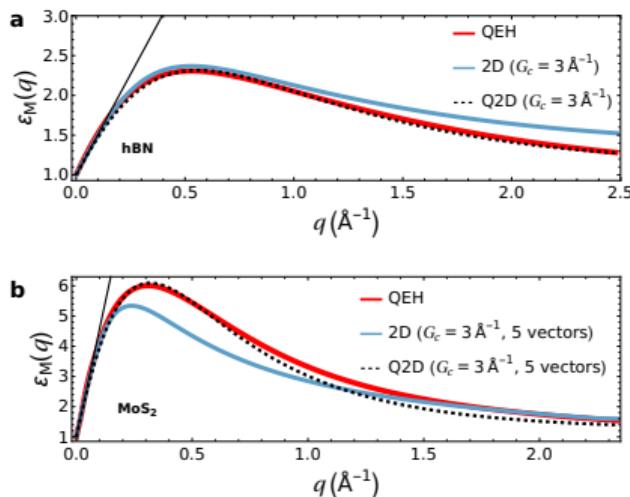
Conclusions: Part II

- 1 Point-like orbital approximation 
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- 4 Exciton binding energy seems to converge 



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- 4 Exciton binding energy seems to converge 
- 5 Panel **b** with 95 points:
 ~ 20 mins for 2D, ~ 30 mins for Q2D 



Acknowledgments

C. Tserkezis



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N. M. R. Peres



J. J. Palacios



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D. Martin-Cano



K. S. Thygesen

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And the audience
Thanks 😊



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Screened potential matrix elements

$$W_{\mathbf{G}\mathbf{G}'}(\mathbf{q}) = \sqrt{v_c(\mathbf{q} + \mathbf{G})} \varepsilon_{\mathbf{G}\mathbf{G}'}^{-1}(\mathbf{q}) \sqrt{v_c(\mathbf{q} + \mathbf{G}')} \quad (1)$$

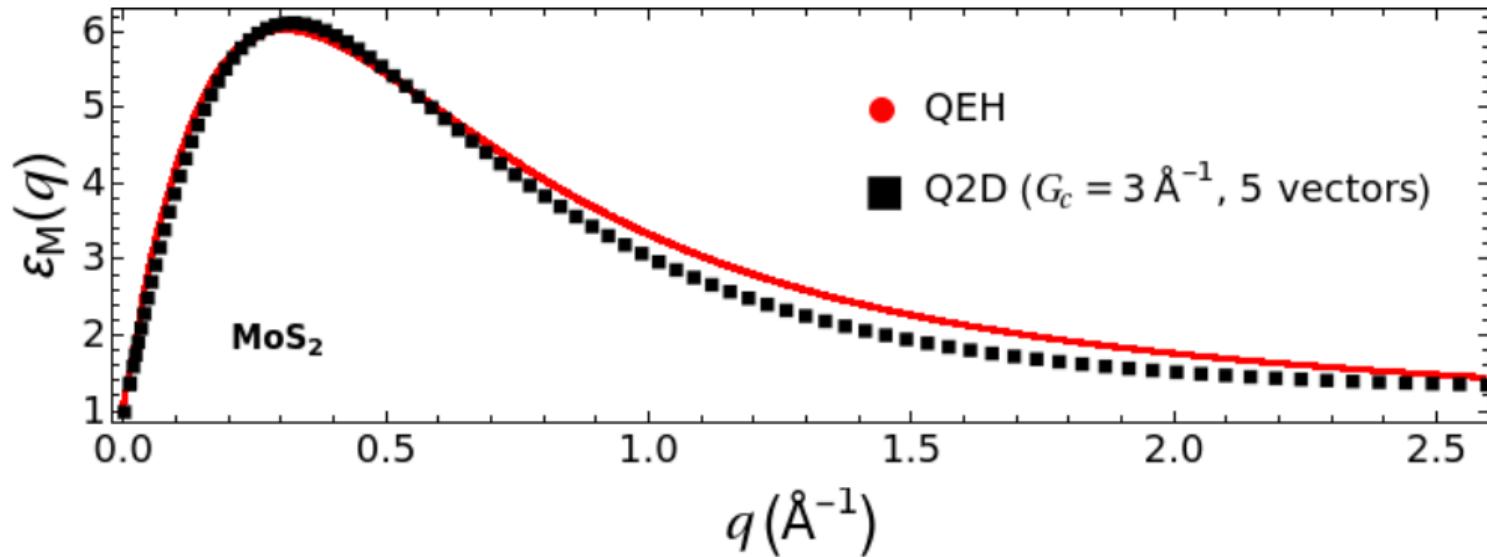
Regularizing the singular terms

$$W_{\mathbf{0}\mathbf{0}}(\mathbf{0}) = \frac{1}{\mathcal{A}_\Gamma} \int_{\mathcal{A}_\Gamma} d\mathbf{q} \varepsilon_{\mathbf{0}\mathbf{0}}^{-1}(\mathbf{q}) v_c(\mathbf{q}) \approx \frac{1}{\mathcal{A}_\Gamma} \int_{\mathcal{A}_\Gamma} d\mathbf{q} v_c(\mathbf{q}) (1 - r_0 q) \quad (2)$$

and for the wing terms

$$W_{\mathbf{G}\mathbf{0}}(\mathbf{0}) = W_{\mathbf{0}\mathbf{G}}(\mathbf{0}) = 0 \quad (3)$$

Q2D dielectric function



Computational Framework: Pre-processing calculations

- DFT w/ Quantum ESPRESSO + Wannier90 (_tb.dat file)
- OR
- DFT w/ CRYSTAL (.oupt file)



System file:

- Wannier90 <filename>_tb.dat file $\xrightarrow{\text{w90 utility}}$.model file as input for xatu
- CRYSTAL <filename>.oupt file as input for xatu

Monolayer MoS₂ Band Structure

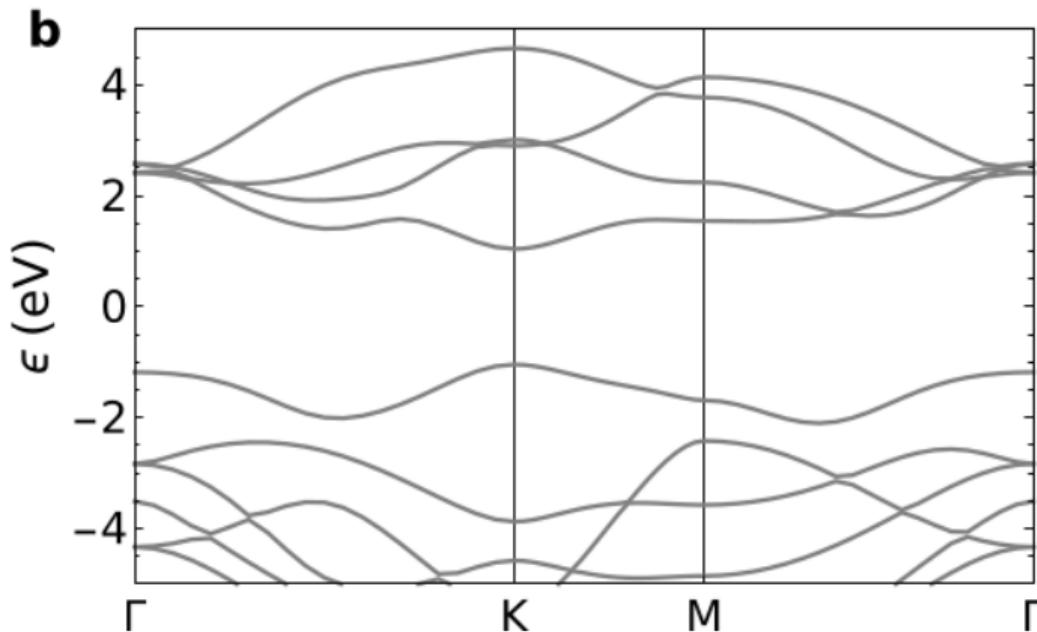


Figure: Band structure of monolayer MoS₂ using CRYSTAL

Excitons in MoS₂: Numerical Results

Table: This table examines the convergence of the excitonic ground state binding energy with the cutoff for the dielectric matrix, G_c^ε , and for the interaction matrix elements, G_c^X , always with $G_c^X < G_c^\varepsilon$. We have used $N_k = 60^2$, $N_c = N_v = 1$, and we have excluded the exchange interaction term. For the size of the regularization region, we used the radius $q_0 = 0.6k_0$, where k_0 is the norm of the wavevector(s) closest to the origin. All values are in eV. $\Delta = 2.08366$ eV

		$G_c^\varepsilon (\text{\AA}^{-1})$					
		0	3	4	5	7	8
G_c^X	0	0.979507	1.567935	1.401440	1.951914	$E_b > \text{gap}$	
	3	0.756373	1.619208	1.785953	$E_b > \text{gap}$	$E_b > \text{gap}$	
	4		0.774599	1.105537	$E_b > \text{gap}$	$E_b > \text{gap}$	
	5			0.778244	$E_b > \text{gap}$	$E_b > \text{gap}$	
	7				0.792309	1.300835	
	8					0.799489	

$E_b > \text{gap}$ -> the exciton comes with negative excitation energy