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

Pedro António Correia Ninhos

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Secondment Host:
Prof. Juan José Palacios

22-01-2026

Ph.D. Defense

List of Publications

- **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)

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Outline

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Solid Materials

Optical Excitations in Matter

Solid Materials $\left\{ \vphantom{\begin{matrix} a\\a\\a\\a\\a \end{matrix}} \right.$

Optical Excitations in Matter

Solid Materials $\left\{ \begin{array}{l} \text{Metals} \\ \\ \\ \\ \end{array} \right.$

Optical Excitations in Matter

Solid Materials $\begin{cases} \text{Metals} \\ \\ \text{Dielectrics} \end{cases}$

Optical Excitations in Matter

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Solid Materials

Metals

Dielectrics

Optical Excitations in Matter

Solid Materials
- Metals
  - Free charges
- Dielectrics

Optical Excitations in Matter

$$\text{Solid Materials}\begin{cases}\text{Metals} & \begin{cases}\text{Free charges}\\ \text{Conducting}\\ \\ \end{cases}\\ \\ \text{Dielectrics}\end{cases}$$

Optical Excitations in Matter

Solid Materials

- Metals
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- Solid Materials
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  - Bound charges
  - Insulating

Optical Excitations in Matter

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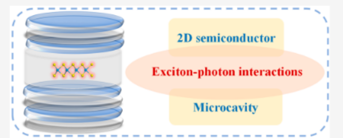
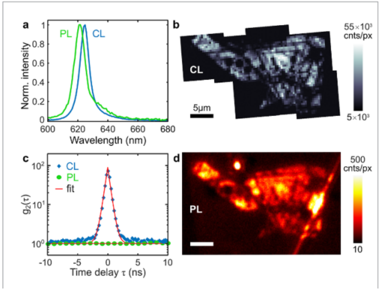
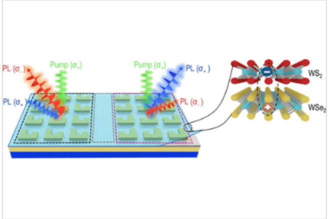
    - Insulating
    - Dipolar excitations (excitons)

Excitons in Photonics

Relevant for:

Light–matter interactions	Quantum Light Sources	Valleytronics
 J. Shang et al. - *ACS Photonics* **10** 7 (2023)	 S. Fiedler et al. - *2D Mater.* **10** 021002 (2023)	 Yi Zhu et al. - *Nano Letters* **25** 21 (2025)

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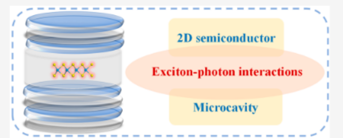

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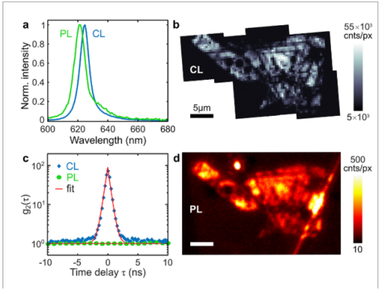

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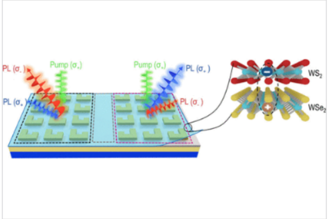

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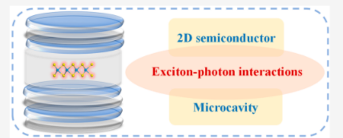

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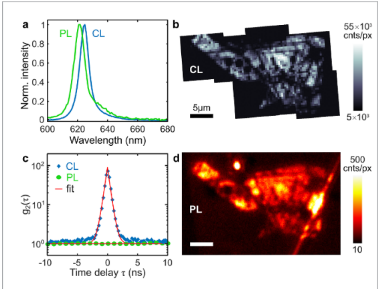

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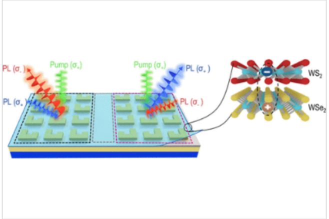

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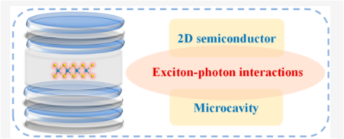

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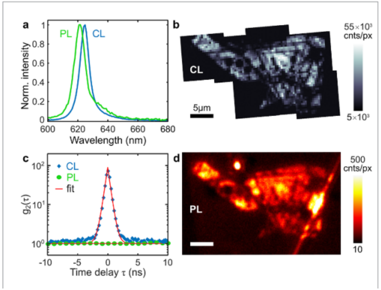

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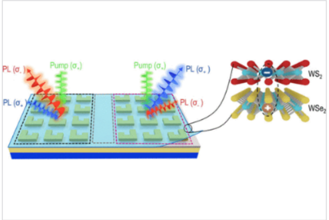

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Excitons in Two-Dimensional Materials

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

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

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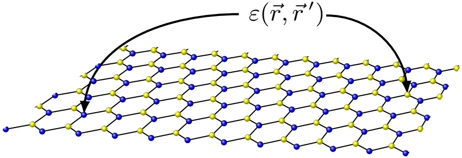

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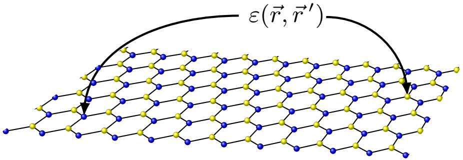

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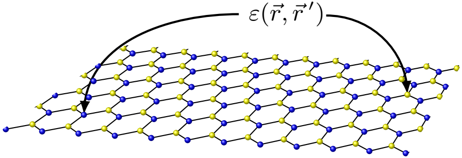

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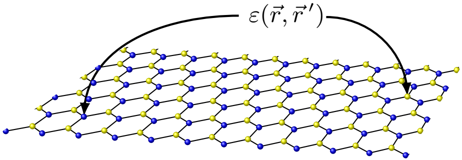

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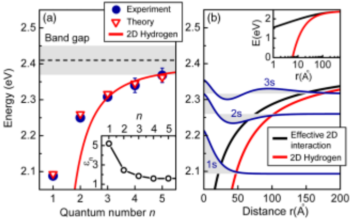

A. Chernikov et al. - *Phys. Rev. Lett.* **113** 076802 (2014)

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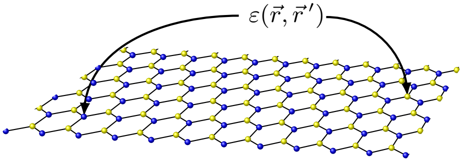

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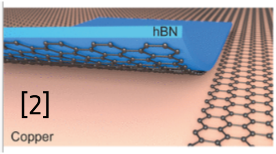

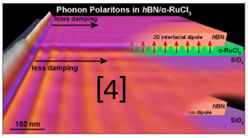

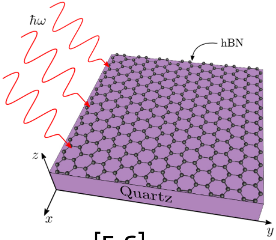

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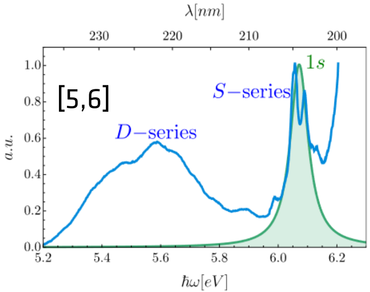

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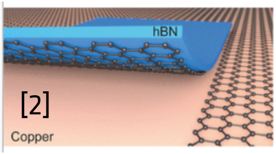

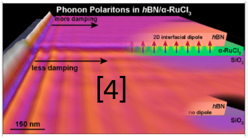

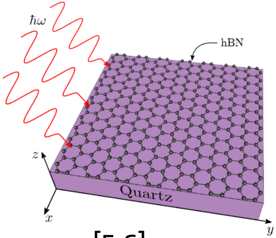

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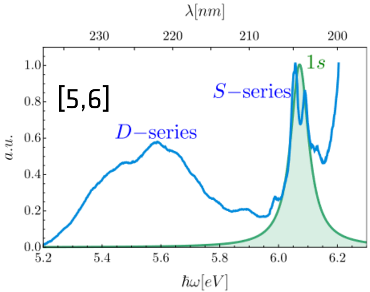

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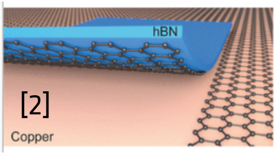

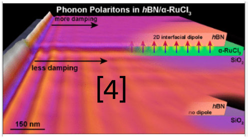

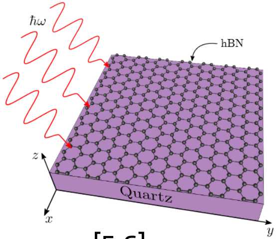

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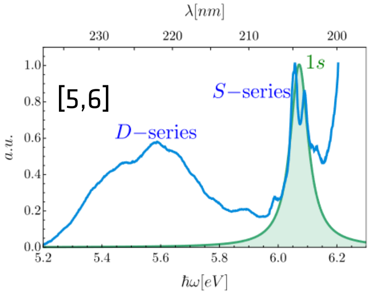

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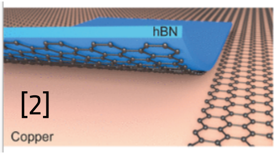

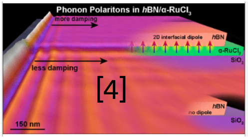

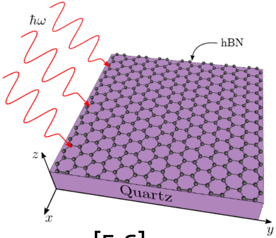

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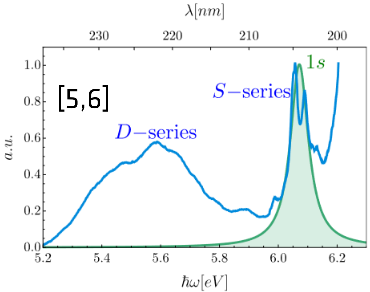

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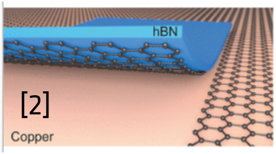

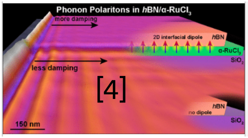

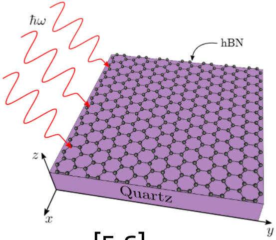

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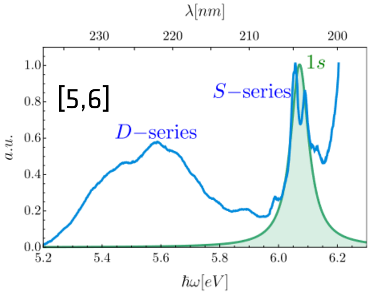

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Motivation

Rytova–Keldysh model

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

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- Intuitive
- Analytical expression

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

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Full numerical *ab initio*

$$\varepsilon_{\boldsymbol{G}\boldsymbol{G}'}(\boldsymbol{q}) = \delta_{\boldsymbol{G}\boldsymbol{G}'} - v_c(\boldsymbol{q} + \boldsymbol{G})\chi^0_{\boldsymbol{G}\boldsymbol{G}'}(\boldsymbol{q})$$

Motivation

Rytova–Keldysh model

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

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

- 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*

$$\varepsilon_{\boldsymbol{G}\boldsymbol{G}'}(\boldsymbol{q}) = \delta_{\boldsymbol{G}\boldsymbol{G}'} - v_c(\boldsymbol{q}+\boldsymbol{G})\chi^0_{\boldsymbol{G}\boldsymbol{G}'}(\boldsymbol{q})$$

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POLIMA

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POLIMA

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Full numerical *ab initio* Can we optimize?

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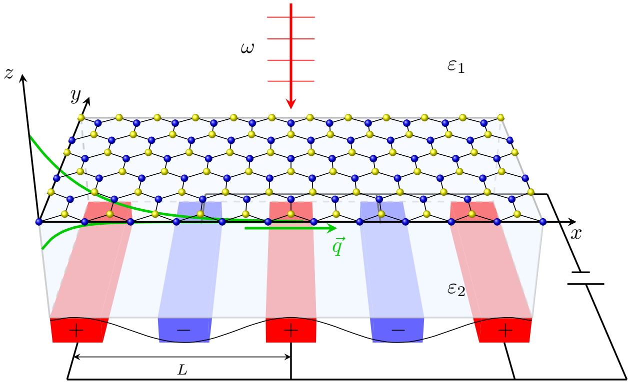
Outline

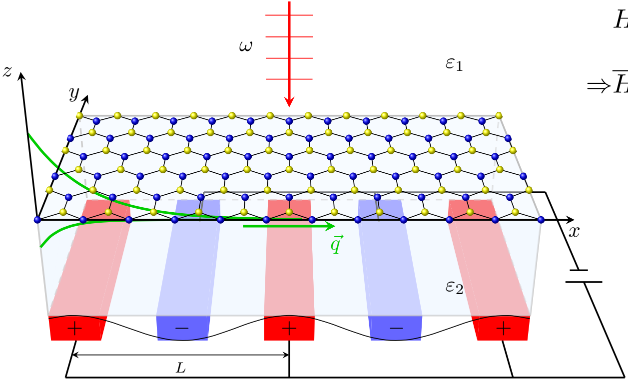
hBN under an external periodic potential

POLIMA



P. Ninhos et. al - *ACS Nano* **18** 31 (2024)

hBN under an external periodic potential



$$H_0 = H_{\mathrm{Dirac}} + V_0 \cos(G_0 x),\ \boldsymbol{G}_0 = \frac{2\pi}{L}\hat{\mathbf{x}}$$

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

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

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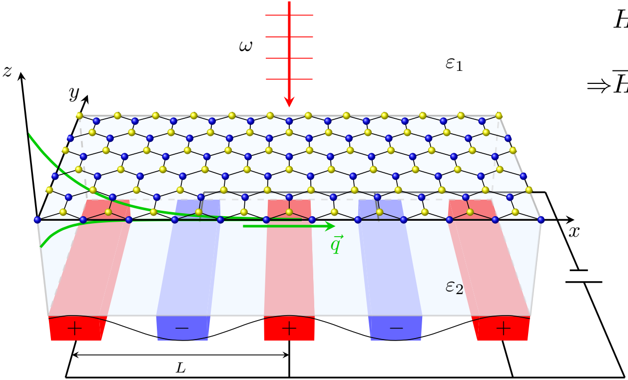

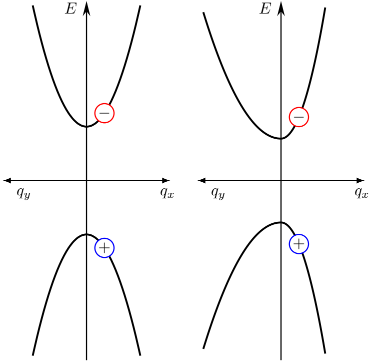

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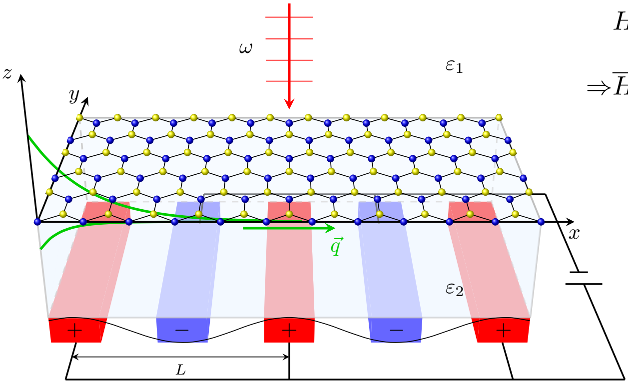

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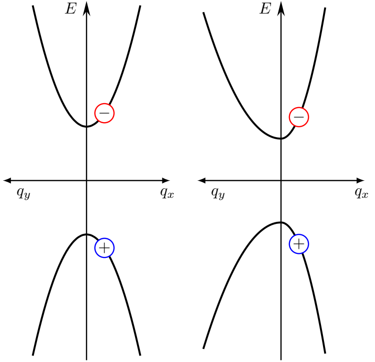

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For $\beta \sim 1$, and $V_0 \sim 40$ meV, $L \sim 40$ nm

Wannier Equation and Variational Method

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Wannier equation [1]

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

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

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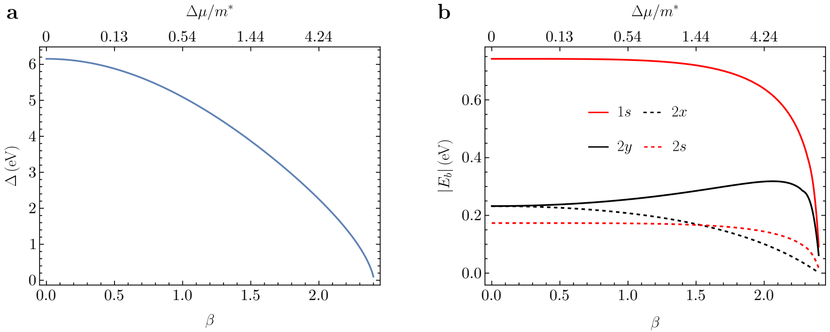

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Optical Conductivity

According to Pedersen [1]

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

[1] T. G. Pedersen - *Phys. Rev. B* **92** 235432 (2015)

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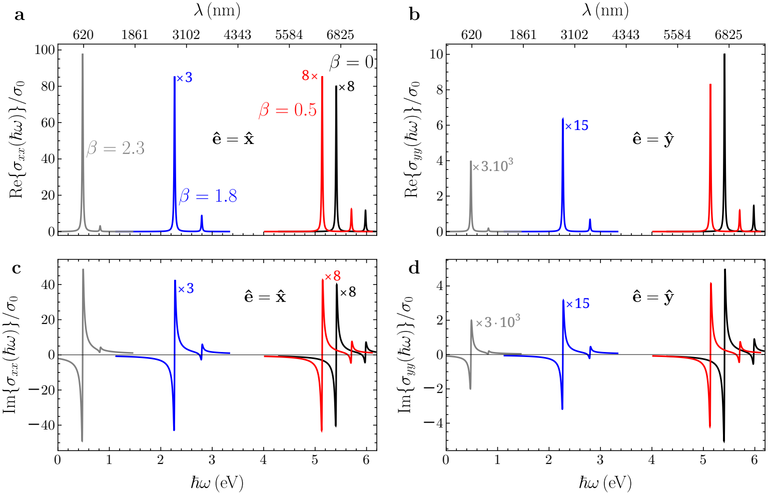

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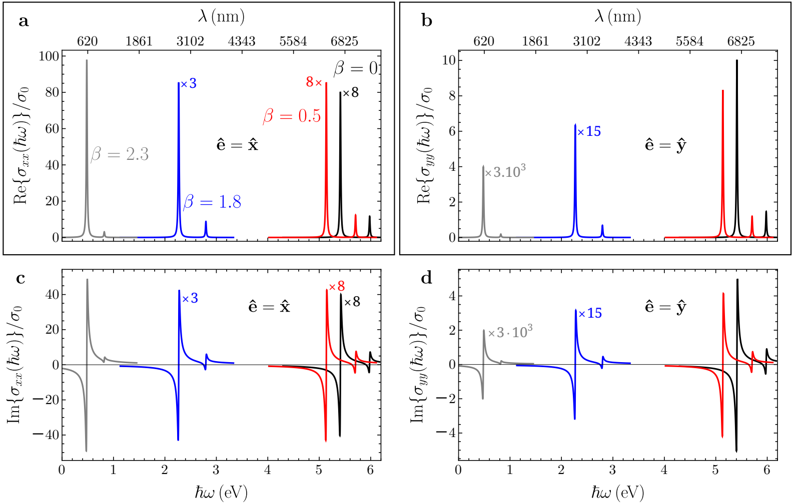

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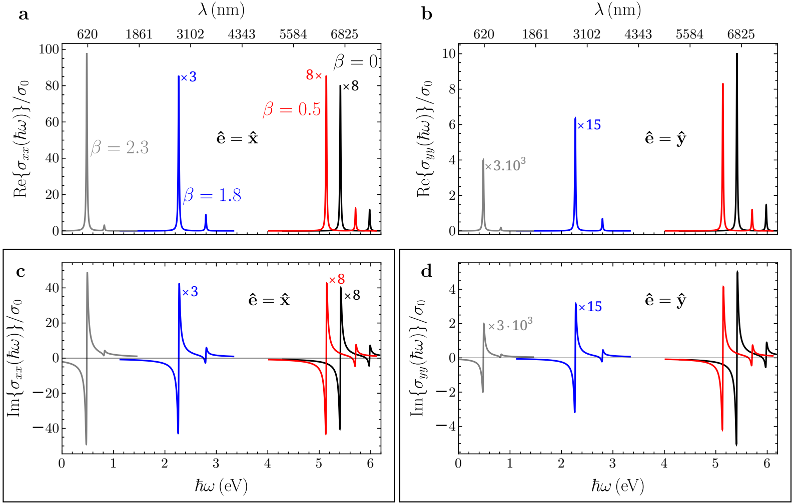

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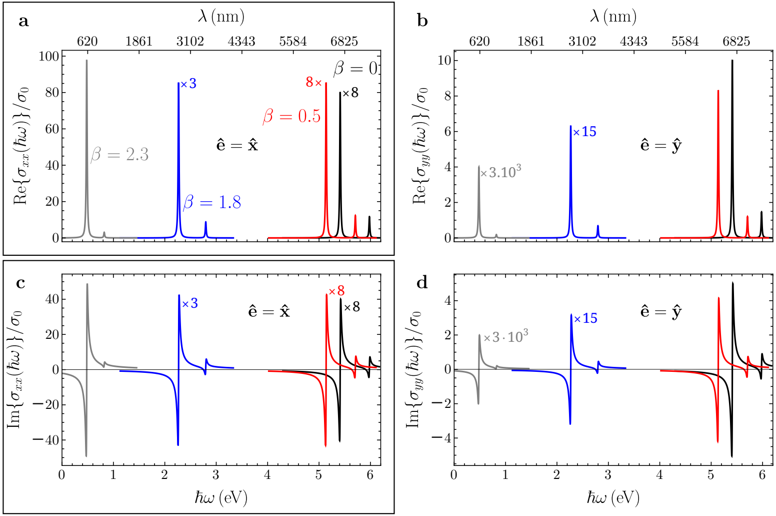

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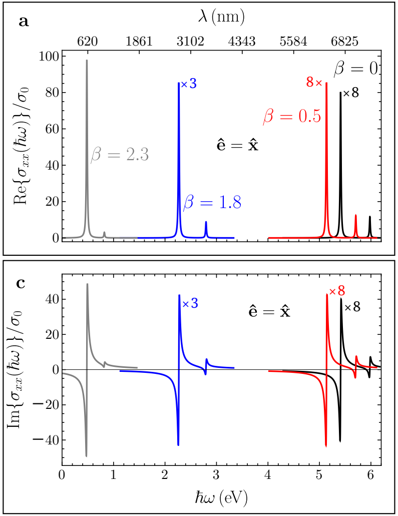

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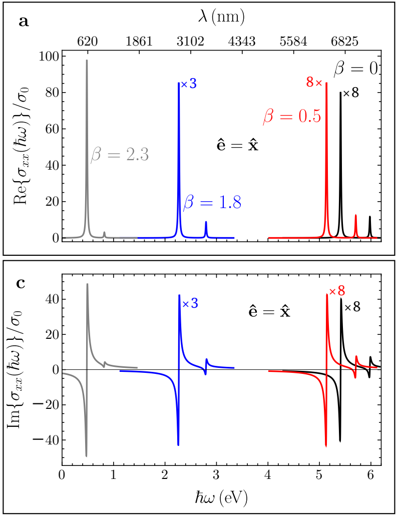

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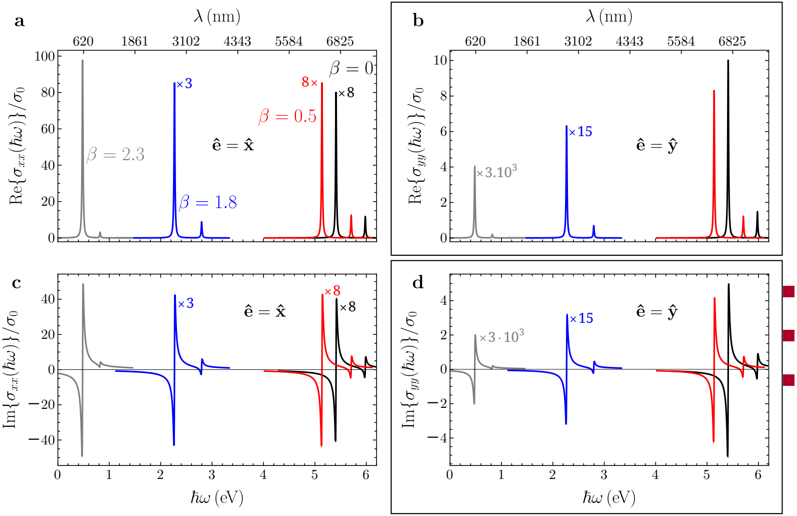
Optical Conductivity

POLIMA



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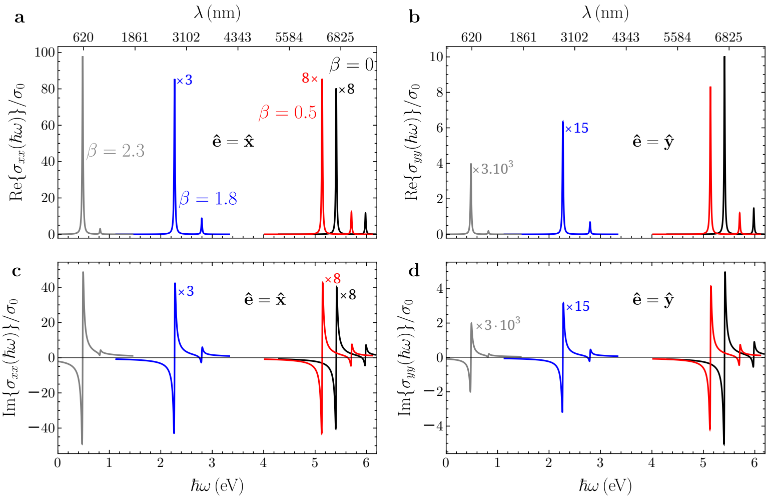

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Optical Absorption

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

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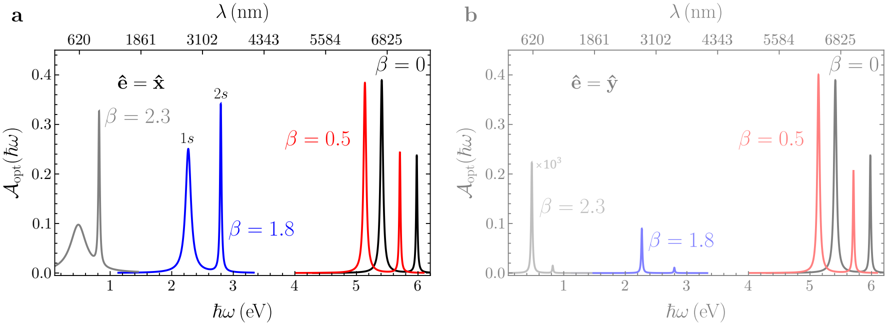

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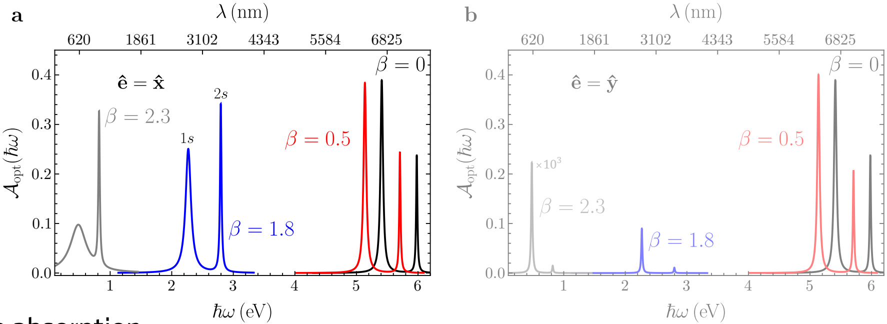

- Tunable absorption
- Non-monotonic behaviour of the absorption
- $2s$ peak higher than $1s$ peak

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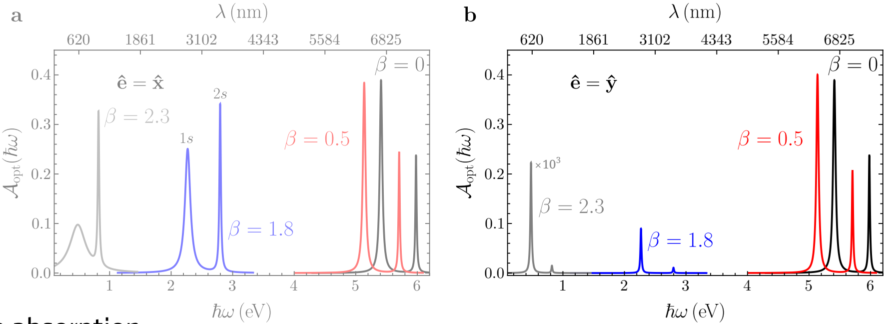

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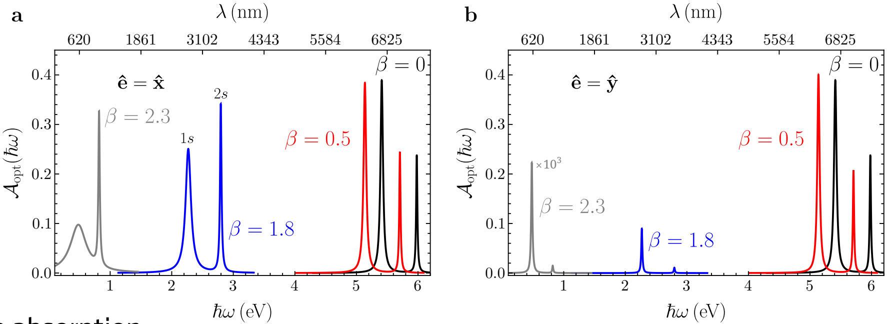

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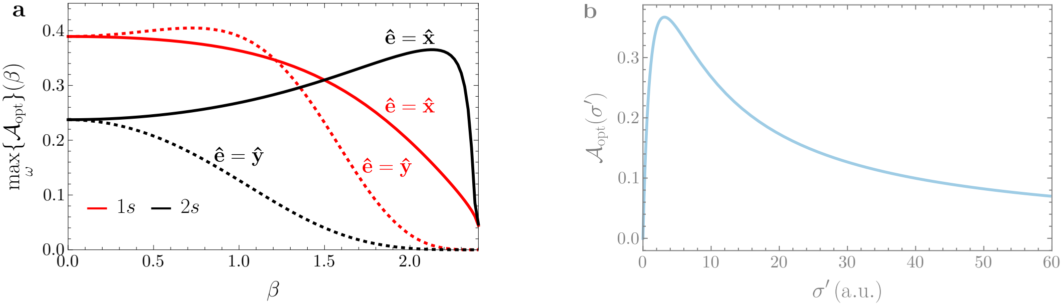
Absorption Peaks

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

Absorption Peaks

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



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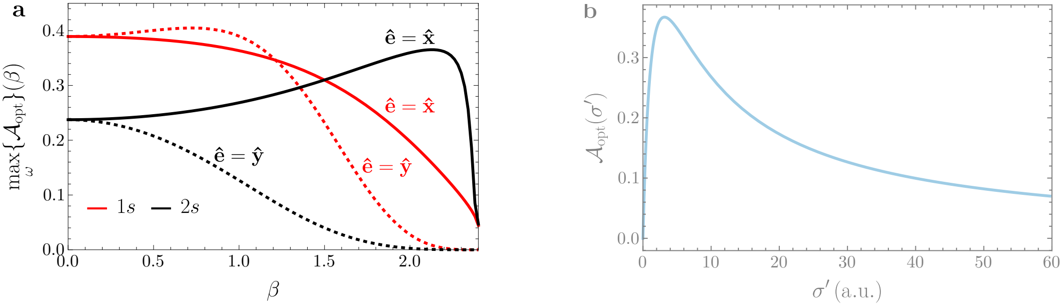

- Tunable absorption
- Different response for different polarizations $\Rightarrow$ grid polarizer

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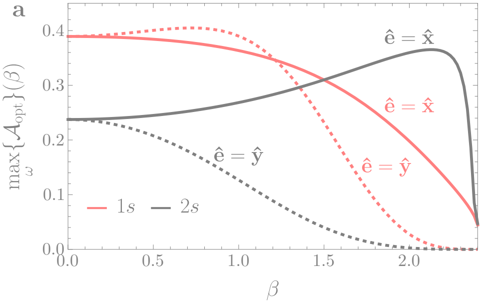

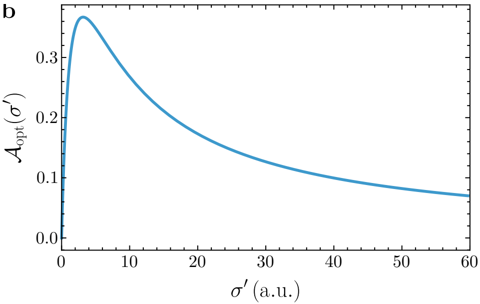

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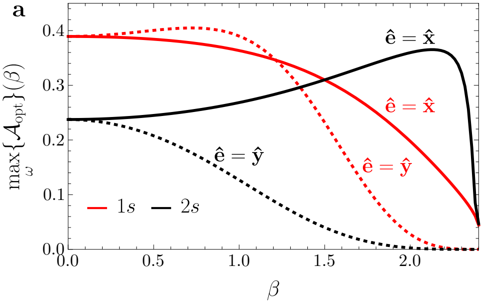

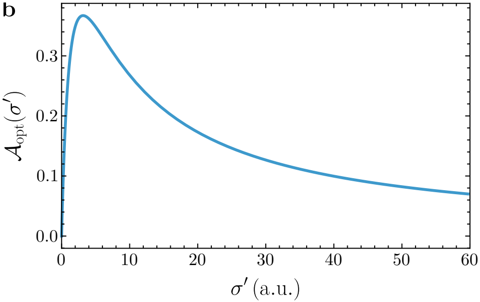

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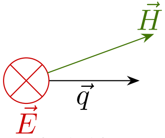
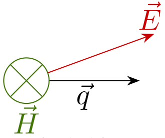
Exciton–Polaritons

Transverse Electric (TE)



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

Transverse Magnetic (TM)



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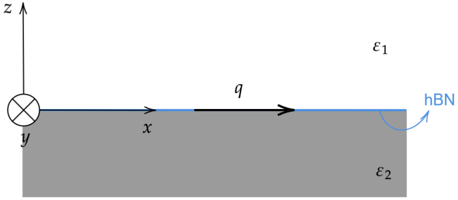

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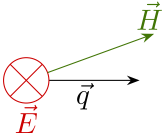

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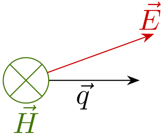

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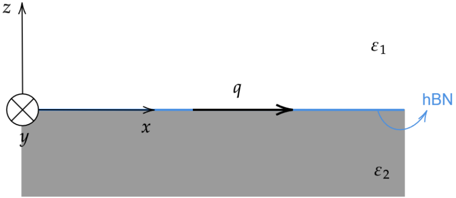


$$\kappa_1 + \kappa_2 - i\omega\mu_0\sigma_{yy}(\omega) = 0$$

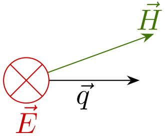
$$\boxed{\frac{\varepsilon_1}{\kappa_1} + \frac{\varepsilon_2}{\kappa_2} + i\frac{\sigma_{xx}(\omega)}{\varepsilon_0\omega} = 0}$$

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

Exciton–Polaritons

POLIMA

Transverse Electric (TE)	Transverse Magnetic (TM)



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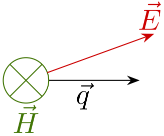

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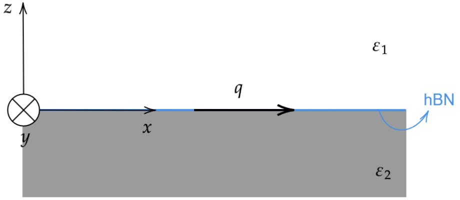

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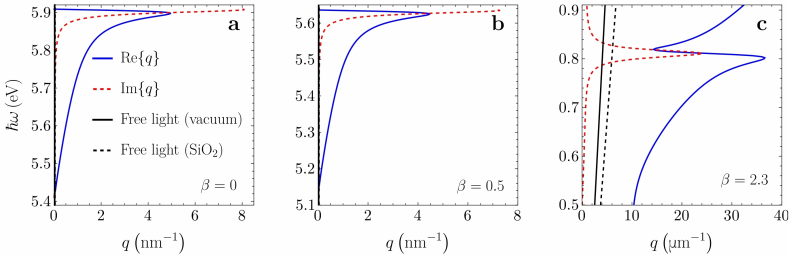

Exciton–Polaritons

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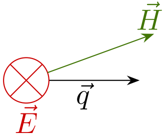

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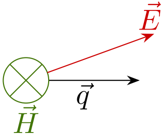

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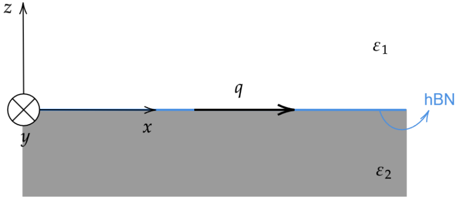

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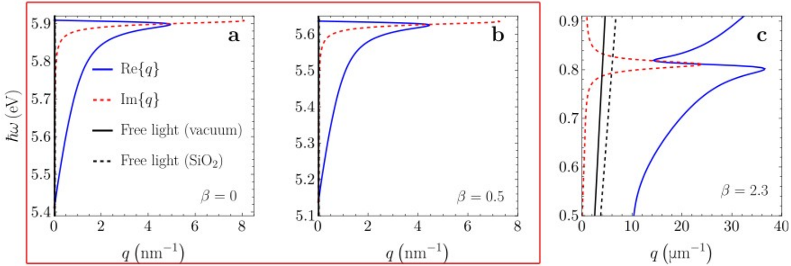

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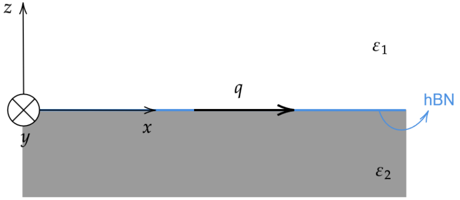

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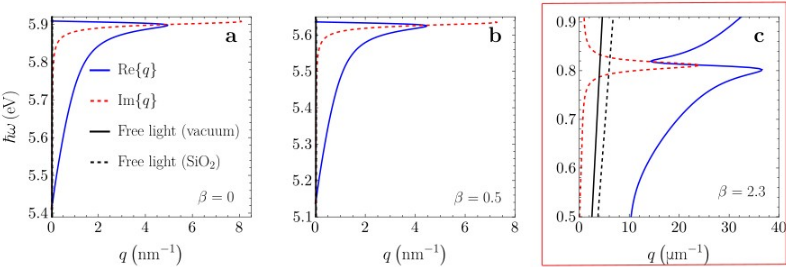

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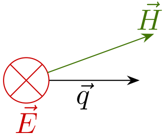

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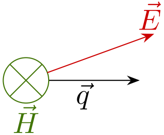

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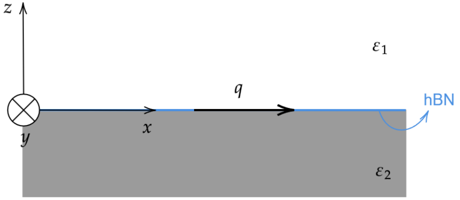

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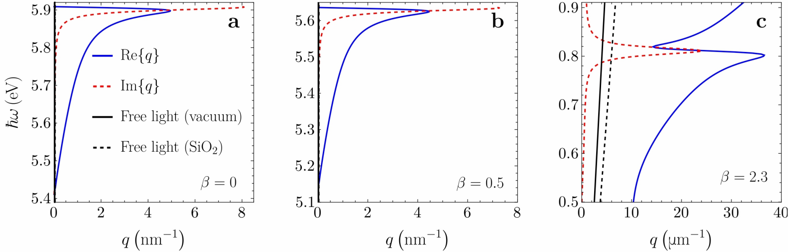
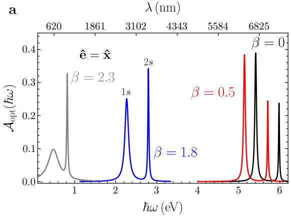


Summary

- Tune the frequency of the optical resonances



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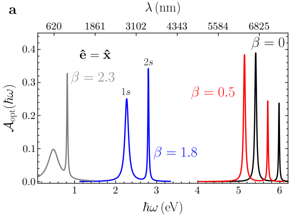

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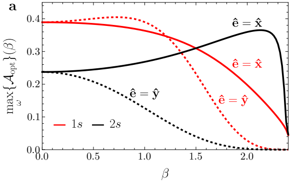

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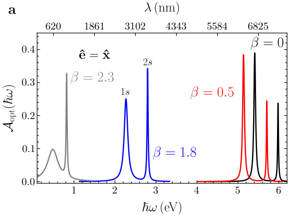

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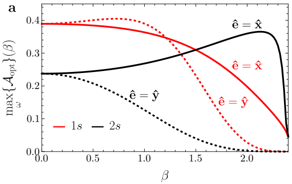

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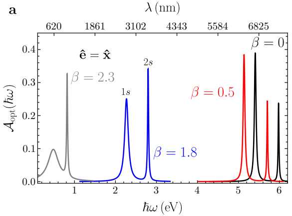

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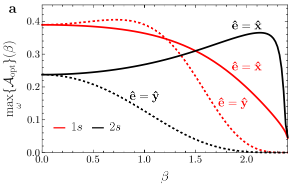

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- $L \sim 40$ nm, $V_0 \sim 40$ meV feasible

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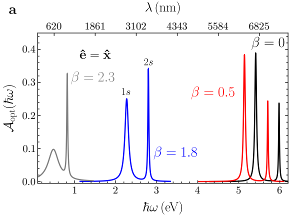

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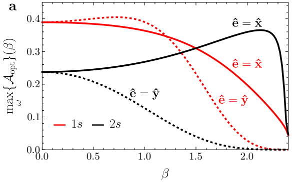

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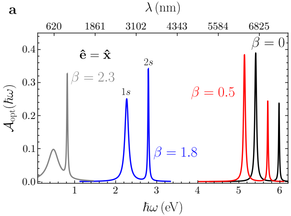

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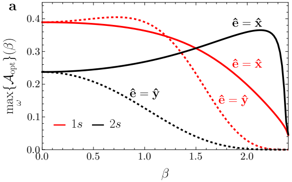

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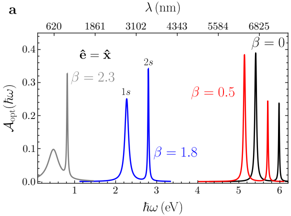

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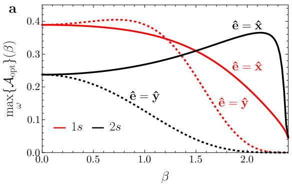

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However....

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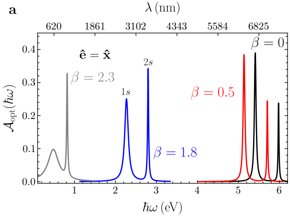

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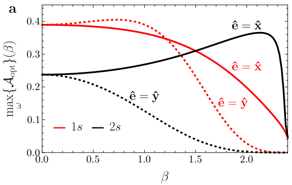

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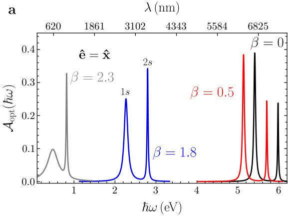
However....

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

Summary

- Tune the frequency of the optical resonances



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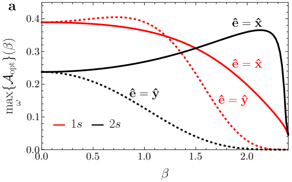

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- How to determine r_0?

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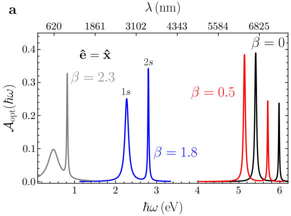

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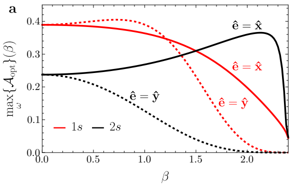

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However....

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

Outline

2D (RPA) Dielectric Function

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

2D (RPA) Dielectric Function

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

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

2D (RPA) Dielectric Function

POLIMA

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

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

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For an insulator/semiconductor

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

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

Macroscopic Dielectric Function

- Screened Coulomb potential in a crystal:
$$W(\boldsymbol{r},\boldsymbol{r}') = \int \mathrm{d}\boldsymbol{r}'' \varepsilon^{-1}(\boldsymbol{r},\boldsymbol{r}'') v_c(\boldsymbol{r}''-\boldsymbol{r}') \xrightarrow{\mathcal{F}} W_{\boldsymbol{G}\boldsymbol{G}'}(\boldsymbol{q}) = \sqrt{v_c(\boldsymbol{q}+\boldsymbol{G})}\varepsilon^{-1}_{\boldsymbol{G}\boldsymbol{G}'}(\boldsymbol{q})\sqrt{v_c(\boldsymbol{q}+\boldsymbol{G}')}$$

Macroscopic Dielectric Function

POLIMA

- Screened Coulomb potential in a crystal:
$$W(\boldsymbol{r},\boldsymbol{r}') = \int \mathrm{d}\boldsymbol{r}''\varepsilon^{-1}(\boldsymbol{r},\boldsymbol{r}'')v_c(\boldsymbol{r}''-\boldsymbol{r}') \xrightarrow{\mathcal{F}} W_{\boldsymbol{G}\boldsymbol{G}'}(\boldsymbol{q}) = \sqrt{v_c(\boldsymbol{q}+\boldsymbol{G})}\varepsilon^{-1}_{\boldsymbol{G}\boldsymbol{G}'}(\boldsymbol{q})\sqrt{v_c(\boldsymbol{q}+\boldsymbol{G}')}$$
- Defining the macroscopic screened potential as:
$$W(\boldsymbol{q}) \equiv W_{\boldsymbol{0}\boldsymbol{0}}(\boldsymbol{q}) = \varepsilon^{-1}_{\boldsymbol{0}\boldsymbol{0}}(\boldsymbol{q})v_c(\boldsymbol{q}) = \frac{v_c(\boldsymbol{q})}{\varepsilon_{\mathrm{M}}(\boldsymbol{q})}$$

Macroscopic Dielectric Function

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- where the macroscopic dielectric function is $\varepsilon_{\mathrm{M}}(\boldsymbol{q}) \equiv \frac{1}{\varepsilon^{-1}_{\mathbf{00}}(\boldsymbol{q})}$

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

Macroscopic Dielectric Function

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$$\varepsilon_{\mathrm{2D}}(\boldsymbol{q}) \equiv \varepsilon_{\mathrm{M}}(\boldsymbol{q}) \overset{q\to 0}{\approx} 1 + r_0 q \equiv \varepsilon_{\mathrm{RK}}(\boldsymbol{q})$$

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Bloch States in the Tight-Binding Approximation

Linear combination of atomic orbitals (LCAO) method

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

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

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

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

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

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

Polarizability in the TB Approximation

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

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Auxiliary calculation:

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Auxiliary calculation:

In the point-like orbital approximation

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

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$$\begin{aligned}\langle n,\boldsymbol{k}|\,\mathrm{e}^{-\mathrm{i}(\boldsymbol{q}+\boldsymbol{G})\cdot\boldsymbol{r}}\,|n',\boldsymbol{k}+\boldsymbol{q}\rangle &= \int_{\mathcal{A}}\mathrm{d}\boldsymbol{r}\,\psi^*_{n,\boldsymbol{k}}(\boldsymbol{r})\,\mathrm{e}^{-\mathrm{i}(\boldsymbol{q}+\boldsymbol{G})\cdot\boldsymbol{r}}\psi_{n',\boldsymbol{k}+\boldsymbol{q}}(\boldsymbol{r}) = \\ &= \sum_{i\alpha}(C^{n\boldsymbol{k}}_{i\alpha})^*C^{n'\boldsymbol{k}+\boldsymbol{q}}_{i\alpha}\mathrm{e}^{-\mathrm{i}(\boldsymbol{q}+\boldsymbol{G})\cdot\boldsymbol{t}_i} \equiv I^{\boldsymbol{G}}_{n\boldsymbol{k},n'\boldsymbol{k}+\boldsymbol{q}}\end{aligned}$$

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$$= \frac{2}{\mathcal{A}}\sum_{vc}\sum_{\boldsymbol{k}\sigma}\frac{I^{\boldsymbol{G}}_{v\boldsymbol{k}+\boldsymbol{q},c\boldsymbol{k}}\left(I^{\boldsymbol{G}'}_{v\boldsymbol{k}+\boldsymbol{q},c\boldsymbol{k}}\right)^*}{\epsilon_{v\boldsymbol{k}+\boldsymbol{q}}-\epsilon_{c\boldsymbol{k}}}$$

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Exciton Computation Scheme with the Xatu Code

1. Diagonalize $H(\boldsymbol{k}+\boldsymbol{q})$ and store all $\{\epsilon_{n\boldsymbol{k}+\boldsymbol{q}}\}$,$\{\mathbf{C}^{n\boldsymbol{k}+\boldsymbol{q}}\}\ \forall\boldsymbol{q}\in\mathrm{BZ},\ \forall\boldsymbol{k}\in\mathrm{BZ}',\mathrm{BZ}\neq\mathrm{BZ}'$
2. Compute dielectric matrix $\varepsilon_{\boldsymbol{G}\boldsymbol{G}'}(\boldsymbol{q})\ \forall\boldsymbol{q}\in\mathrm{BZ}$
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4. Compute the exciton (following slides)

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Example: Monolayer hBN

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

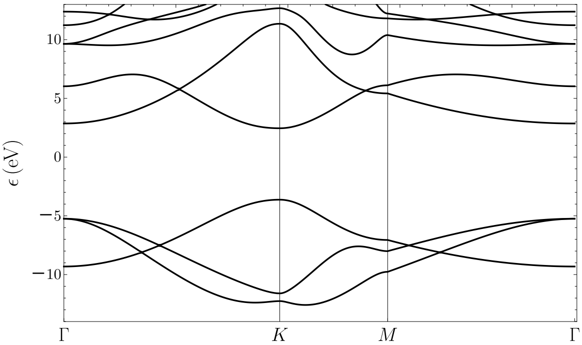

Figure: *Band structure of monolayer hBN*

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

Macroscopic Dielectric Function: Results

Does $\varepsilon^{-1}_{\boldsymbol{G}\boldsymbol{G}'}(\boldsymbol{q})$ converge?

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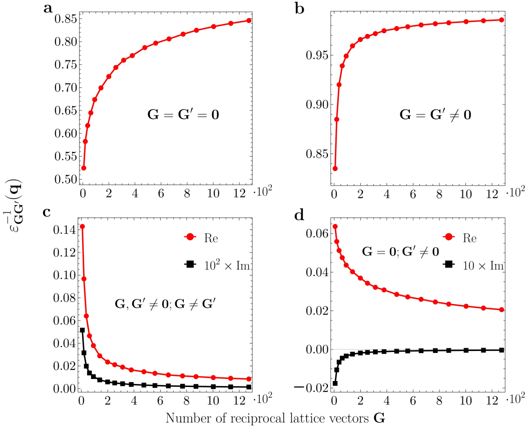

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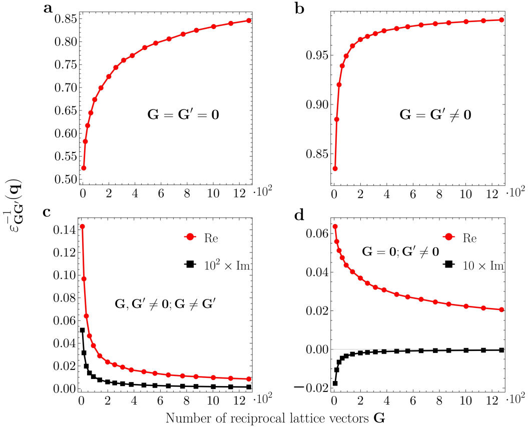
Does $\varepsilon^{-1}_{\boldsymbol{G}\boldsymbol{G}'}(\boldsymbol{q})$ converge? No!



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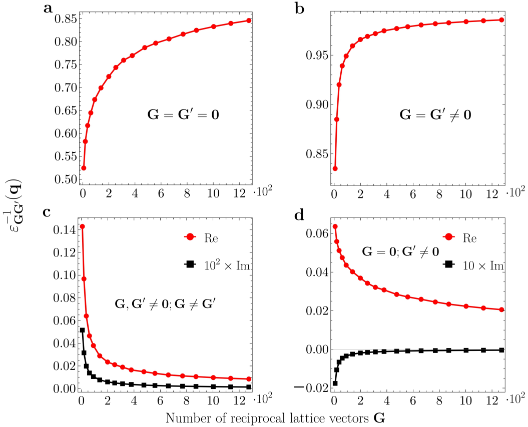

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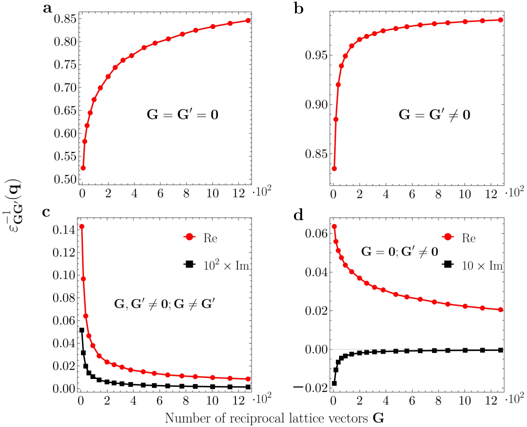

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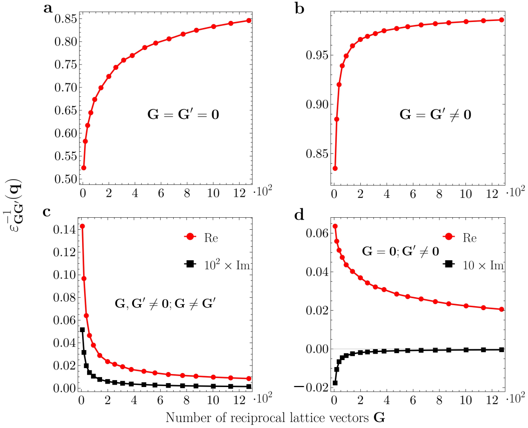

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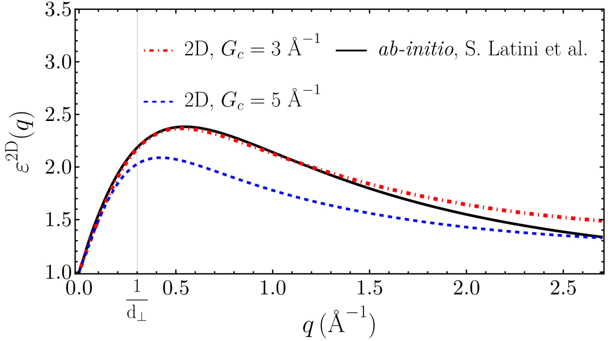

S. Latini, T. Olsen, K. S. Thygesen - *Phys. Rev. B* **92** 245123 (2015)

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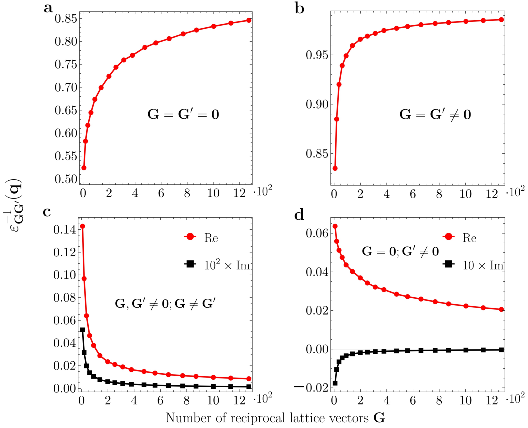
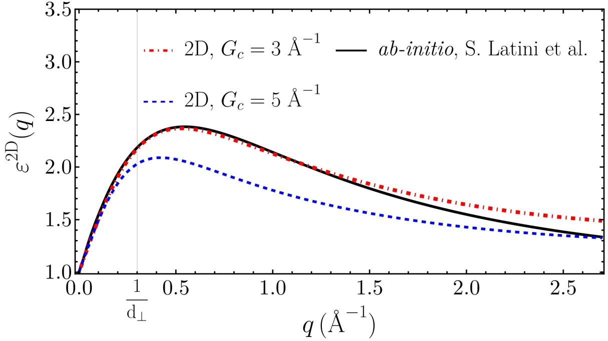


But still,

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



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Macroscopic Dielectric Function: 2D vs. *Ab initio*

2D approach

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

Ab initio

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2. invert $\varepsilon_{\boldsymbol{G}\boldsymbol{G}'}(\boldsymbol{q})$
3. $\varepsilon^{-1}_{00}(\boldsymbol{q}, z, z') = \frac{1}{L_\perp}\sum_{G_z, G'_z} \mathrm{e}^{\mathrm{i}G_z z}\varepsilon^{-1}_{G_z\hat{z}G'_z\hat{z}}(\boldsymbol{q})\mathrm{e}^{-\mathrm{i}G'_z z'}$
4. $\varepsilon^{2\mathrm{D}}(\boldsymbol{q}) = 1/\langle\varepsilon^{-1}_{00}(\boldsymbol{q}, z, z')\rangle_{\text{off-plane}}$

Also, the Coulomb potential is truncated as $v_c(\boldsymbol{r}) = \frac{\Theta(R_c - z)}{r}$, with $R_c \to \infty$

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Macroscopic Dielectric Function: 2D vs. *Ab initio*

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$$\boxed{(\epsilon_{c\boldsymbol{k}+\boldsymbol{Q}} - \epsilon_{v\boldsymbol{k}})A^{\boldsymbol{Q}}_{vc}(\boldsymbol{k}) + \sum_{v'c',\boldsymbol{k}'} K_{vc,v'c'}(\boldsymbol{k},\boldsymbol{k}',\boldsymbol{Q})A^{\boldsymbol{Q}}_{v'c'}(\boldsymbol{k}') = E_X A^{\boldsymbol{Q}}_{vc}(\boldsymbol{k})}$$

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POLIMA

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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	$E_b >$ 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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Quasi-2D Approach for Screening

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

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

Q2D Dielectric Function

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

Q2D Dielectric Function

POLIMA

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

Q2D Dielectric Function: Results

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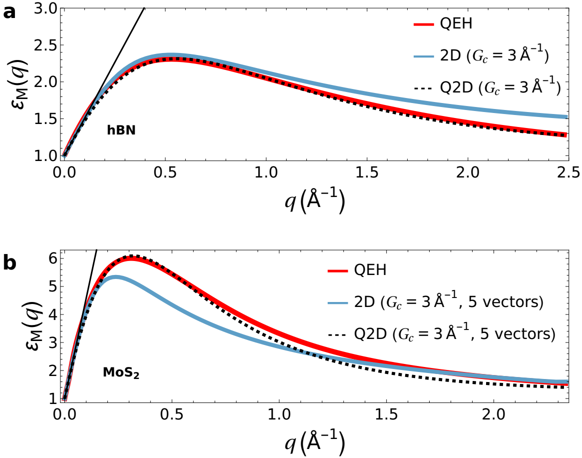

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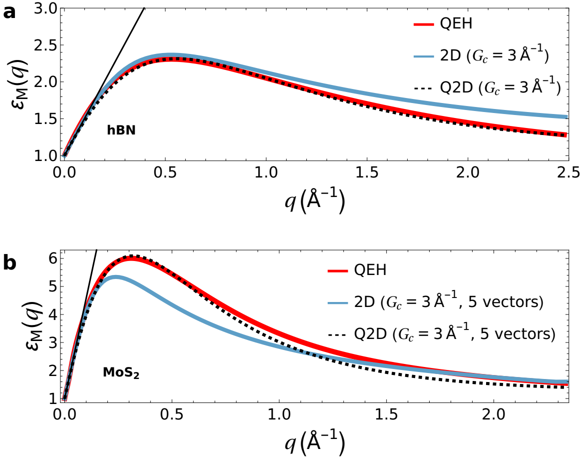

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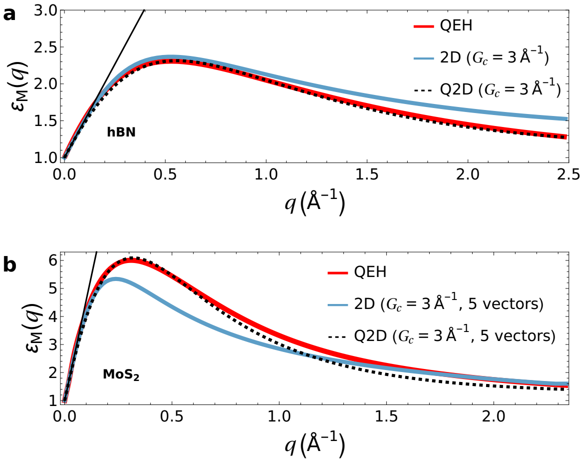

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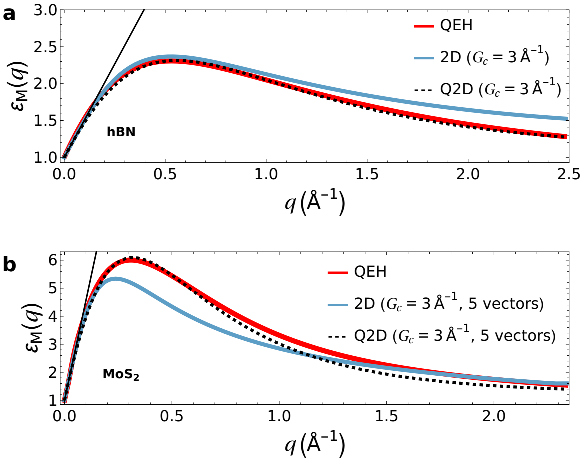

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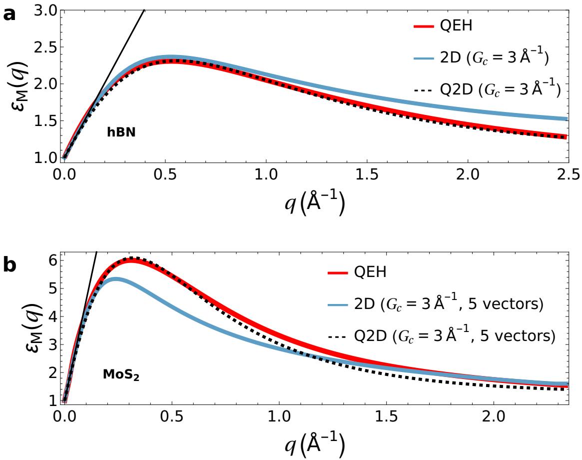

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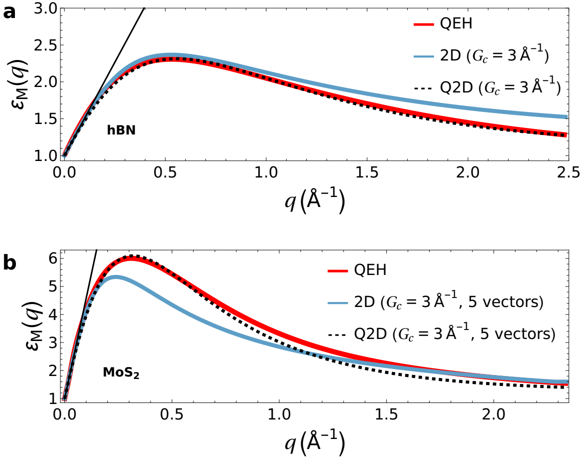

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- r_0 can be very well estimated with vanishing computational cost!
- Very good agreement with the literature! For MoS_2 $r_0 \approx 32$ Å; for GeS $r_0 \approx 20$ Å

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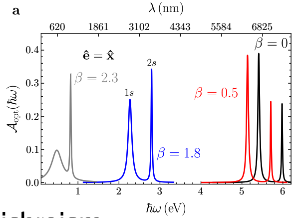
Outline

Conclusions: Part I

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



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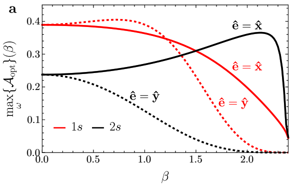

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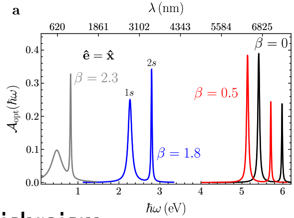

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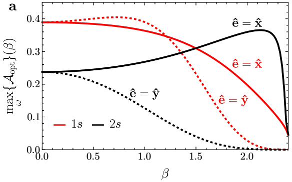

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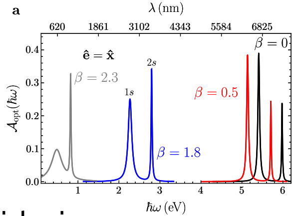

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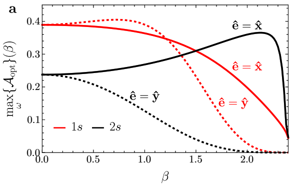

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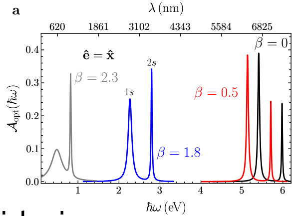

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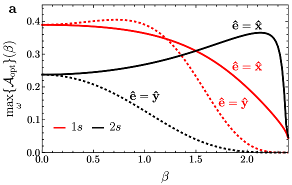

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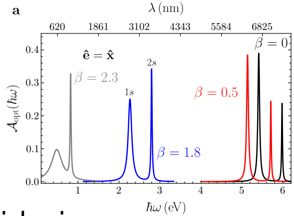

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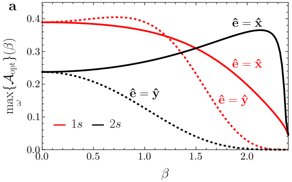

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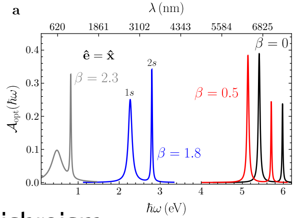

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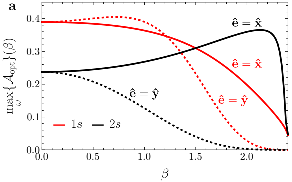

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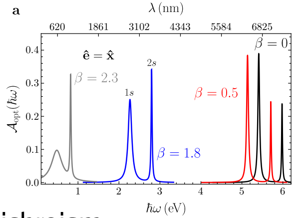

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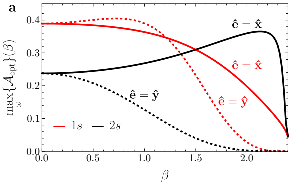

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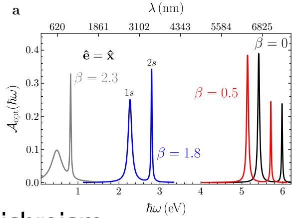

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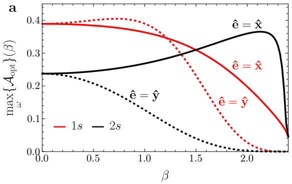

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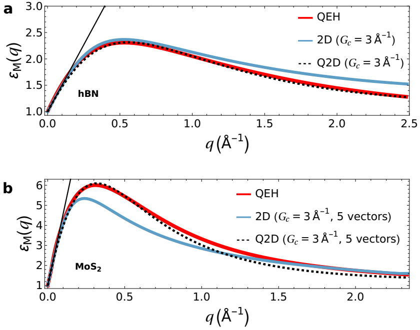

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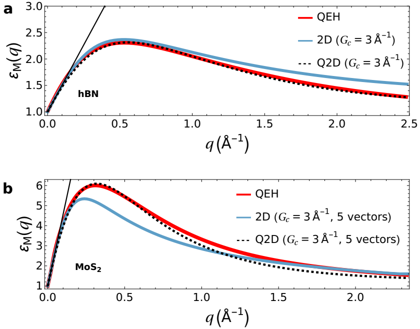

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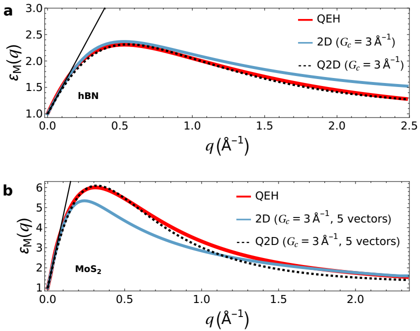

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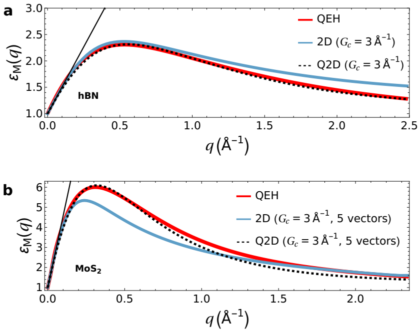
5. Panel **b** with 95 points:
   $\sim$ 20 mins for 2D, $\sim$ 30 mins for Q2D ⏱️



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And the audience

Thanks 😊

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Screened potential matrix elements

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$$W_{\boldsymbol{G}\boldsymbol{G}'}(\boldsymbol{q}) = \sqrt{v_c(\boldsymbol{q}+\boldsymbol{G})}\varepsilon^{-1}_{\boldsymbol{G}\boldsymbol{G}'}(\boldsymbol{q})\sqrt{v_c(\boldsymbol{q}+\boldsymbol{G}')} \tag{1}$$

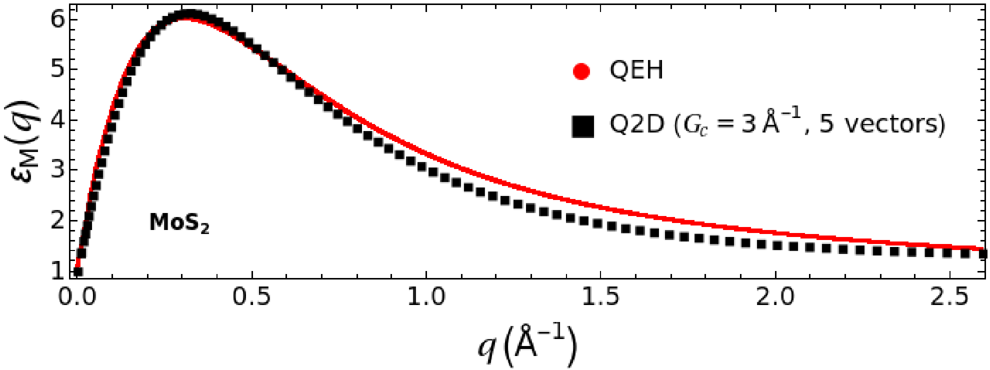
Regularizing the singular terms

$$W_{\boldsymbol{0}\boldsymbol{0}}(\boldsymbol{0}) = \frac{1}{\mathcal{A}_\Gamma}\int_{\mathcal{A}_\Gamma} \mathrm{d}\boldsymbol{q}\, \varepsilon^{-1}_{\boldsymbol{0}\boldsymbol{0}}(\boldsymbol{q}) v_c(\boldsymbol{q}) \approx \frac{1}{\mathcal{A}_\Gamma}\int_{\mathcal{A}_\Gamma} \mathrm{d}\boldsymbol{q}\, v_c(\boldsymbol{q})\big(1 - r_0 q\big) \tag{2}$$

and for the wing terms

$$W_{\boldsymbol{G}\boldsymbol{0}}(\boldsymbol{0}) = W_{\boldsymbol{0}\boldsymbol{G}}(\boldsymbol{0}) = 0 \tag{3}$$

Q2D dielectric function



Computational Framework: Pre-processing calculations

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

$\downarrow$

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 MoS_2 Band Structure

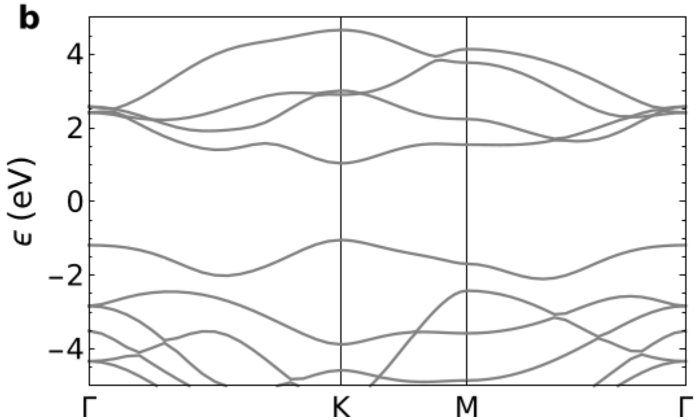


Figure: *Band structure of monolayer MoS_2 using CRYSTAL*

Excitons in MoS_2: 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^{ε} (Å^{-1})					
		0	3	4	5	7	8
G_c^X	0		0.979507	1.567935	1.401440	1.951914	$E_b >$ gap
	3		0.756373	1.619208	1.785953	$E_b >$ gap	$E_b >$ gap
	4			0.774599	1.105537	$E_b >$ gap	$E_b >$ gap
	5				0.778244	$E_b >$ gap	$E_b >$ gap
	7					0.792309	1.300835
	8						0.799489

$E_b >$ gap -> the exciton comes with negative excitation energy

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