

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

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POLIMA: Center for Polariton-driven Light-Matter Interactions

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Ph.D. Defense

# 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

- 2D Dielectric function
- Dielectric function in the Tight-Binding approximation
- Dielectric function: numerical results
- Excitons
- Quasi-2D approach for screening

## 4 Conclusions

## 5 Acknowledgements

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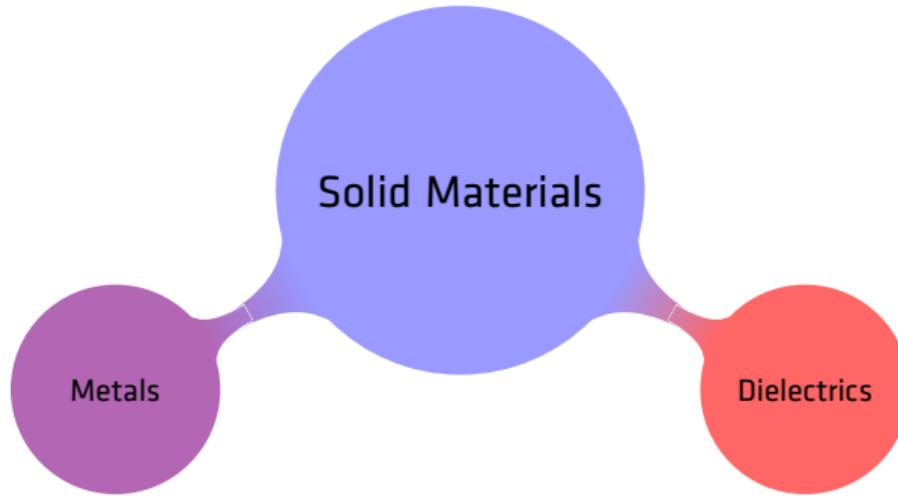
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## 3 Part II: Screening in 2D materials

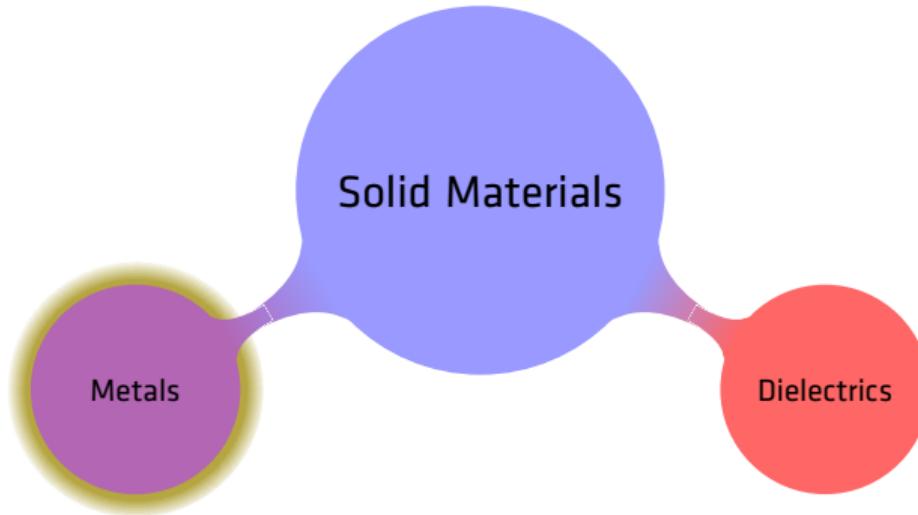
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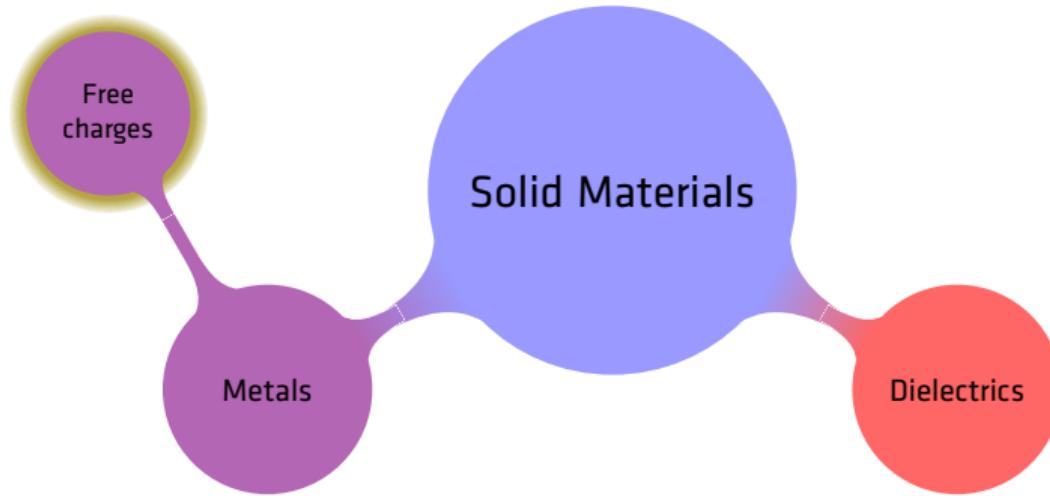
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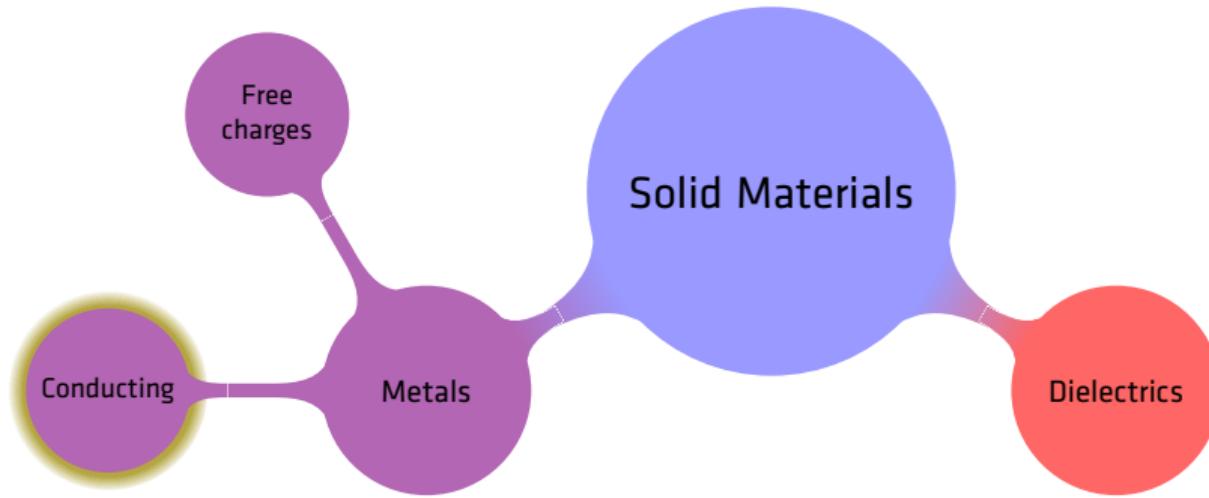
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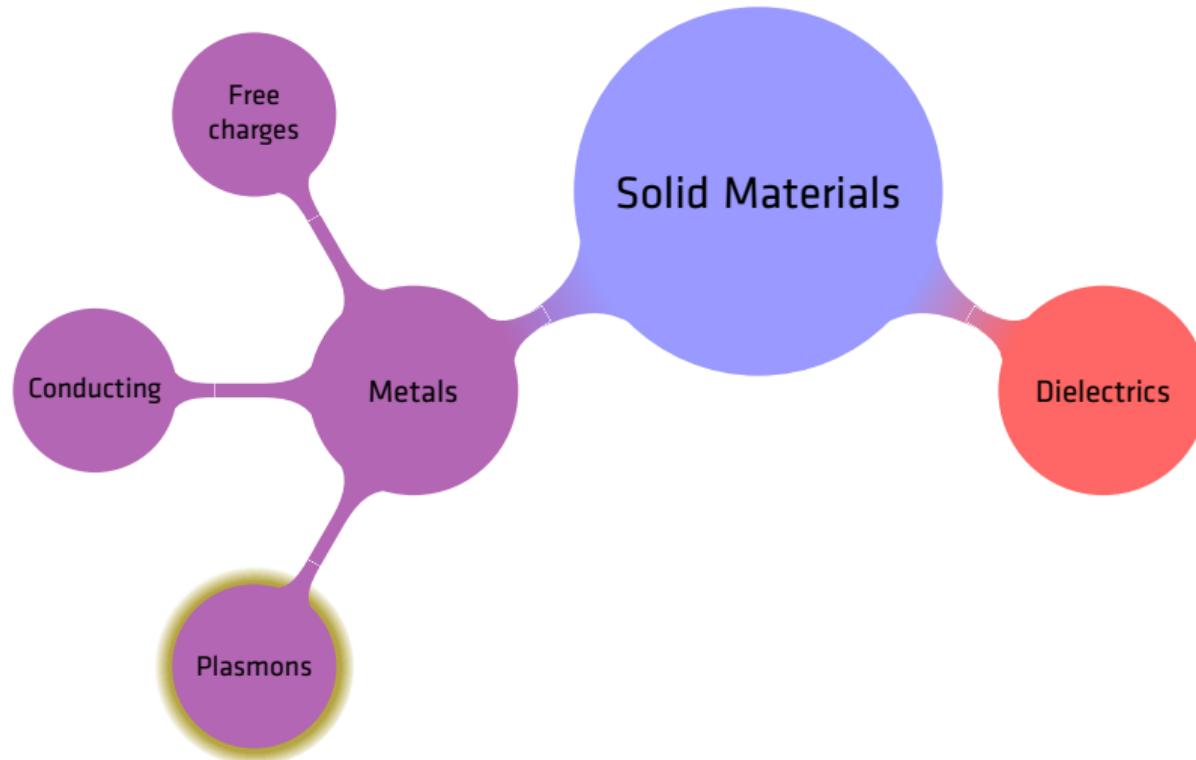
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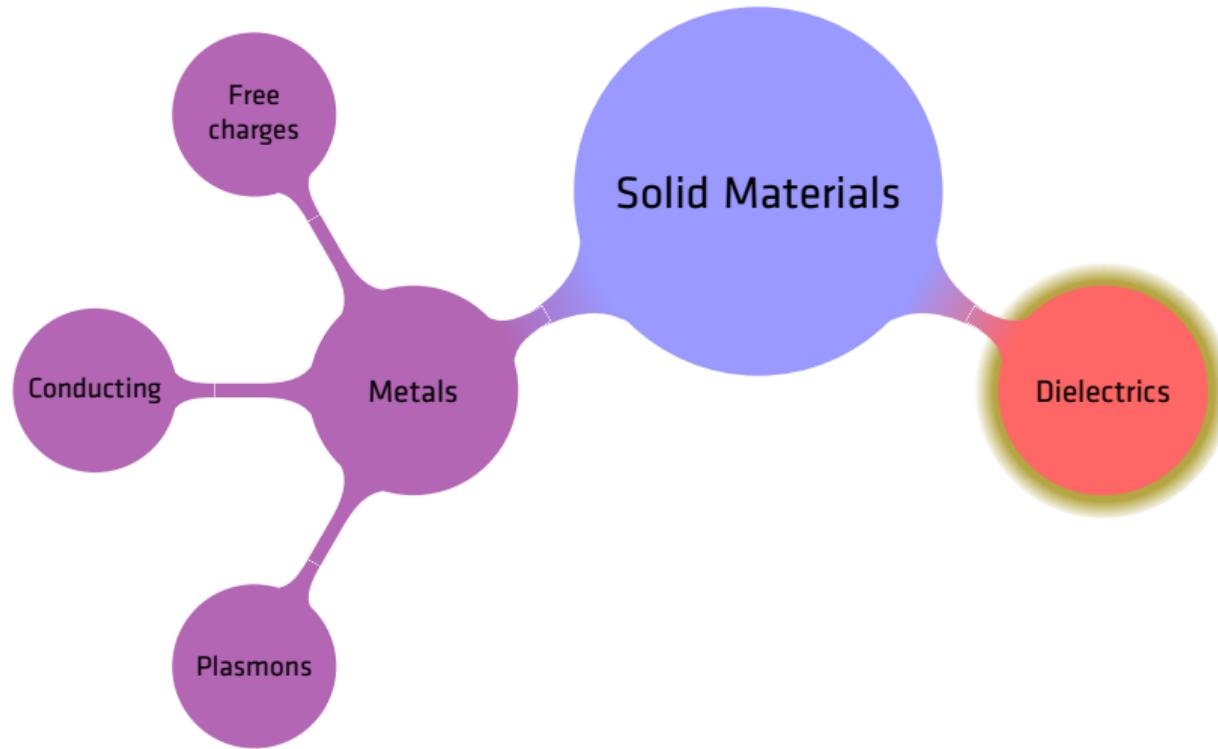
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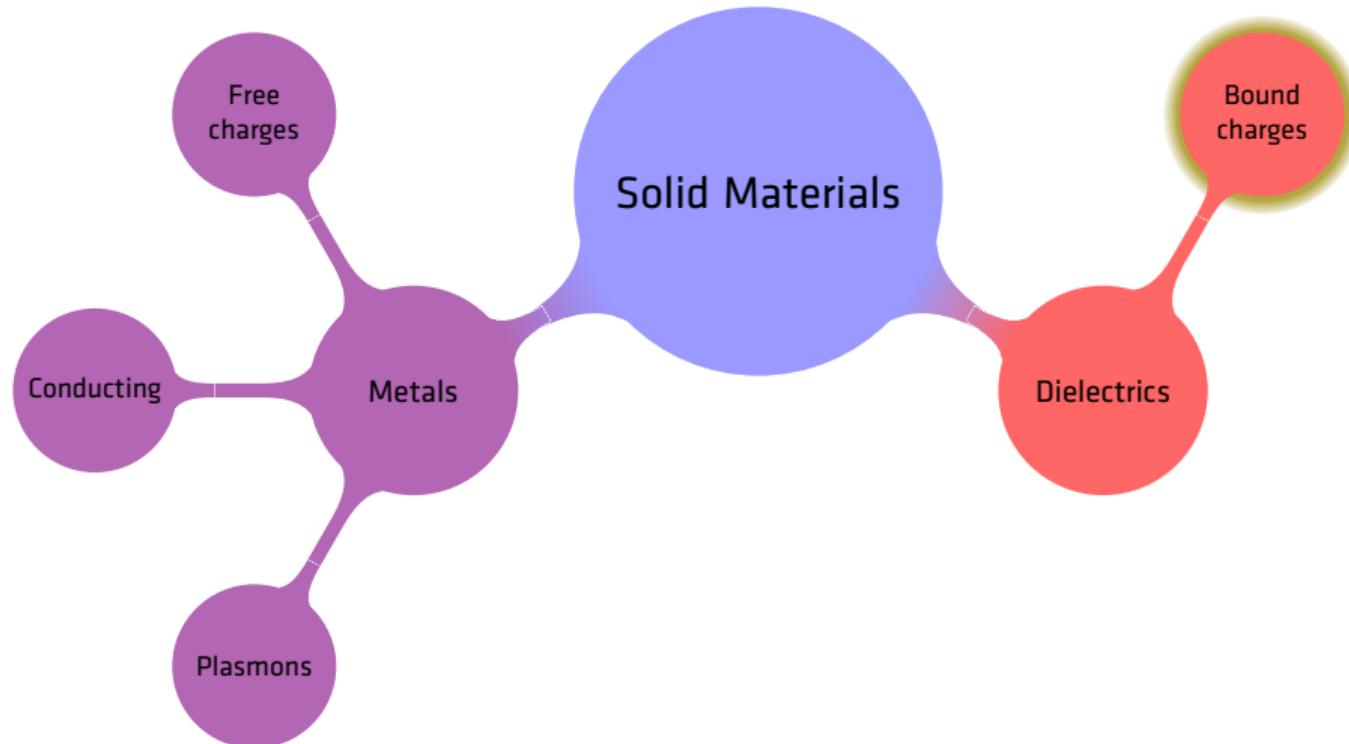
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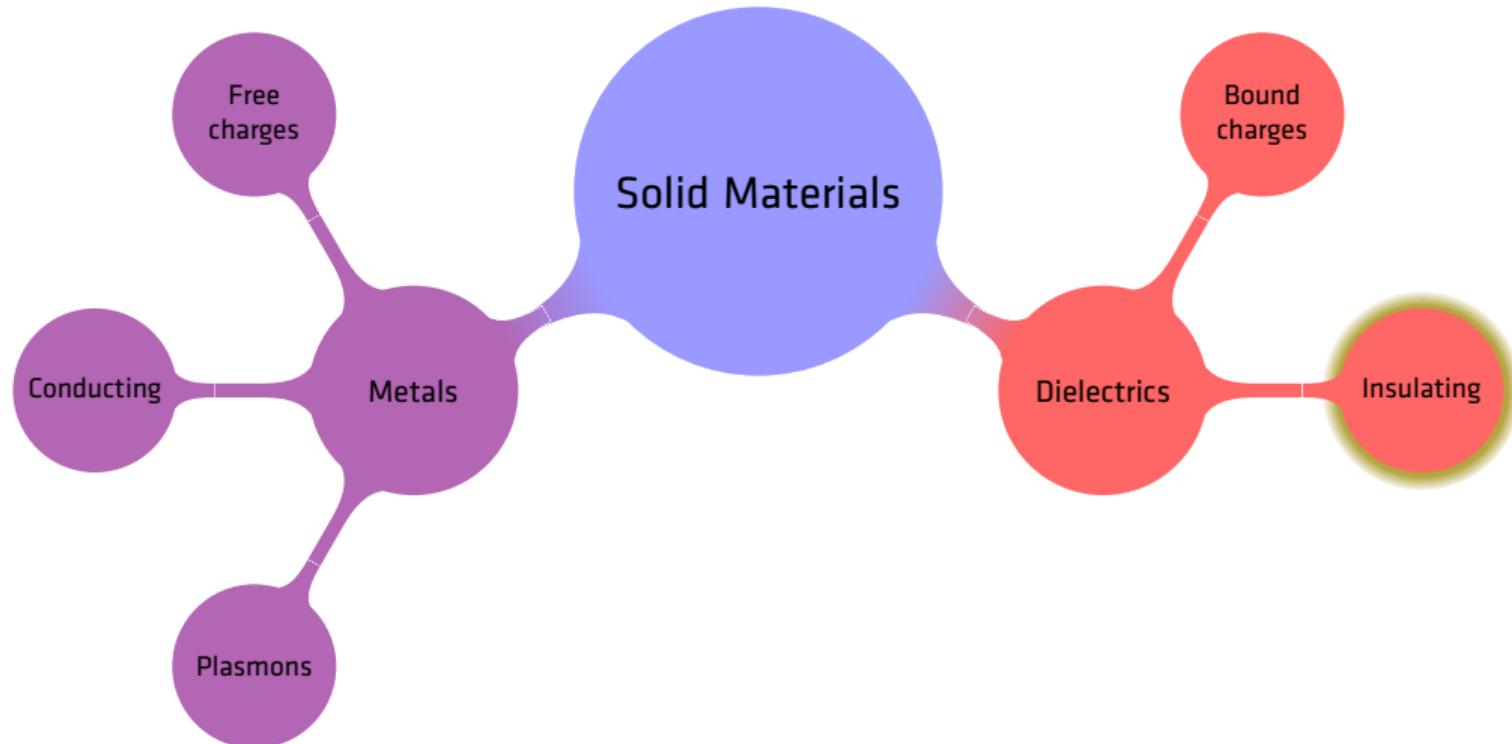
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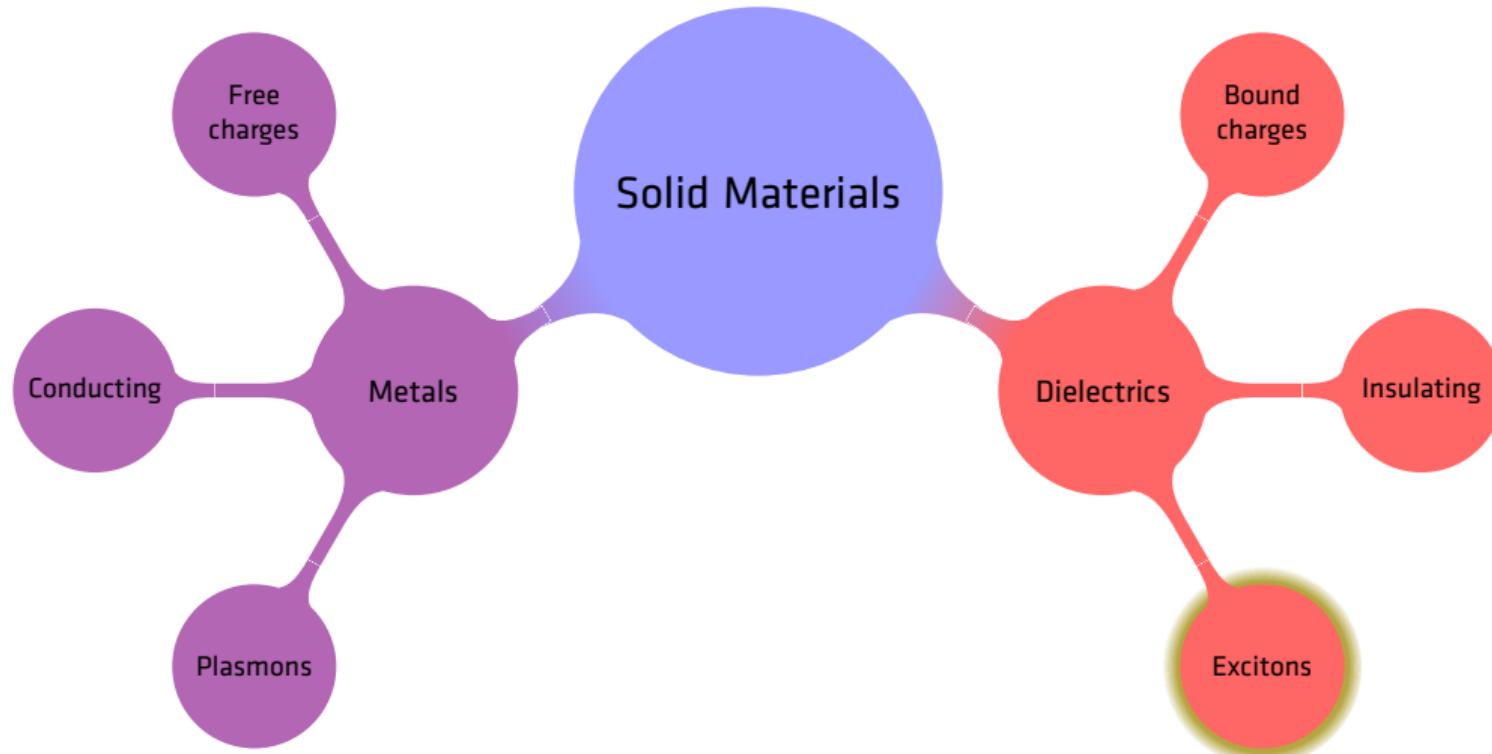
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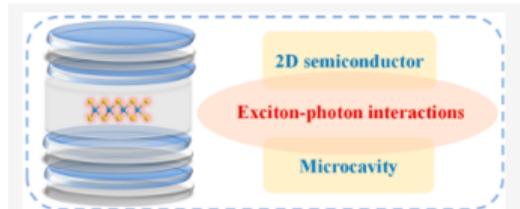
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# Excitons in photonics

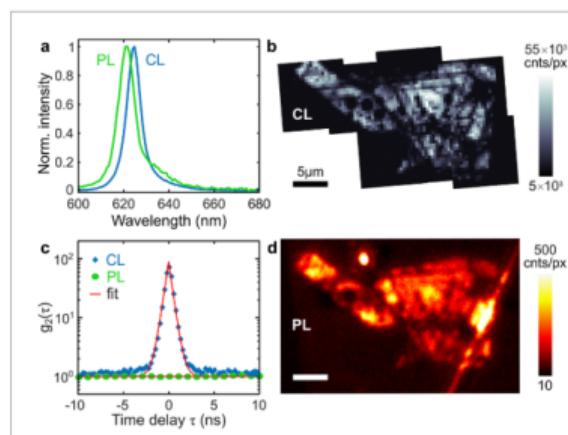
Relevant for:

Light-matter interactions



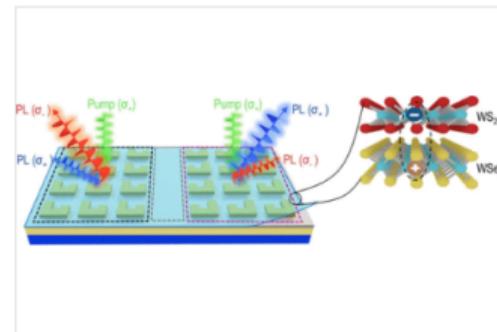
J. Shang et al. - ACS Photonics  
2023, 10, 2064–2077

Quantum Light Sources



S. Fiedler et al. - 2D Mater.  
10 021002 (2023)

Optical Communication



Yi Zhu et al. - Nano Letters  
2025, 25 (21)

# Excitons in two-dimensional materials

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

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

$$R^* = \frac{2\mu_{eh}^2 e^4}{\hbar^2 (8\pi\epsilon\epsilon_0)^2}$$

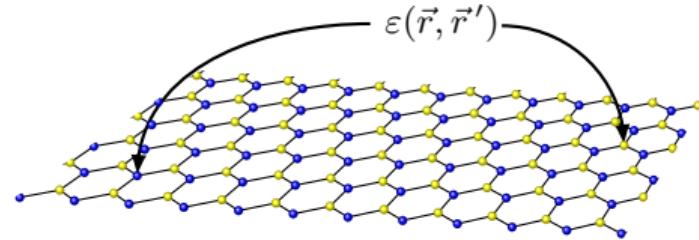
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But for a 2D (insulating) material



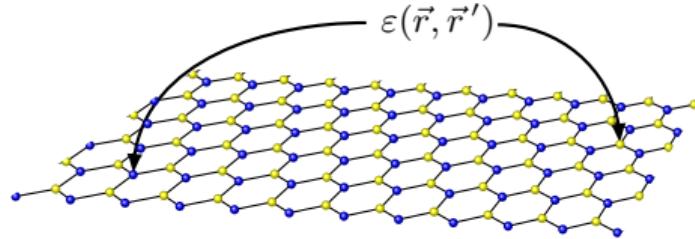
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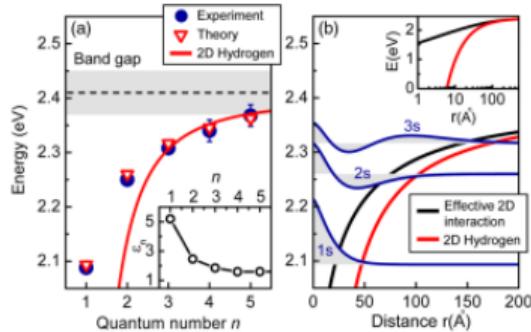
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- Dielectric "constant"  
 $\epsilon = \lim_{q \rightarrow 0} \lim_{\omega \rightarrow 0} \epsilon(q, \omega) = 1$
- $\epsilon(q)$  highly dependent on  $q$   
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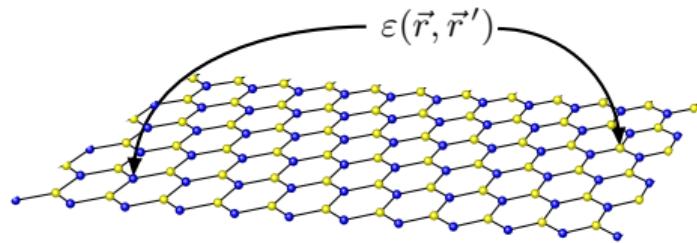
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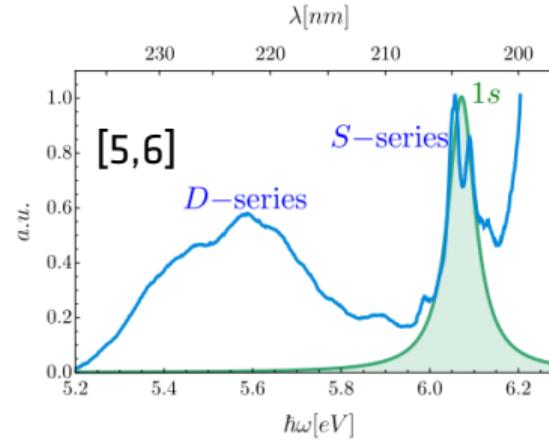
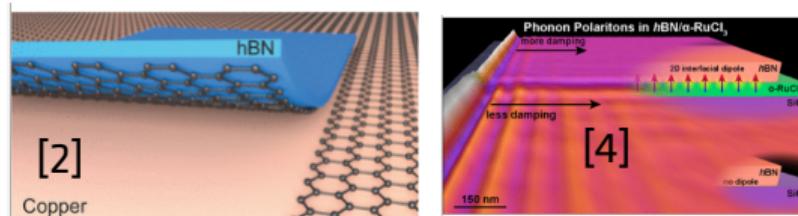
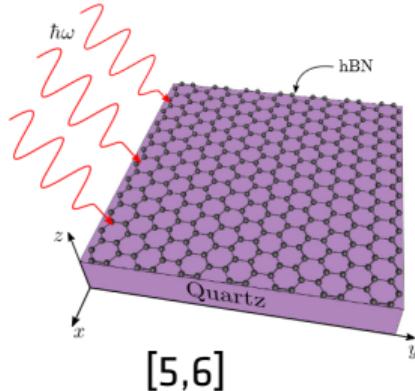


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Alexey Chernikov et al., Phys. Rev. Lett. 113, 076802 (2014)

# 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)  
[2] L. Banszerus et al., *Nano Lett.* 16, 1387-1391 (2016)  
[3] J. D. Caldwell et al., *Nat. Rev. Mat.* 4, 5221 (2019)

- [4] D. Rizzo et al., *Nano Lett.* 23, 18, 8426-8435 (2023)  
[5] J. Henriques et al., *J. Phys.: Cond. Matter* 32, 025304 (2019)  
[6] C. Elias et al., *Nat. Comm.* 10, 2639 (2019)

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$$\varepsilon_{\text{RK}}(q) = 1 + r_0 q$$

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- Computationally heavy
- Technically involved/Less accessible
- Systems are always 3D

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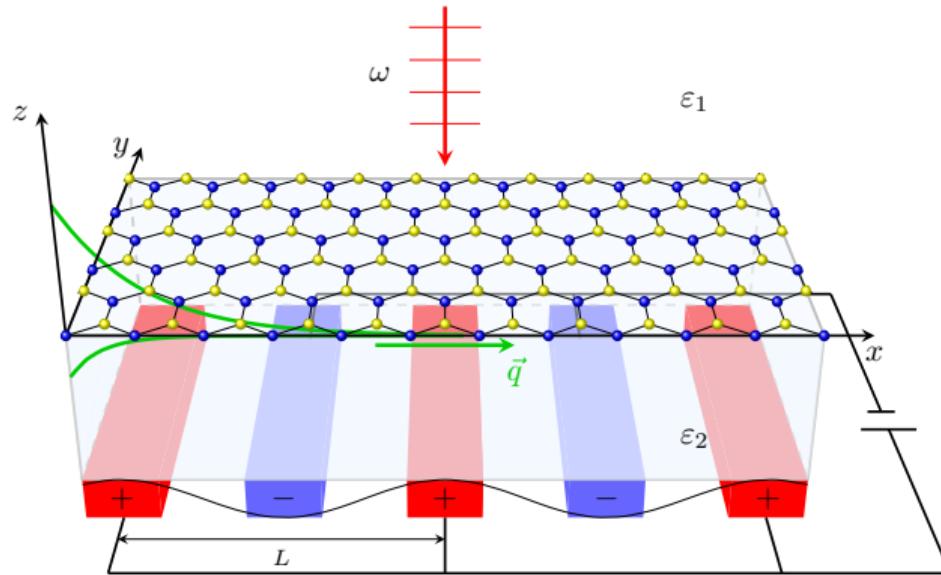
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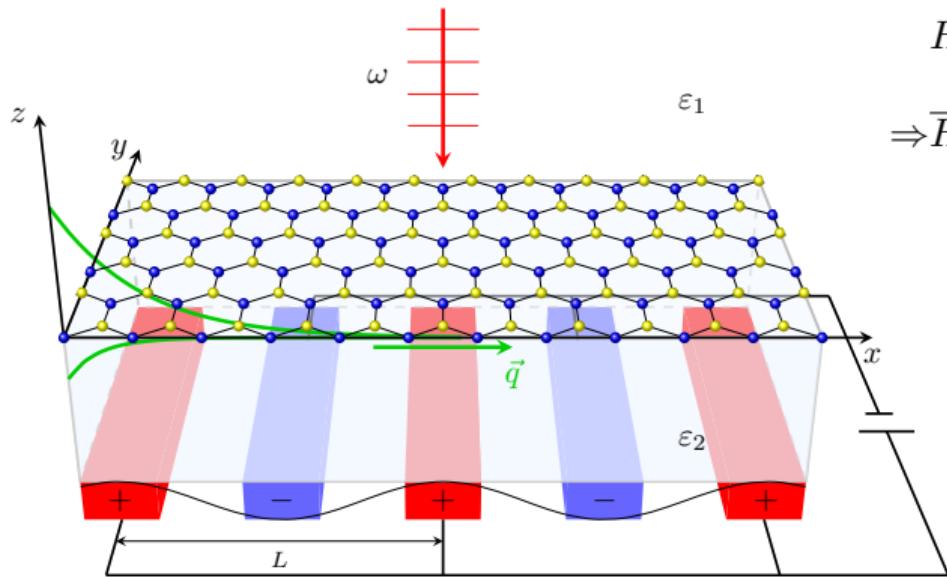
# hBN under an external periodic potential



“Tunable Exciton Polaritons in Band-Gap Engineered hBN”

P. Ninhos, C. Tserkezis, N. A. Mortensen, N. M. R. Peres, ACS Nano 18, 31, (2024)

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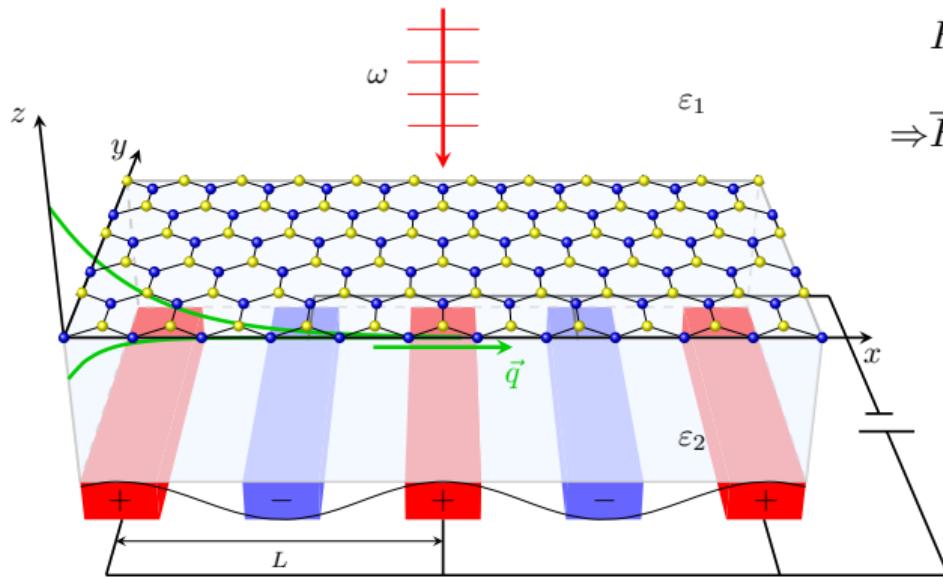


$$H_0 = H_{\text{Dirac}} + V_0 \cos(G_0 x), \quad G_0 = \frac{2\pi}{L} \hat{\mathbf{x}}$$

$$\Rightarrow \overline{H}_0 = \hbar v_F [q_x \sigma_x + J_0(\beta) q_y \sigma_y] - \frac{E_g}{2} J_0(\beta) \sigma_z$$

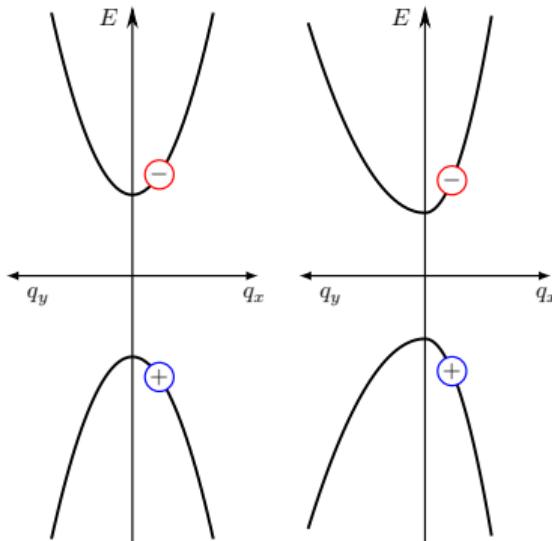
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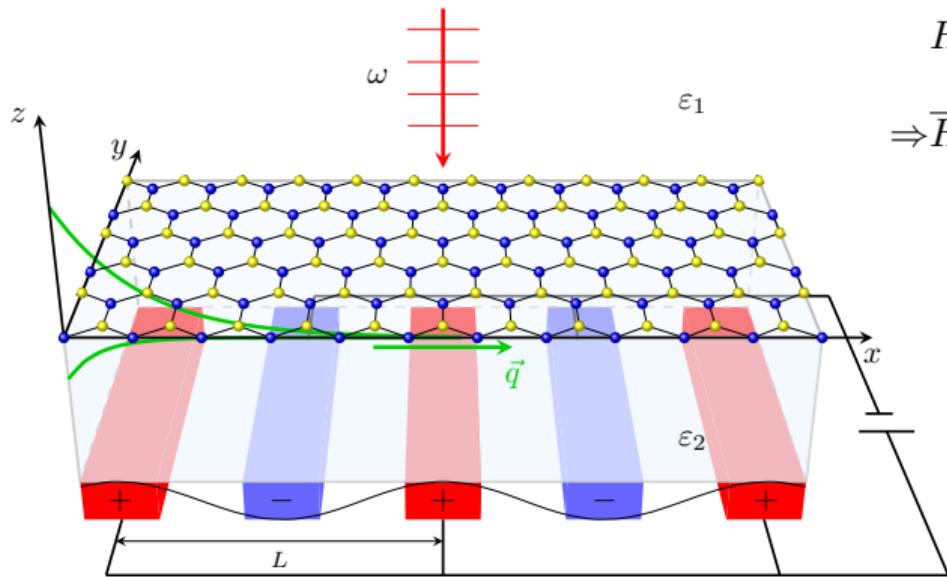
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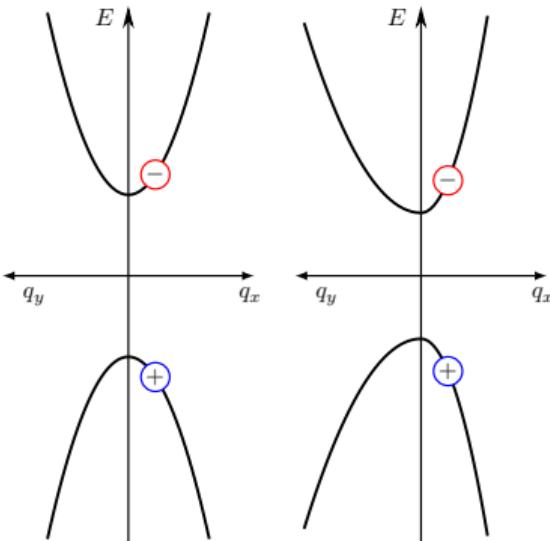
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$$\beta = V_0 L / (\pi \hbar v_F)$$

# Wannier equation and variational method

Wannier equation

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

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$$\rho_\nu = \sqrt{a_\nu x^2 + b_\nu y^2}$$

$$\nu = 1s, 2x, 2y, 2s$$

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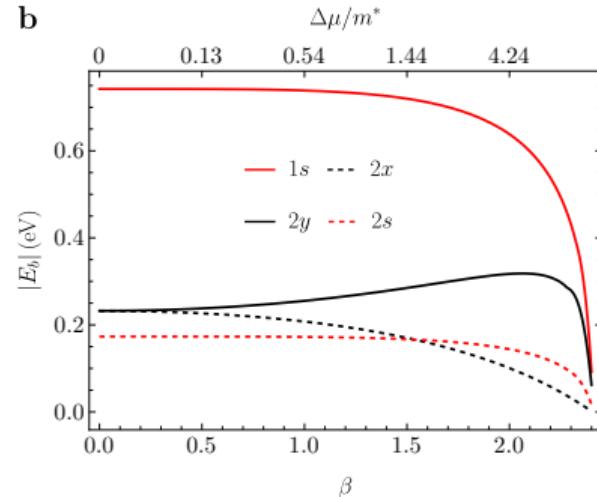
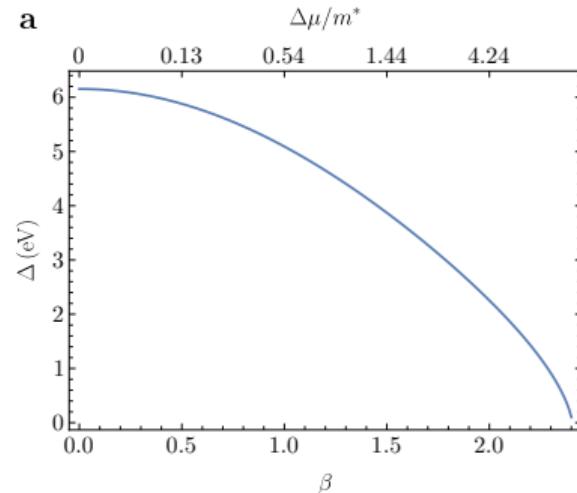
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# Optical Conductivity

According to T. 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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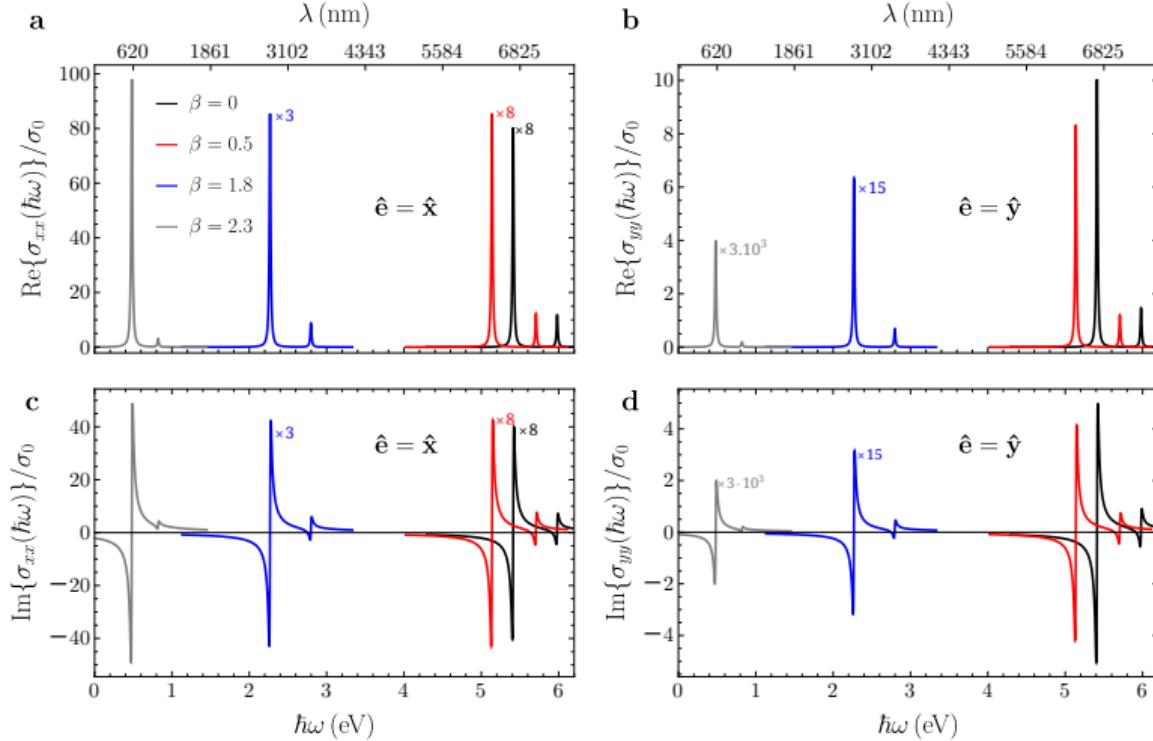
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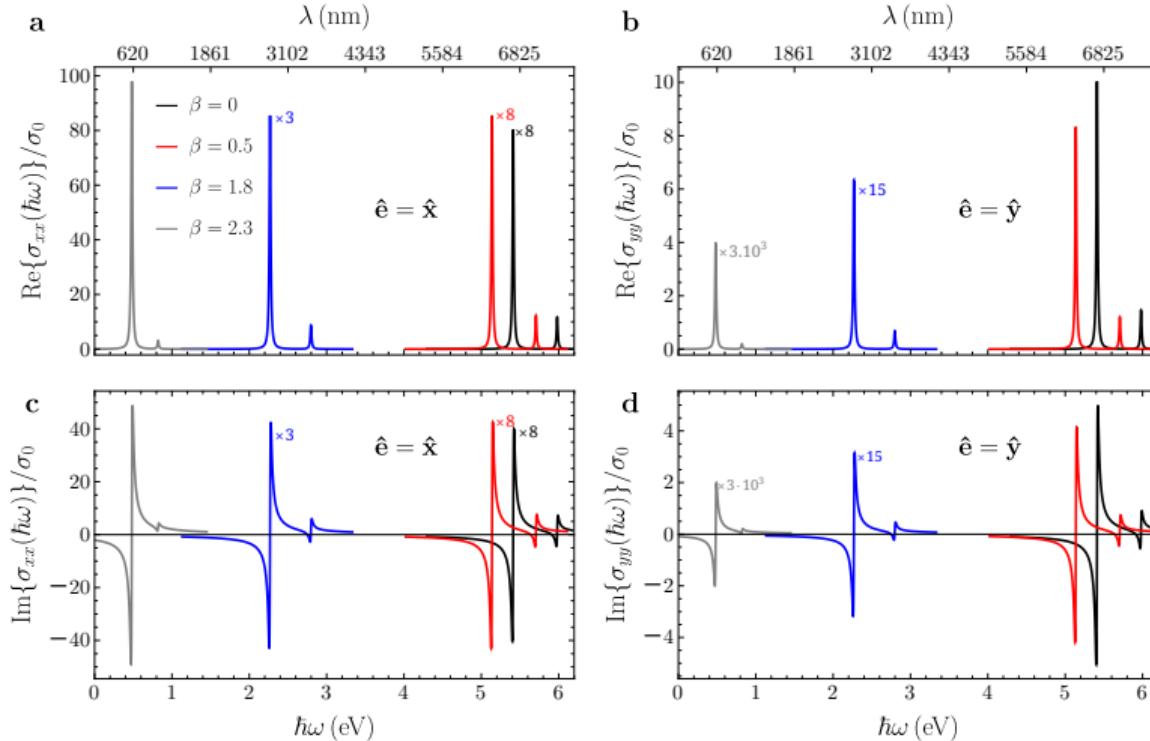
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- Increasing peak intensity
- $\text{Im}\{\sigma\}$  only one zero for  $\beta = 2.3$
- $\hat{\mathbf{e}}_j = \hat{\mathbf{y}}, \sigma_{yy}(\omega)$  is attenuated

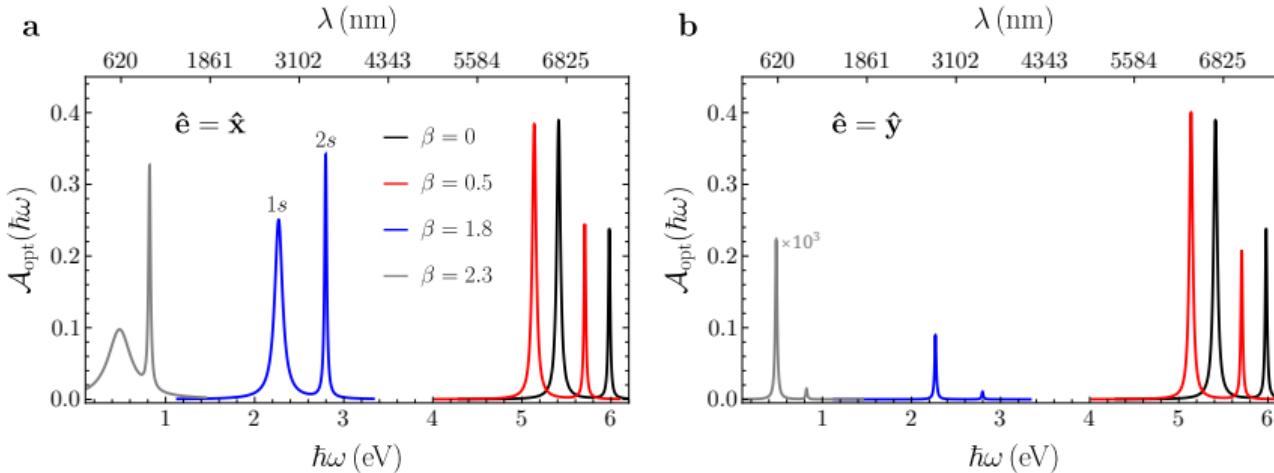
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# Optical absorption

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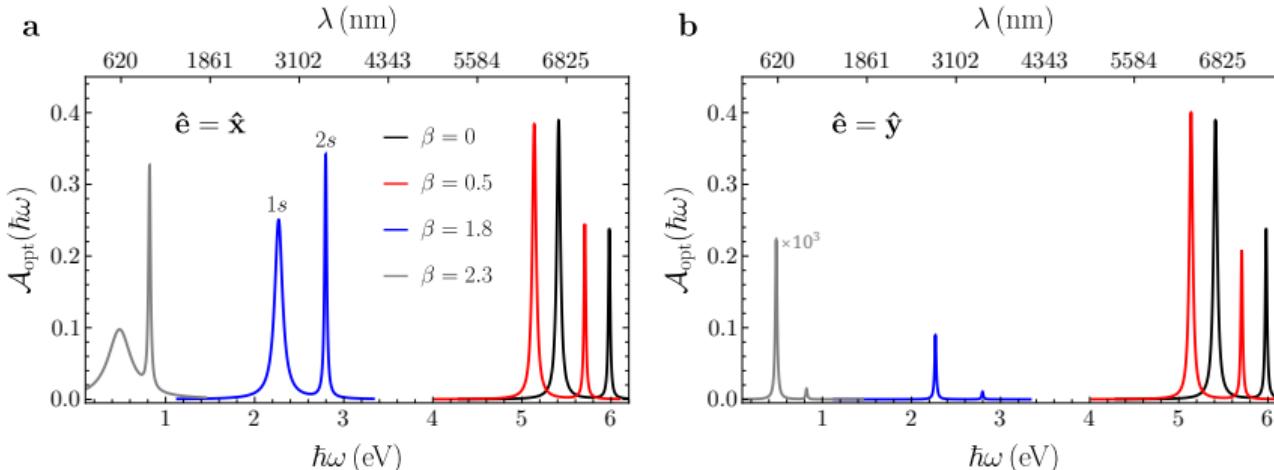
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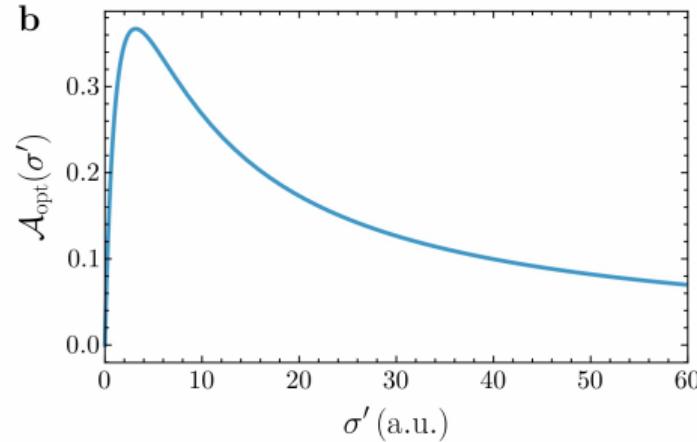
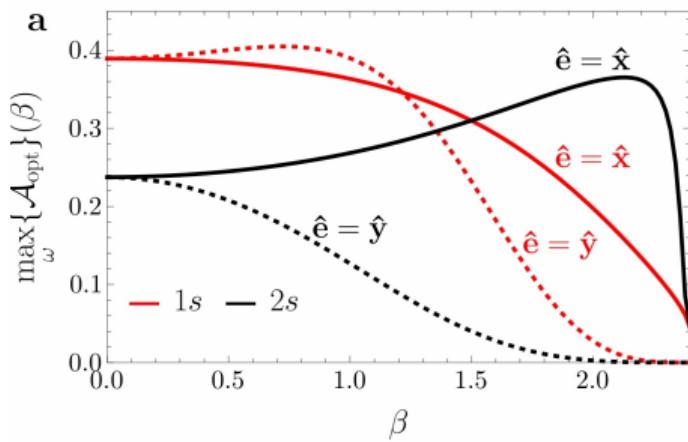
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- Tunable absorption
- Non-monotonic behaviour of the absorption
- Different response for different polarizations
- Red-shift of the resonances
- 2s peak higher than 1s peak
- For  $y$  pol. absorption is suppressed

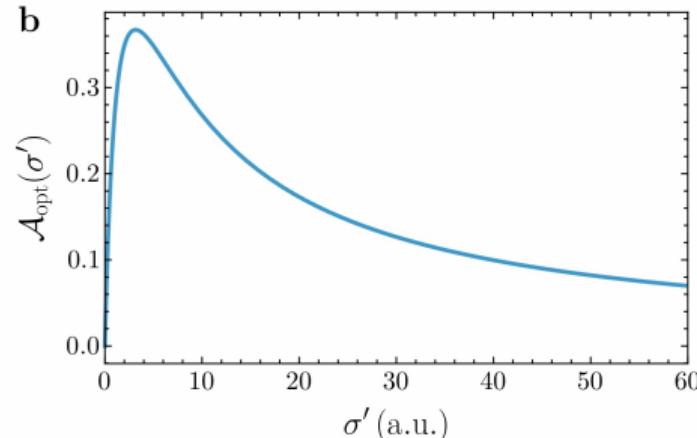
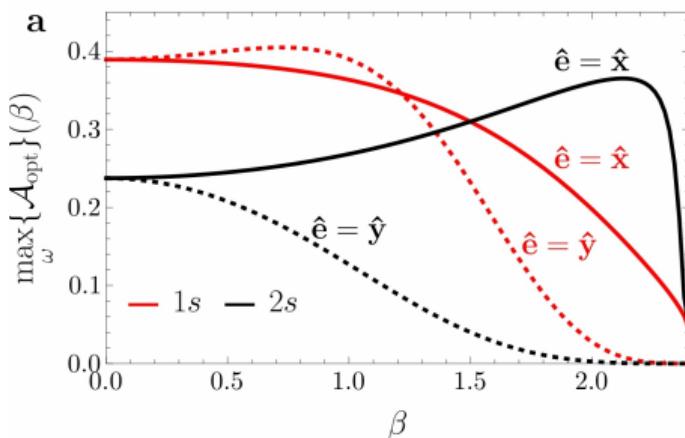
# Absorption peaks

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



# Absorption peaks

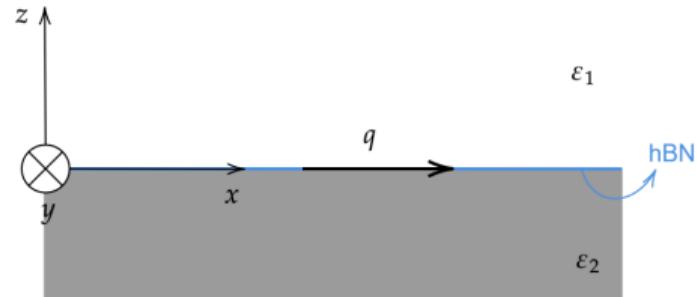
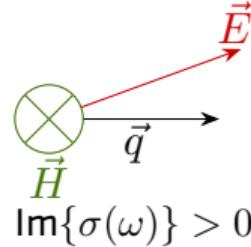
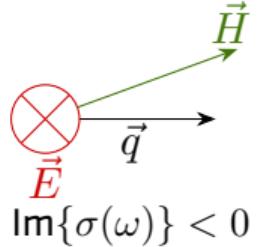
$$\max_{\omega} \mathcal{A}_{\text{opt}} = \frac{4\sqrt{\varepsilon_1}\sigma'}{(\sqrt{\varepsilon_2} + \sqrt{\varepsilon_1} + \sigma')^2}, \omega = E_{\nu}/\hbar, \nu = 1s, 2s$$



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

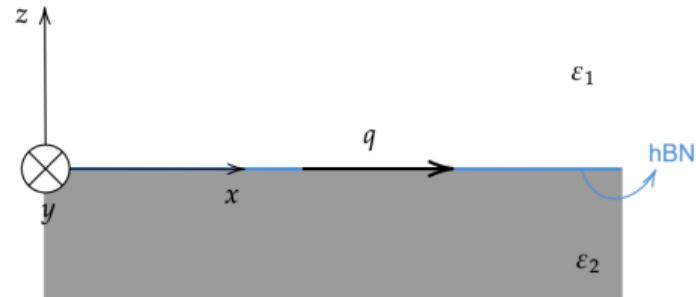
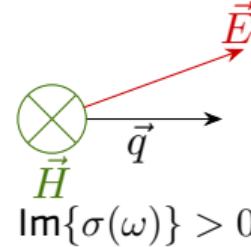
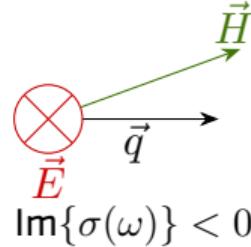
# Exciton-polaritons

Transverse Electric (TE) Transverse Magnetic (TM)



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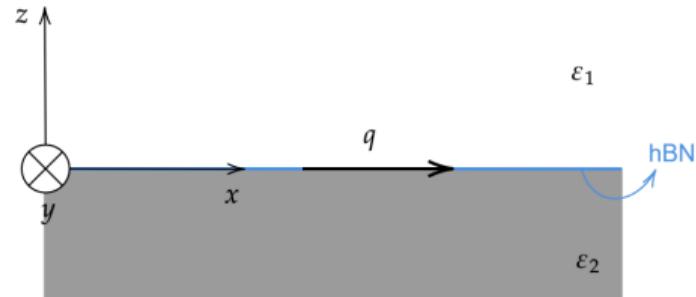
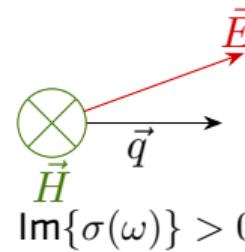
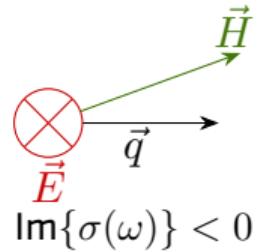
$$\kappa_1 + \kappa_2 - i\omega\mu_0\sigma_{yy}(\omega) = 0$$

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

$$\kappa_j = \sqrt{q^2 - \varepsilon_j(\omega)\frac{\omega^2}{c^2}}, \quad j = 1, 2$$

# Exciton-polaritons

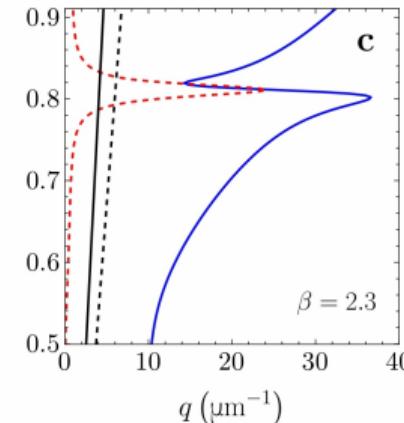
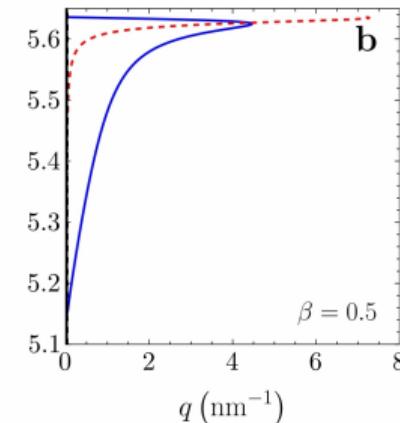
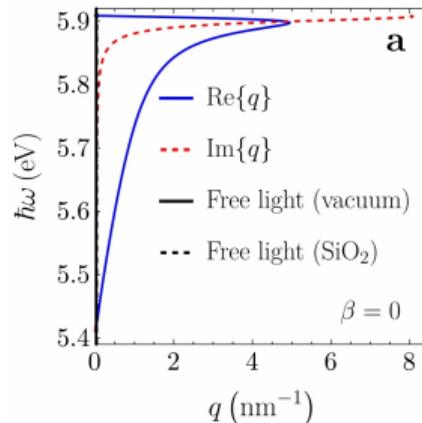
Transverse Electric (TE) Transverse Magnetic (TM)



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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

- 2D Dielectric function
- Dielectric function in the Tight-Binding approximation
- Dielectric function: numerical results
- Excitons
- Quasi-2D approach for screening

4 Conclusions

5 Acknowledgements

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

For an insulator/semiconductor

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

[1] Jack Deslippe et al., “BerkeleyGW: A massively parallel computer package for the calculation of the quasiparticle and optical properties of materials and nanostructures”, Computer Physics Communications 183.6 (2012)

# Macroscopic dielectric function

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

# Macroscopic dielectric function

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

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$$W(\mathbf{q}) = \frac{v_c(\mathbf{q})}{\varepsilon_M(\mathbf{q})}$$

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For a 2D semiconductor/insulator  $\varepsilon_M(\mathbf{q}) = \varepsilon_{2D}(\mathbf{q}) \xrightarrow{q \rightarrow 0} 1 + r_0 q \equiv \varepsilon_{RK}(\mathbf{q})$

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

# Bloch states in the TB approx.

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

$C_{i\alpha}^{n\mathbf{k}}$  → TB coefficients

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$C_{i\alpha}^{n\mathbf{k}}$  → TB coefficients

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

# Polarizability in the TB approximation

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

$$\begin{aligned}\chi_{GG'}^0(\mathbf{q}) &= \frac{2}{\mathcal{A}} \sum_{vc} \sum_{\mathbf{k}\sigma} \frac{\langle c, \mathbf{k} | e^{-i(\mathbf{q}+\mathbf{G}) \cdot \mathbf{r}} | v, \mathbf{k} + \mathbf{q} \rangle \langle v, \mathbf{k} + \mathbf{q} | e^{i(\mathbf{q}+\mathbf{G}') \cdot \mathbf{r}} | c, \mathbf{k} \rangle}{\epsilon_{v\mathbf{k}+\mathbf{q}} - \epsilon_{c\mathbf{k}}} = \\ &= \frac{2}{\mathcal{A}} \sum_{vc} \sum_{\mathbf{k}\sigma} \frac{I_{v\mathbf{k}+\mathbf{q}, c\mathbf{k}}^G \left( I_{v\mathbf{k}+\mathbf{q}, c\mathbf{k}}^{G'} \right)^*}{\epsilon_{v\mathbf{k}+\mathbf{q}} - \epsilon_{c\mathbf{k}}}\end{aligned}$$

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

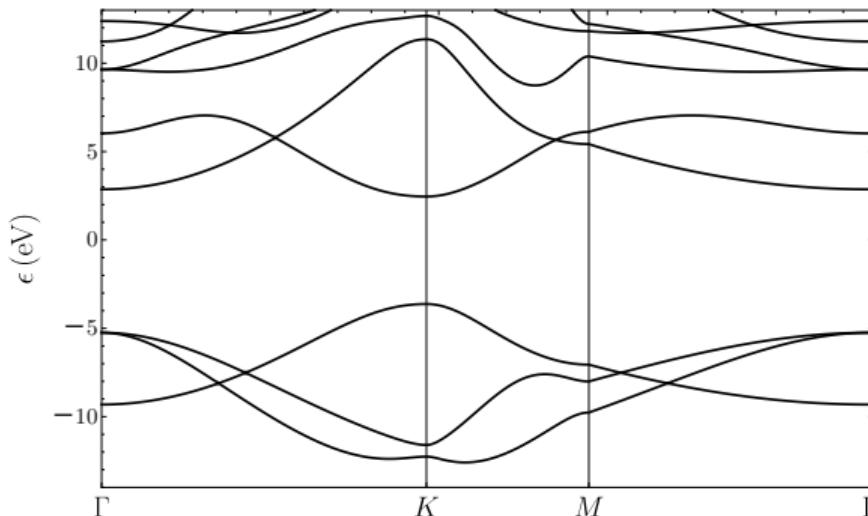
$$\begin{aligned}\Rightarrow I_{n\mathbf{k}, n'\mathbf{k}+\mathbf{q}}^G &\equiv \langle n, \mathbf{k} | e^{-i(\mathbf{q}+\mathbf{G}) \cdot \mathbf{r}} | n', \mathbf{k} + \mathbf{q} \rangle = \int_{\mathcal{A}} d\mathbf{r} \psi_{n, \mathbf{k}}^*(\mathbf{r}) e^{-i(\mathbf{q}+\mathbf{G}) \cdot \mathbf{r}} \psi_{n', \mathbf{k}+\mathbf{q}}(\mathbf{r}) = \\ &= \sum_{i\alpha} (C_{i\alpha}^{n\mathbf{k}})^* C_{i\alpha}^{n'\mathbf{k}+\mathbf{q}} e^{-i(\mathbf{q}+\mathbf{G}) \cdot \mathbf{t}_i}\end{aligned}$$

# Exciton computation scheme with the Xatu code

- ① Diagonalize  $H(\mathbf{k} + \mathbf{q})$  and store all  $\{\epsilon_{n\mathbf{k}+\mathbf{q}}\}, \{\mathbf{C}^{n\mathbf{k}+\mathbf{q}}\}$   $\forall \mathbf{q} \in \text{BZ}, \forall \mathbf{k} \in \text{BZ}', \text{BZ} \neq \text{BZ}'$
- ② Compute dielectric matrix  $\varepsilon_{GG'}(\mathbf{q}) \forall \mathbf{q} \in \text{BZ}$
- ③ Invert  $\varepsilon_{GG'}(\mathbf{q}) \forall \mathbf{q} \in \text{BZ}$
- ④ Compute the exciton

# Example: Monolayer hBN

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

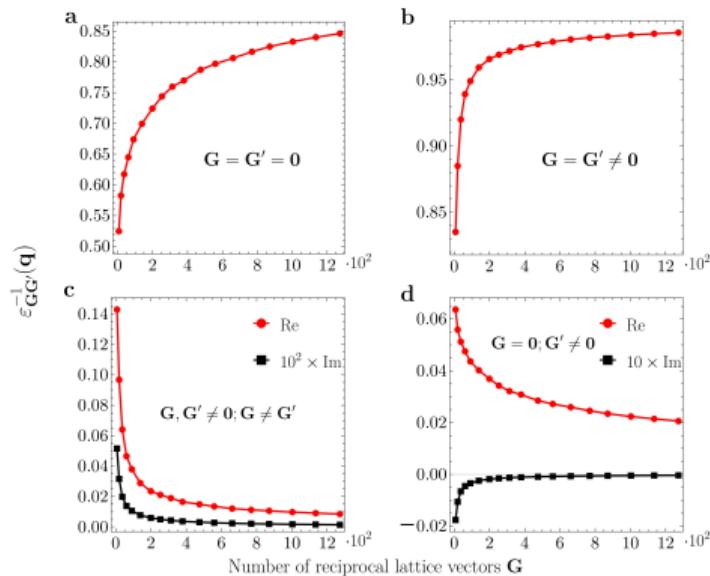


**Figure:** Band structure of monolayer hBN

- [1] A Erba et al., Journal of Chemical Theory and Computation 13.10 (2017)

# Convergence of the inverse dielectric function

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



**Figure:** Convergence of the inverse dielectric matrix. Selection of inverse dielectric function matrix elements  $\varepsilon_{GG'}^{-1}(q)$  computed at a point  $q \neq 0$  in the BZ for hBN. We display the head element in panel **a**, a diagonal body element in panel **b**, an off-diagonal body element in panel **c**, and a wing element in panel **d**. The cutoff  $G_c$  increases by  $3 \text{ \AA}^{-1}$  for each point, from  $G_c = 3 \text{ \AA}^{-1}$  up to  $G_c = 54 \text{ \AA}^{-1}$ .

# Macroscopic dielectric function: results

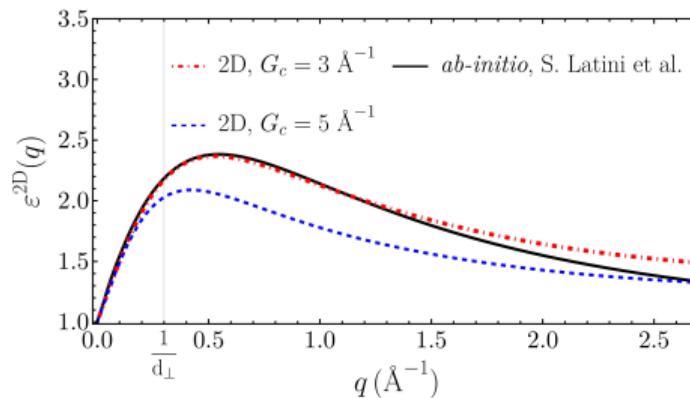
Defined as

$$\varepsilon^{2D}(\mathbf{q}) \equiv \frac{1}{\varepsilon_{00}^{-1}(\mathbf{q})}$$

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**Figure:** The black curve was obtained by Simone Latini, Thomas Olsen and Kristian Thygesen in Phys. Rev. B 92 (24 2015-12) through *ab initio* methods, applying a cutoff of 150 eV for the reciprocal lattice vectors. Therein, the band structure of hBN was obtained through DFT calculations within LDA. The dielectric function was calculated as a post-processing step. We computed the dielectric function along the symmetry line  $\Gamma - K$ . A vertical line indicating  $qd_\perp = 1$  is included, with  $d_\perp = 3.33 \text{\AA}$ .

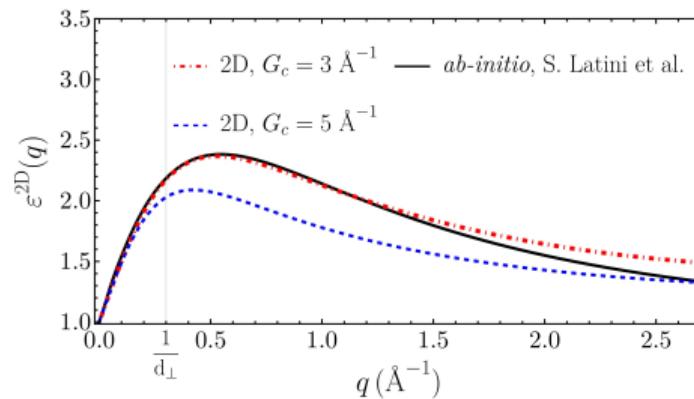
# Macroscopic dielectric function: results

Defined as

$$\varepsilon^{2D}(\mathbf{q}) \equiv \frac{1}{\varepsilon_{00}^{-1}(\mathbf{q})}$$

We recover:

- Rytova-Keldysh model
- $\varepsilon^{2D}(\mathbf{0}) = 1$
- $\varepsilon^{2D}(\mathbf{q}) \rightarrow 1$  w/  $q \rightarrow \infty$



**Figure:** The black curve was obtained by Simone Latini, Thomas Olsen and Kristian Thygesen in Phys. Rev. B 92 (24 2015-12) through *ab initio* methods, applying a cutoff of 150 eV for the reciprocal lattice vectors. Therein, the band structure of hBN was obtained through DFT calculations within LDA. The dielectric function was calculated as a post-processing step. We computed the dielectric function along the symmetry line  $\Gamma - K$ . A vertical line indicating  $qd_{\perp} = 1$  is included, with  $d_{\perp} = 3.33 \text{ \AA}$ .

# 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*

- ①  $\varepsilon_{GG'}(\mathbf{q}) = \delta_{GG'} - \frac{e^2}{|\mathbf{q} + \mathbf{G}|^2 \varepsilon_0} \chi_{GG'}^0(\mathbf{q})$  w/  
 $\langle n, \mathbf{k} | e^{-i(\mathbf{q} + \mathbf{G}) \cdot \mathbf{r}} | n', \mathbf{k}' \rangle$  via FFT
- ② invert  $\varepsilon_{GG'}(\mathbf{q})$
- ③  $\varepsilon_{00}^{-1}(\mathbf{q}, z, z') = \frac{1}{L_\perp} \sum_{G_z, G'_z} e^{iG_z z} \varepsilon_{G_z \hat{z} G'_z \hat{z}}^{-1}(\mathbf{q}) e^{-iG'_z z'}$
- ④  $\varepsilon^{2D}(\mathbf{q}) = 1 / \langle \varepsilon_{00}^{-1}(\mathbf{q}, z, z') \rangle$

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

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

# Excitons with the Xatu code

Bethe-Salpeter Equation (BSE)

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

In the interaction kernel  $K \equiv -(D - X)$ , the direct  $D$  and exchange  $X$  interaction terms read

$$\begin{aligned} D_{vc,v'c'}(\mathbf{k}, \mathbf{k}', \mathbf{Q}) &= \int d\mathbf{r} \int d\mathbf{r}' \psi_{c,\mathbf{k}+\mathbf{Q}}^*(\mathbf{r}) \psi_{v',\mathbf{k}'}^*(\mathbf{r}') W(\mathbf{r}, \mathbf{r}') \psi_{c',\mathbf{k}'+\mathbf{Q}}(\mathbf{r}) \psi_{v,\mathbf{k}}(\mathbf{r}') = \\ &= \frac{1}{\mathcal{A}} \sum_{G,G'} \left( I_{c'\mathbf{k}'+\mathbf{Q}, c\mathbf{k}+\mathbf{Q}}^{\mathbf{G}} \right)^* W_{GG'}(\mathbf{k} - \mathbf{k}') I_{v'\mathbf{k}', v\mathbf{k}}^{\mathbf{G}'}, \end{aligned}$$

and (albeit in *ab initio*  $X$  uses the bare potential  $v_c$ )

$$X_{vc,v'c'}(\mathbf{k}, \mathbf{k}', \mathbf{Q}) = \int_{\mathcal{A}} d\mathbf{r} \int_{\mathcal{A}} d\mathbf{r}' \psi_{c,\mathbf{k}+\mathbf{Q}}^*(\mathbf{r}) \psi_{v',\mathbf{k}'}^*(\mathbf{r}') W(\mathbf{r}, \mathbf{r}') \psi_{v,\mathbf{k}}(\mathbf{r}) \psi_{c',\mathbf{k}'+\mathbf{Q}}(\mathbf{r}') \rightarrow 0$$

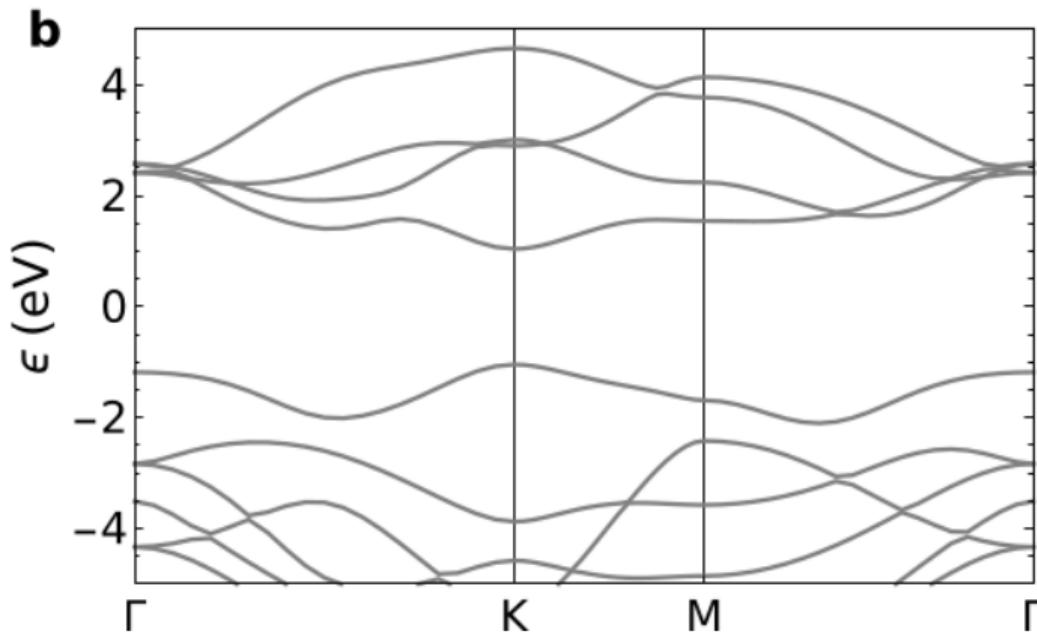
# Excitons in hBN: numerical results

**Table:** This table examines the convergence of the excitonic ground state binding energy with the cutoff for the dielectric matrix,  $G_c^\varepsilon$ , 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

		$G_c^\varepsilon$					
		0	3	5.1	6	8	9
$G_c^X$	0	X	4.14935	5.5566	5.75416	6.011076	-
	3	X	2.503138	4.380231	3.803146	3.811565	4.326392
	5.1	X	X	2.797365	2.99418	3.888089	4.630105
	6	X	X	X	2.83405	3.492424	4.330678
	8	X	X	X	X	2.900768	5.811998
	9	X	X	X	X	X	3.018396

Cell with – means that the output result does not make physical sense

# Monolayer MoS<sub>2</sub> band structure



**Figure:** Band structure of monolayer MoS<sub>2</sub> using CRYSTAL

# Excitons in MoS<sub>2</sub>: numerical results

**Table:** This table examines the convergence of the excitonic ground state binding energy with the cutoff for the dielectric matrix,  $G_c^\varepsilon$ , 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	X	0.979507	1.567935	1.401440	1.951914	-
	3	X	0.756373	1.619208	1.785953	-	-
	4	X	X	0.774599	1.105537	-	-
	5	X	X	X	0.778244	-	-
	7	X	X	X	X	0.792309	1.300835
	8	X	X	X	X	X	0.799489

Cell with - means that the output result does not make physical sense

At least apparent numerical convergence

# The quasi-2D approach for screening

Introducing the bare Coulomb potential in the mixed  $(\mathbf{q}, z)$ -representation

$$v_c(\mathbf{q}, z - z') = \frac{e}{2\epsilon_0 q} e^{-q|z-z'|}, \quad (1)$$

Within a quasi-2D (Q2D) framework, with the dielectric function in the mixed representation as

$$\varepsilon_{GG'}(\mathbf{q}, z, z') = \delta_{GG'} \delta(z - z') - \frac{e}{2\epsilon_0 |\mathbf{q} + \mathbf{G}|} \int_{-\infty}^{\infty} dz'' e^{-|\mathbf{q} + \mathbf{G}| |z - z''|} \chi_{GG'}^0(\mathbf{q}, z'', z') \quad (2)$$

and with the  $(\mathbf{q}, z)$ -resolved polarizability

$$\chi_{GG'}^0(\mathbf{q}, z, z') = \int_{\mathcal{A}} d\mathbf{r}_{||} \int_{\mathcal{A}} d\mathbf{r}'_{||} e^{-i(\mathbf{q} + \mathbf{G}) \cdot \mathbf{r}} \chi^0(\mathbf{r}, \mathbf{r}') e^{i(\mathbf{q}' + \mathbf{G}') \cdot \mathbf{r}'} \quad (3)$$

# The Q2D dielectric function

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

$$\bar{\varepsilon}_{GG'}(\mathbf{q}) \equiv \frac{1}{d_{\perp}} \int_{-d_{\perp}/2}^{d_{\perp}/2} \int_{-d_{\perp}/2}^{d_{\perp}/2} \varepsilon_{GG'}(\mathbf{q}, z, z') dz dz' \quad (4)$$

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$$\varepsilon_{GG'}(\mathbf{q}) = \lim_{d_{\perp} \rightarrow 0} \frac{1}{d_{\perp}} \int_{-d_{\perp}/2}^{d_{\perp}/2} \int_{-d_{\perp}/2}^{d_{\perp}/2} \varepsilon_{GG'}(\mathbf{q}, z, z') dz dz' \quad (5)$$

# The Q2D dielectric function

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

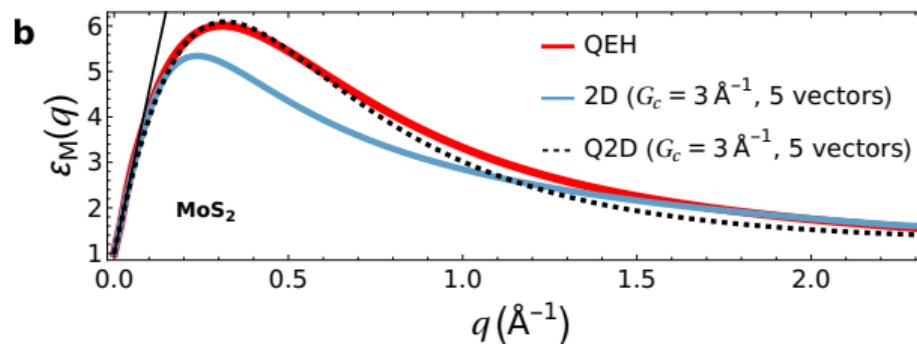
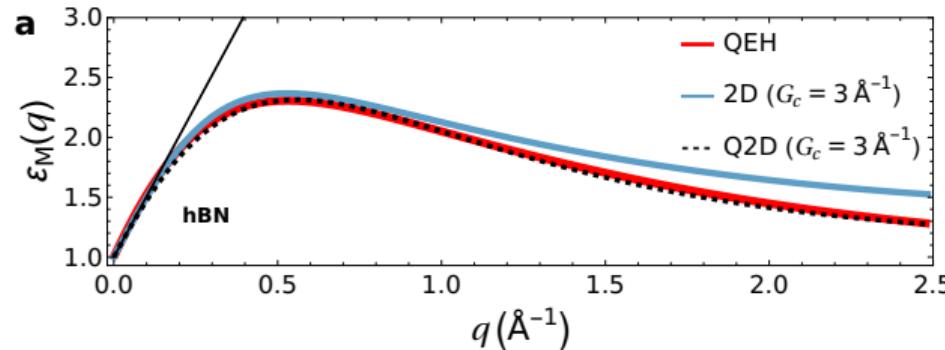
$$\bar{\varepsilon}_{GG'}(\mathbf{q}) \equiv \frac{1}{d_{\perp}} \int_{-d_{\perp}/2}^{d_{\perp}/2} \int_{-d_{\perp}/2}^{d_{\perp}/2} \varepsilon_{GG'}(\mathbf{q}, z, z') dz dz' \quad (4)$$

$$\varepsilon_{GG'}(\mathbf{q}) = \lim_{d_{\perp} \rightarrow 0} \frac{1}{d_{\perp}} \int_{-d_{\perp}/2}^{d_{\perp}/2} \int_{-d_{\perp}/2}^{d_{\perp}/2} \varepsilon_{GG'}(\mathbf{q}, z, z') dz dz' \quad (5)$$

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

# The Q2D dielectric function: numerical results

For hBN and MoS<sub>2</sub> CRYSTAL models



# 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
- 4 Conclusions
- 5 Acknowledgements

# Summary

- hBN as a promising material for UV polaritonics
- 1D superlattice with tunable periodicity: from deep-UV to the visible
- Tunable absorption
- Different response for different polarizations
- Confined EM modes with tunable frequency
- the point-like (and orthogonal) orbital approximation does not set us back
- $v_c(q) \sim 1/q$  brings numerical and practical benefits; Also, no need to truncate  $v_c$
- 2D, Q2D and *ab-initio* approaches agree in the very low  $q$  limit, or when  $qd_{\perp} \lesssim 1$
- size of  $\varepsilon_{GG'}(q)$  scales much slower than 3D
- inverting the dielectric matrix poses no hindrance in the processing time
- direct inversion of  $\varepsilon_{GG'}(q)$  gives  $\varepsilon^{2D}(q)$ ; Our  $r_0$  agrees well with the literature
- exciton binding energy seems to converge; numerical coincidence?

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