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

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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

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

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Optical Excitations in Matter

Solid Materials

Optical Excitations in Matter

Solid Materials $\left\{ \vphantom{\begin{matrix} a \\ b \\ c \\ d \\ e \\ f \end{matrix}} \right.$

Optical Excitations in Matter

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

Optical Excitations in Matter

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

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Optical Excitations in Matter

Solid Materials
- Metals
  - Free charges
- Dielectrics

Optical Excitations in Matter

Solid Materials
- Metals
  - Free charges
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Optical Excitations in Matter

Solid Materials
- Metals
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POLIMA

- Solid Materials
  - Metals
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  - Dielectrics
    - Bound charges

Optical Excitations in Matter

Solid Materials
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  - Bound charges
  - Insulating

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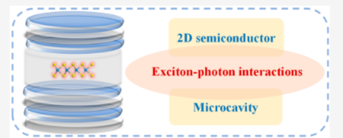
    - Insulating
    - Dipolar excitations (excitons)

Excitons in Photonics

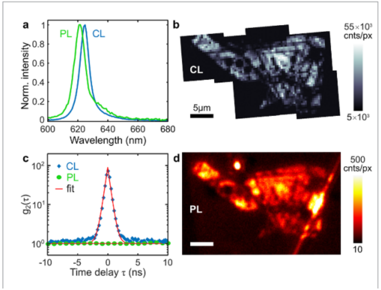
Relevant for:

Light–matter interactions



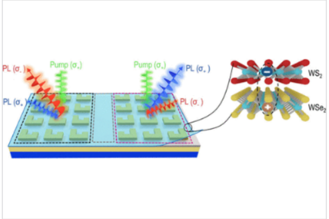
J. Shang et al. - *ACS Photonics* **10** 7 (2023)

Quantum Light Sources



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

Valleytronics



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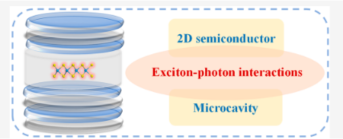

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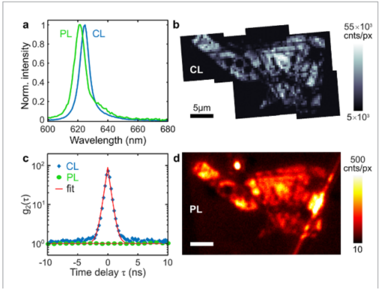

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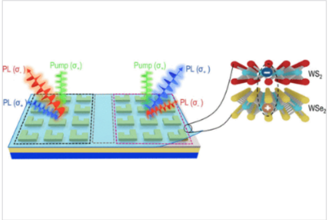

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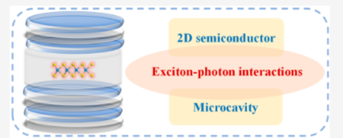

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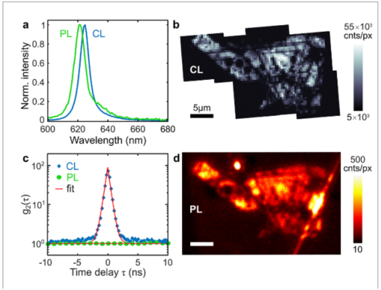

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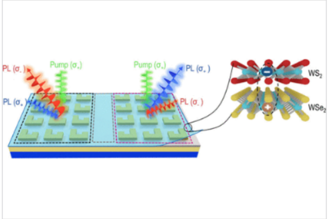

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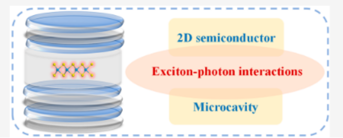

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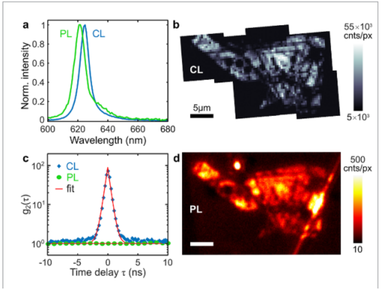

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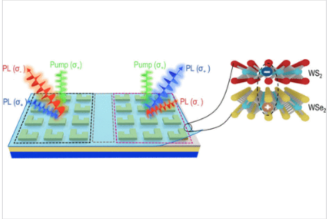

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Excitons in Two-Dimensional Materials

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

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

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

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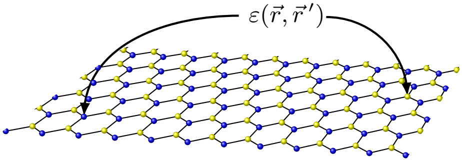

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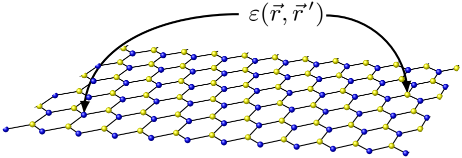

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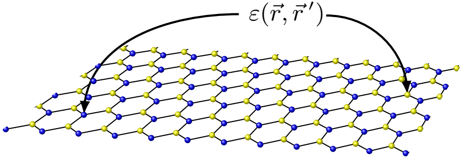

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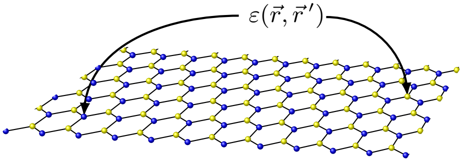

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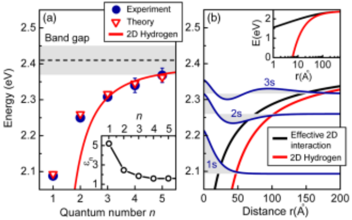

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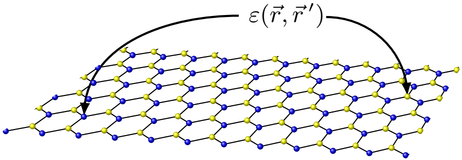

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Hexagonal Boron Nitride in Photonics

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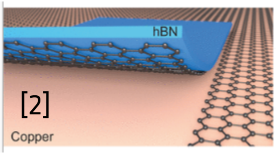
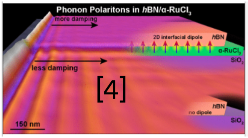
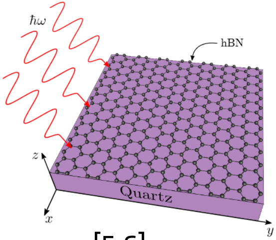
- Ballistic transport in graphene [2]
- Hyperbolic material (MIR) [3]
- Polaritonics in the MIR [4]







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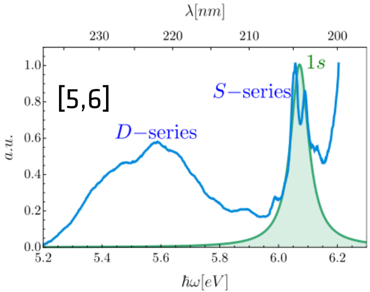

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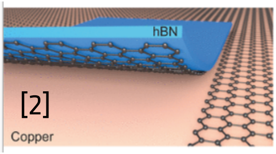

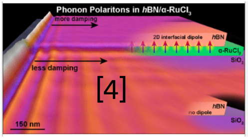

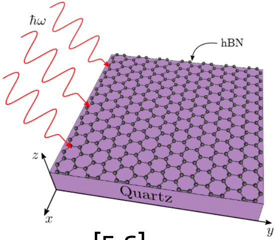

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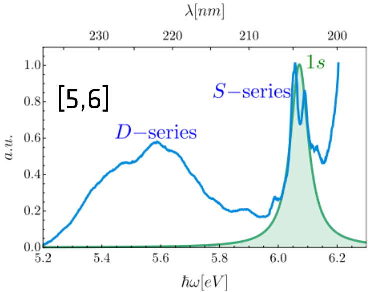

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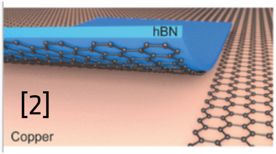

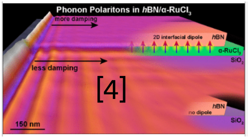

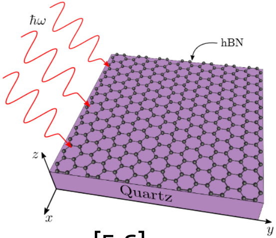

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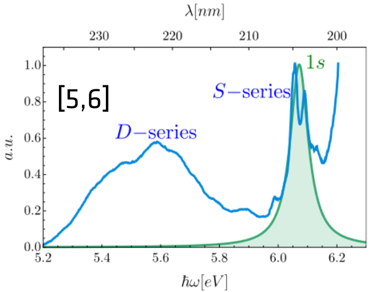

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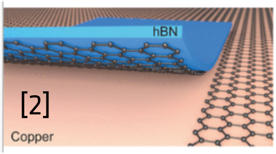

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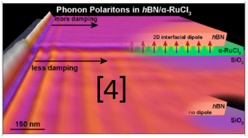

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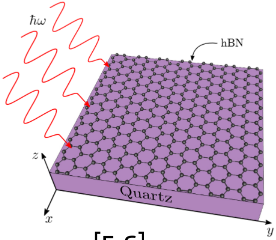

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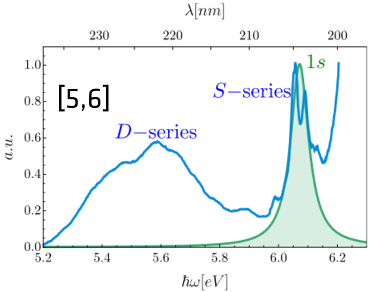

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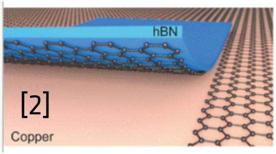

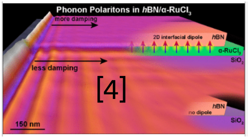

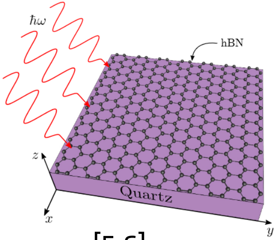

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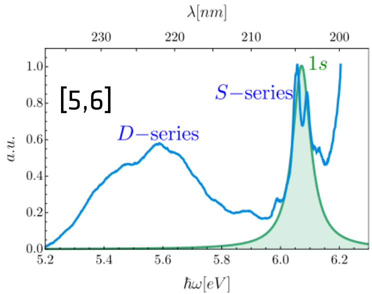

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Motivation

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

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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Full numerical *ab initio* Can we optimize?

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Outline

1 Introduction to Excitons in 2D Materials

2 Part I: Exciton–Polaritons in a 1D hBN Superlattice
- Setup
- Excitonic States
- Optical Response
- Exciton–Polaritons

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

4 Conclusions

hBN under an external periodic potential

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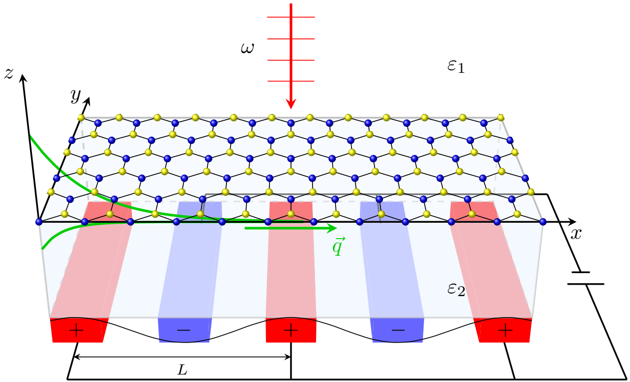
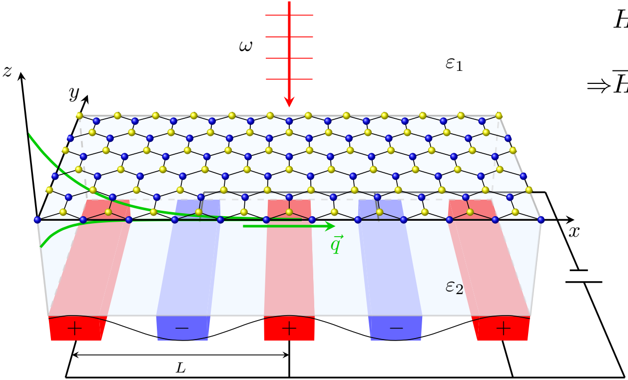


P. Ninhos et. al - *ACS Nano* **18** 31 (2024)

hBN under an external periodic potential



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

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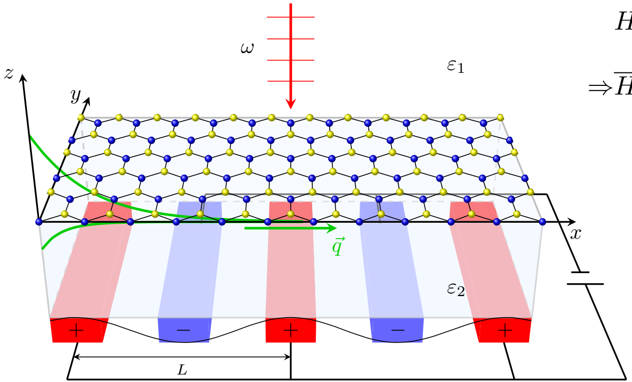

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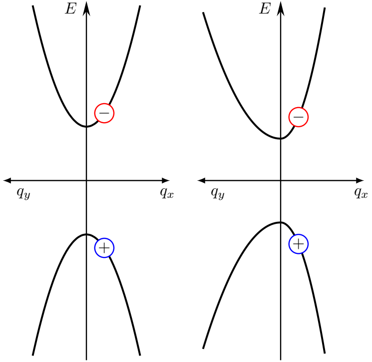

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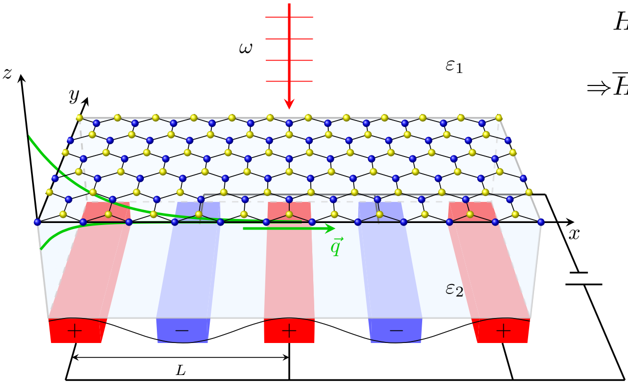

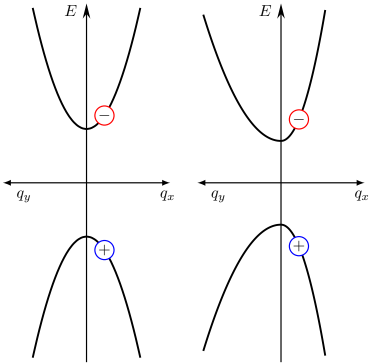

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For $\beta \sim 1$, and $V_0 \sim 40$ meV, $L \sim 40$ nm

Wannier Equation and Variational Method

Wannier equation [1]

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

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

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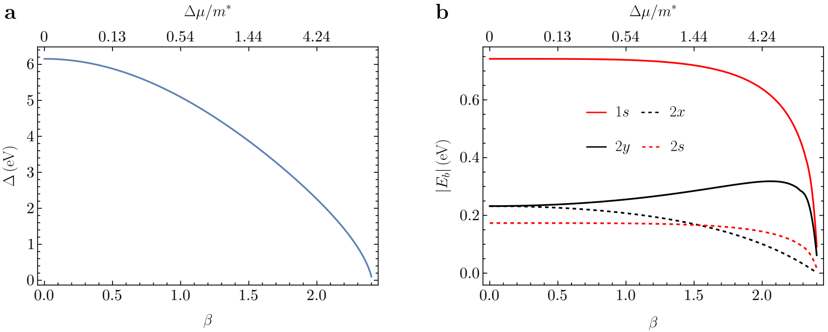

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Optical Conductivity

According to Pedersen [1]

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

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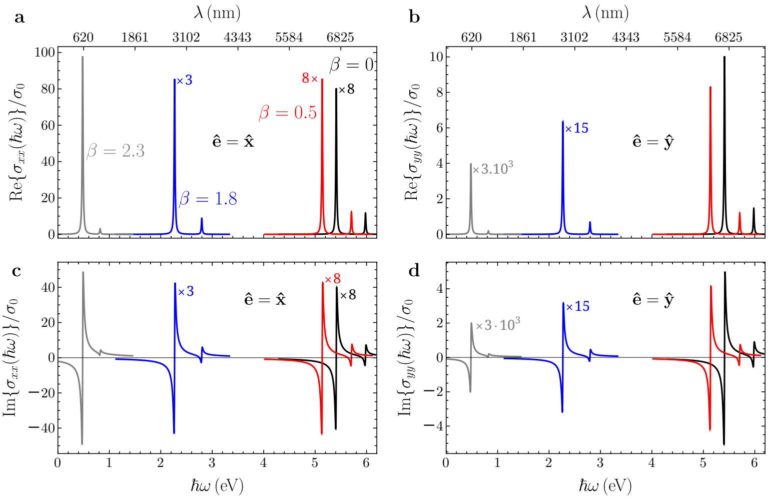

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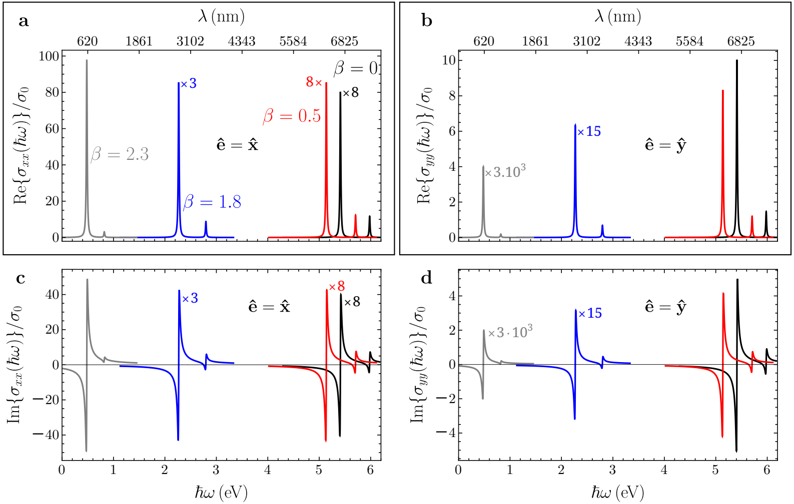

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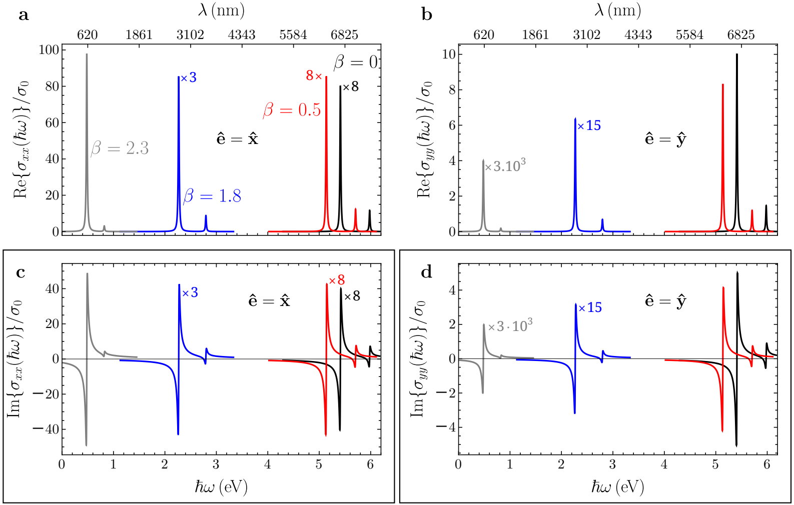

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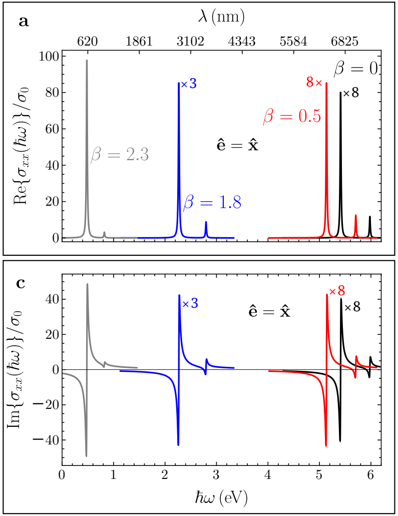

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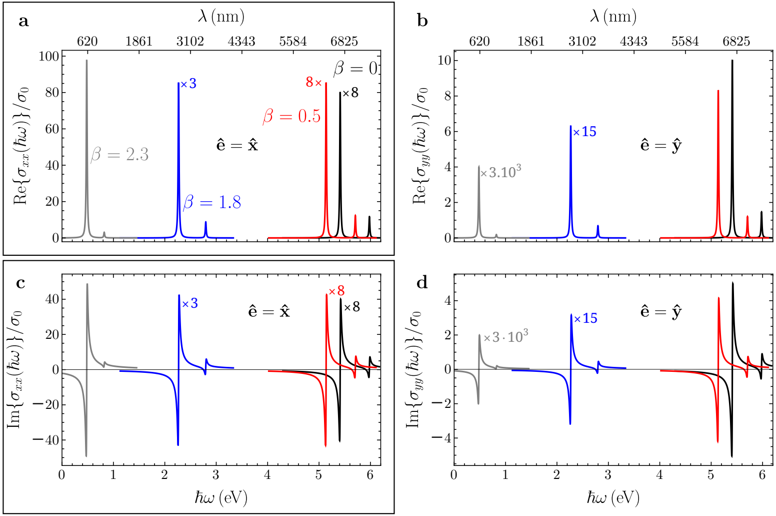

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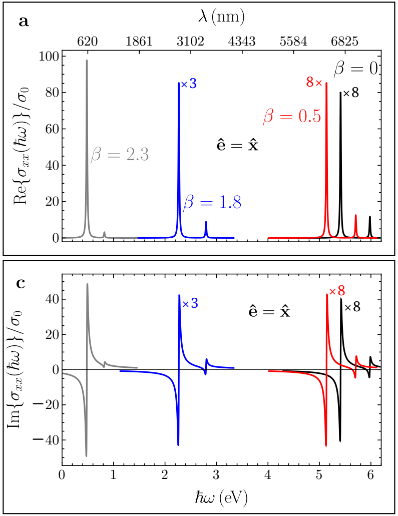

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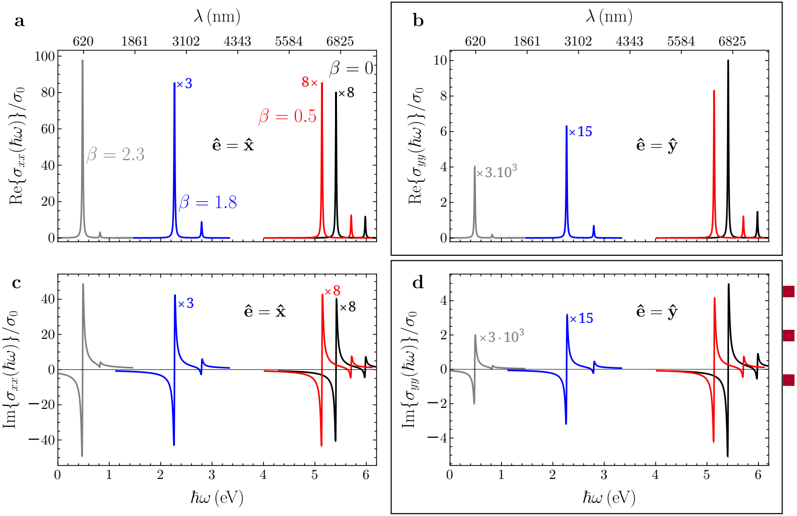

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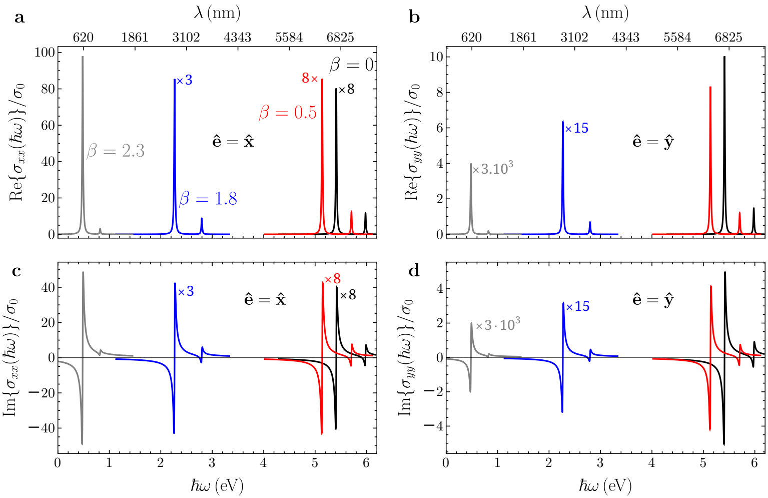

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$$\mathcal{A}_{\text{opt}} = 1 - \mathcal{R} - \frac{\mathrm{Re}\{\sqrt{\varepsilon_2}\}}{\mathrm{Re}\{\sqrt{\varepsilon_1}\}}\mathcal{T}\,, \quad \mathcal{R} = \left| \frac{\sqrt{\varepsilon_2} - \sqrt{\varepsilon_1} + \frac{\sigma}{\varepsilon_0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

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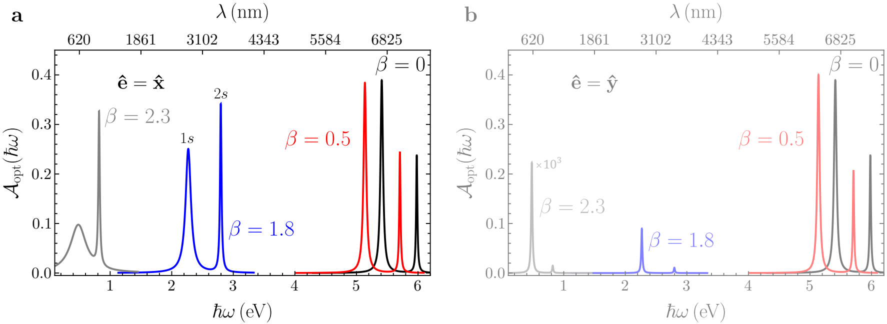

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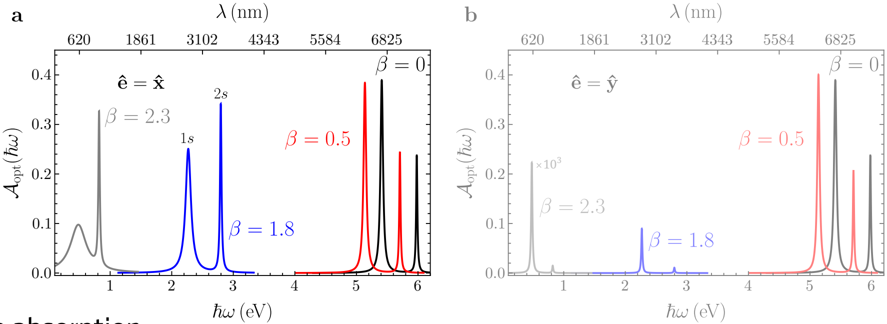

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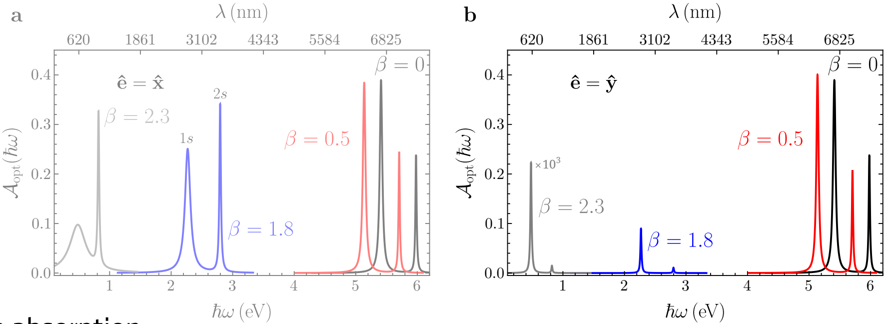

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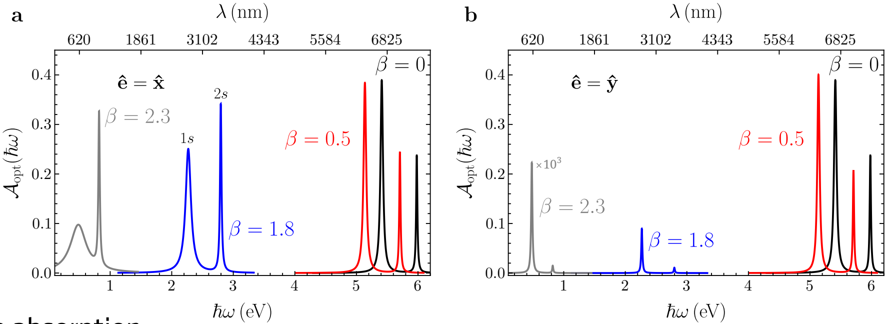
- For y pol. absorption is suppressed

Optical Absorption

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



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

- For y pol. absorption is suppressed

Absorption Peaks

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

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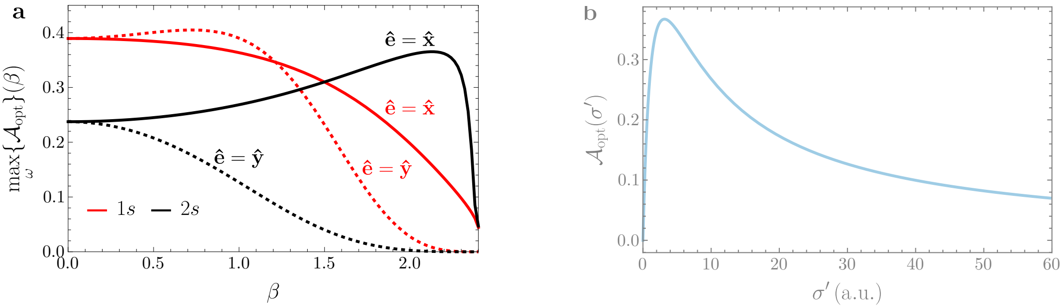

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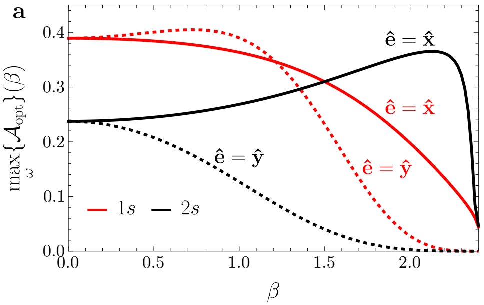

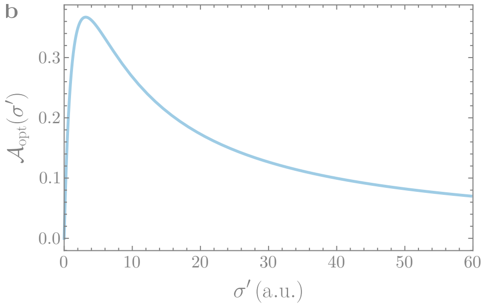

- Tunable absorption
- Different response for different polarizations $\Rightarrow$ grid polarizer

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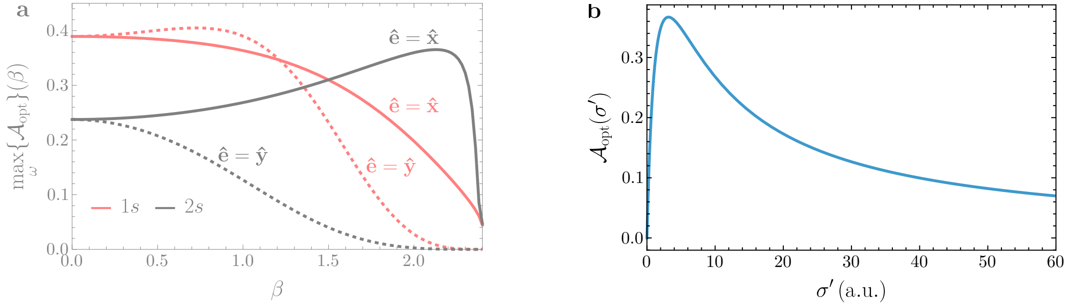

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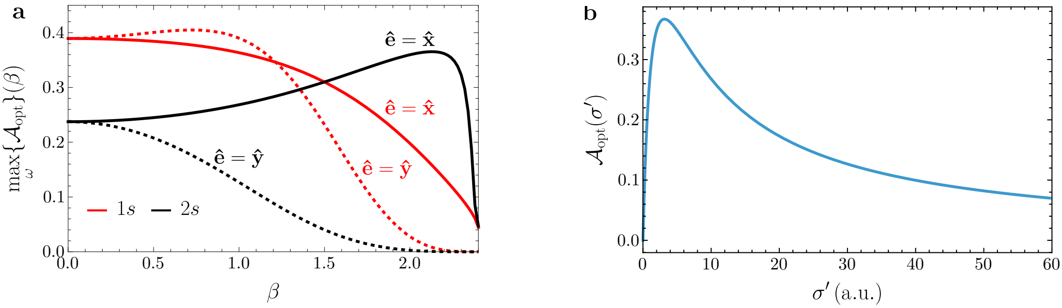

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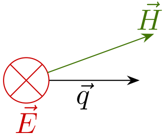
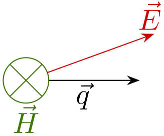
Exciton–Polaritons

Transverse Electric (TE)



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

Transverse Magnetic (TM)



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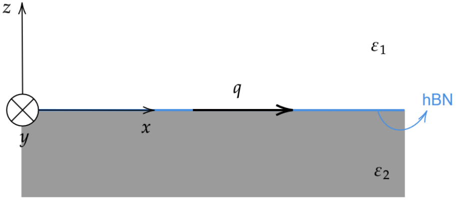
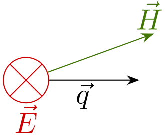


Exciton–Polaritons

Transverse Electric (TE) Transverse Magnetic (TM)



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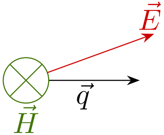

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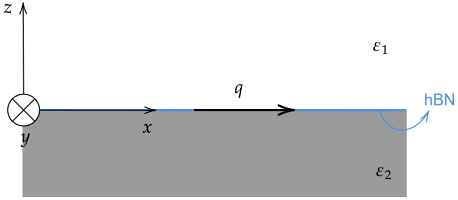

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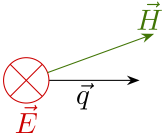

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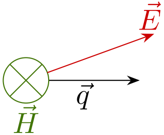

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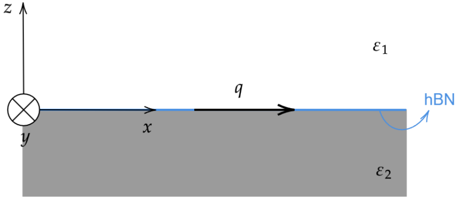

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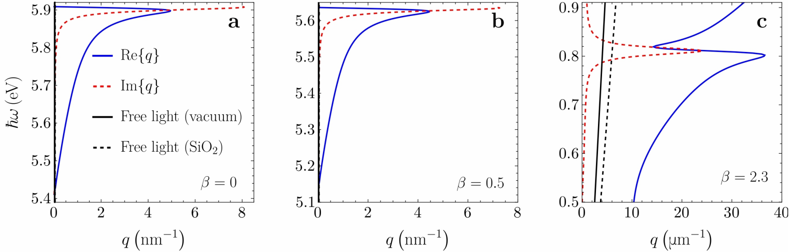

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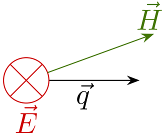

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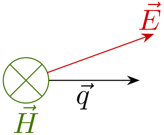

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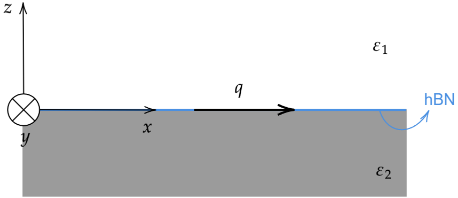

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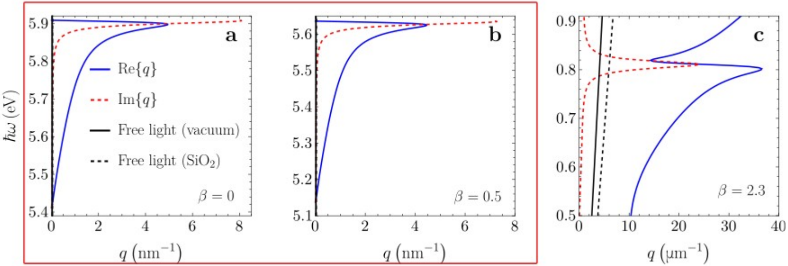

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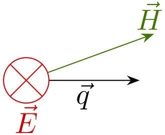

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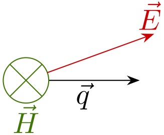

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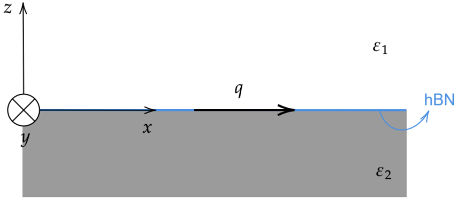

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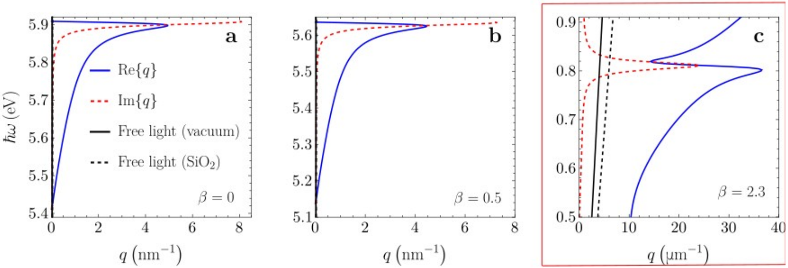

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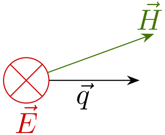

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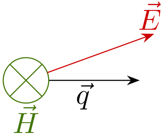

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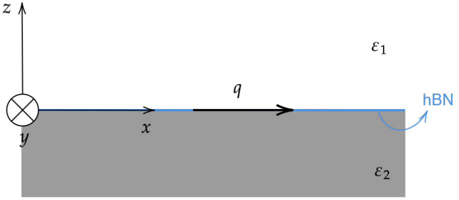

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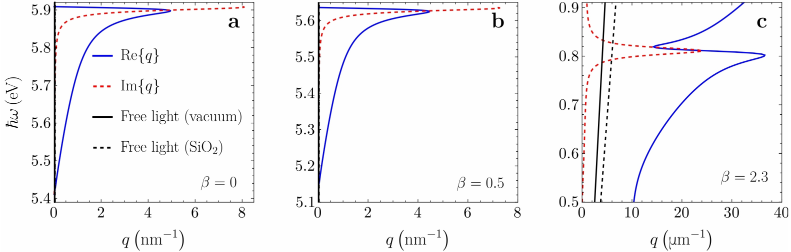
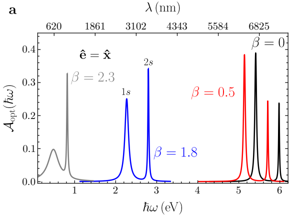


Summary

- Tune the frequency of the optical resonances



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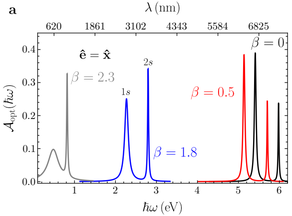

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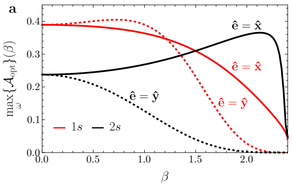

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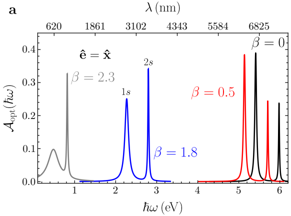

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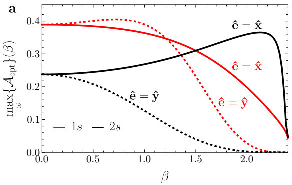

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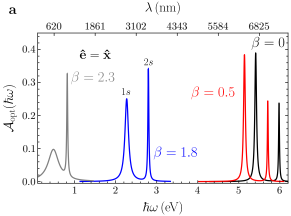

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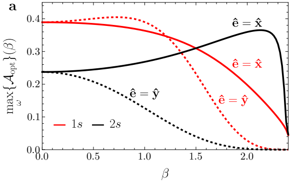

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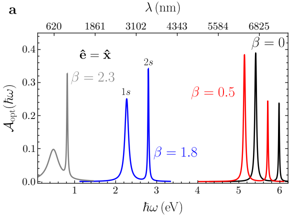

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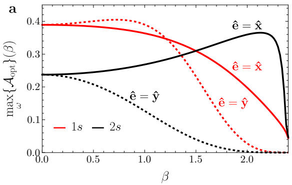

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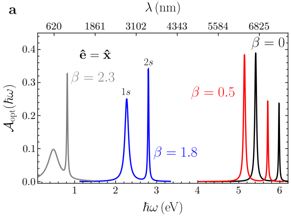

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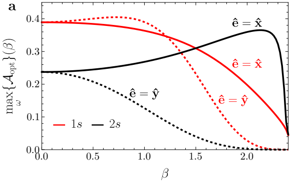

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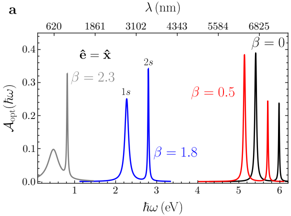

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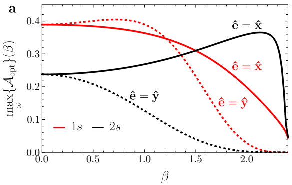

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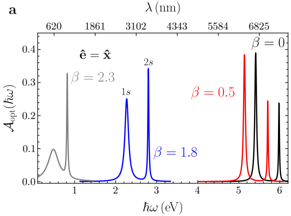

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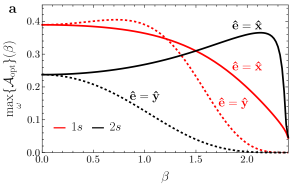

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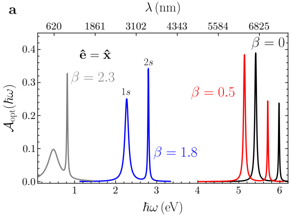
However....

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

Summary

- Tune the frequency of the optical resonances



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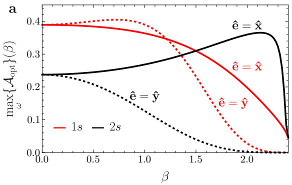

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- How to determine r_0?

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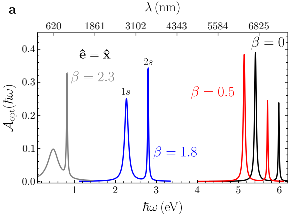

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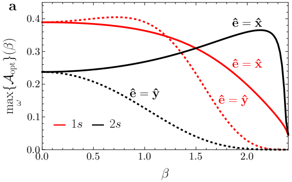

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However....

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

Outline

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

2D (RPA) Dielectric Function

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

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

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

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

2D (RPA) Dielectric Function

POLIMA

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

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

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

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

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- Defining the macroscopic screened potential as:
$W(\boldsymbol{q}) \equiv W_{\mathbf{00}}(\boldsymbol{q}) = \varepsilon^{-1}_{\mathbf{00}}(\boldsymbol{q})v_c(\boldsymbol{q}) = \frac{v_c(\boldsymbol{q})}{\varepsilon_{\mathrm{M}}(\boldsymbol{q})}$

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

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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

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

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

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

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

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Exciton Computation Scheme with the Xatu Code

POLIMA

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 $\varepsilon_{\boldsymbol{G}\boldsymbol{G}'}(\boldsymbol{q})\,\forall\boldsymbol{q}\in\mathrm{BZ}$
3. Invert $\varepsilon_{\boldsymbol{G}\boldsymbol{G}'}(\boldsymbol{q})\,\forall\boldsymbol{q}\in\mathrm{BZ}$
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A. J. Uría-Alvárez et al. - *Comp. Phys. Comm.* **295** 109001 (2024) $\leftarrow$ 1st version of Xatu

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

Example: Monolayer hBN

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

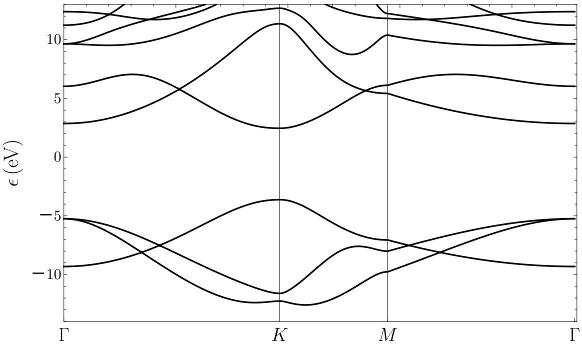

Figure: *Band structure of monolayer hBN*

- [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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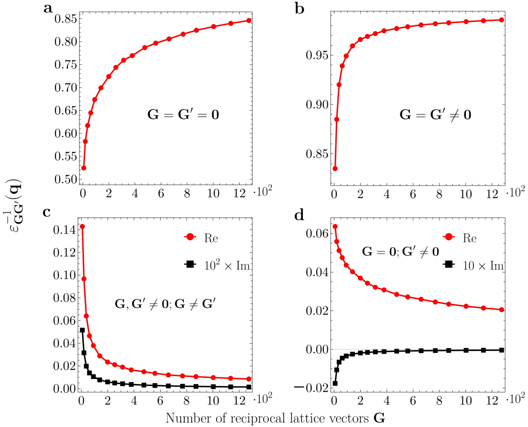
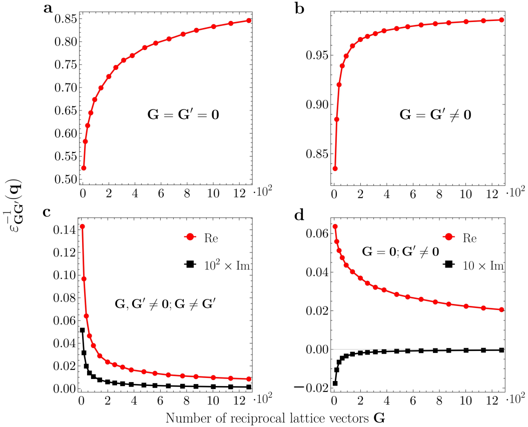


Macroscopic Dielectric Function: Results

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



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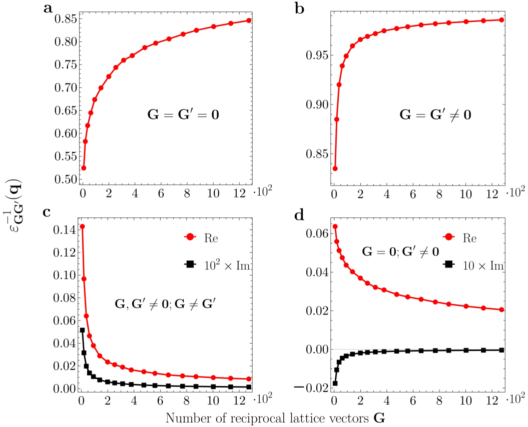
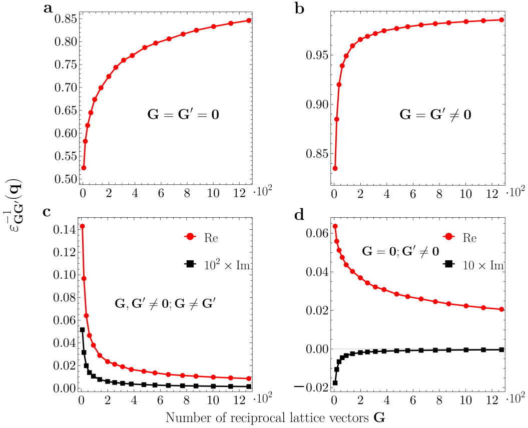


But still,

Macroscopic Dielectric Function: Results

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



But still,

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

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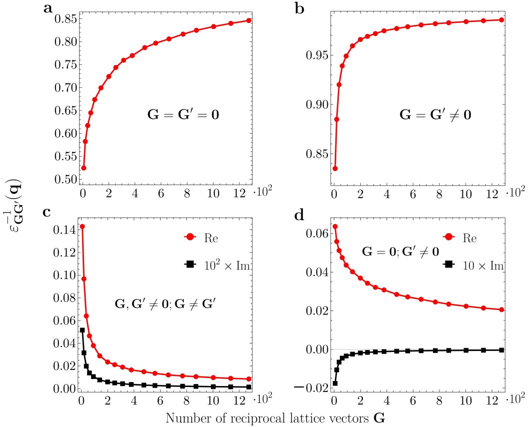

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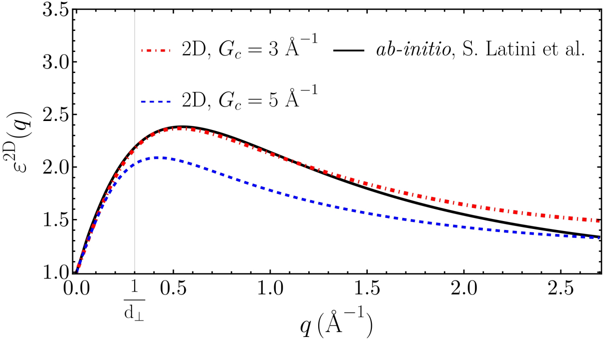

S. Latini, T. Olsen, K. S. Thygesen - *Phys. Rev. B* **92** 245123 (2015)

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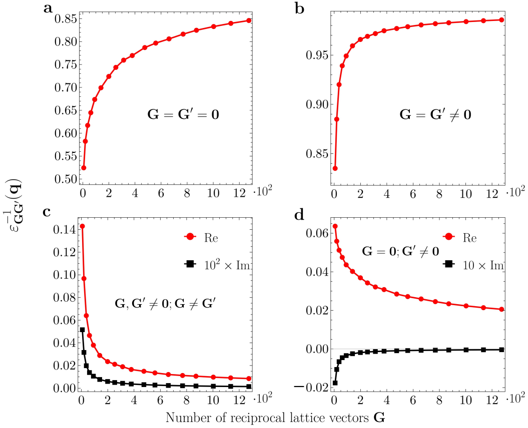
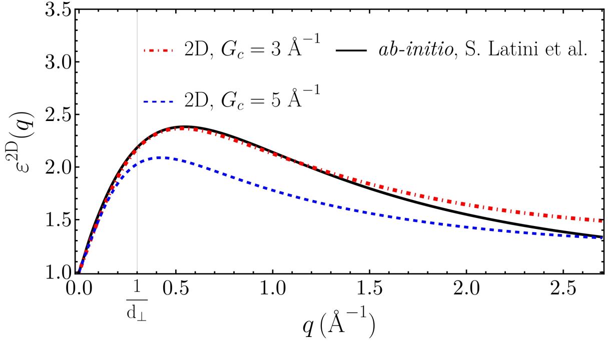


But still,

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



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

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 $\varepsilon^{\mathrm{2D}}(\boldsymbol{q}) = \frac{1}{\varepsilon^{-1}_{00}(\boldsymbol{q})}$

Ab initio

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

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$$\Downarrow \mathcal{F}_{||}$$

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$$v_c(\boldsymbol{r}-\boldsymbol{r}') = v_c(\boldsymbol{r}_{||}-\boldsymbol{r}'_{||}, z-z') \xrightarrow{\mathcal{F}_{||}} v_c(\boldsymbol{q}, z-z') = \frac{e}{2\varepsilon_0 q}\,\mathrm{e}^{-q|z-z'|}$$

Within a quasi-2D (Q2D) framework, the diele. function

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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

POLIMA

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

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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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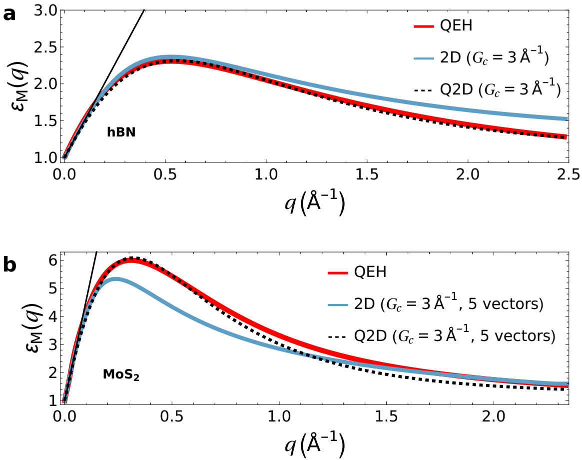

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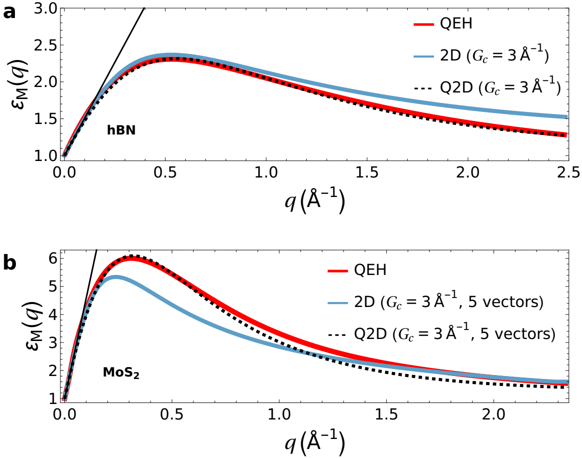

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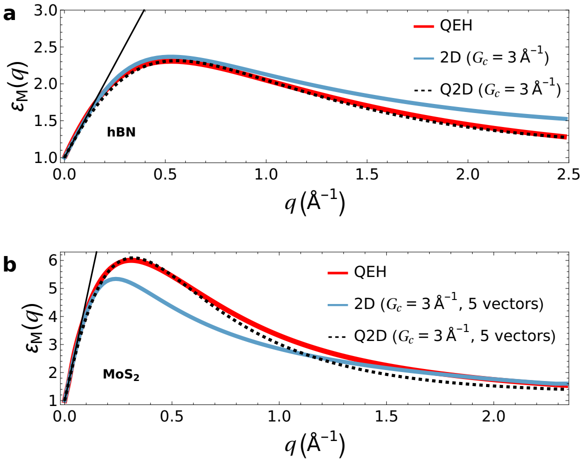

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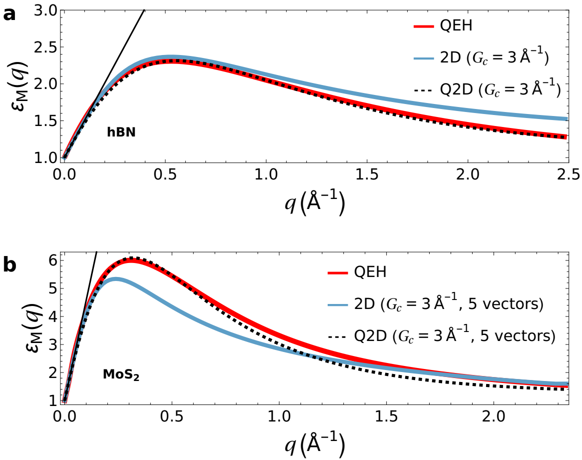

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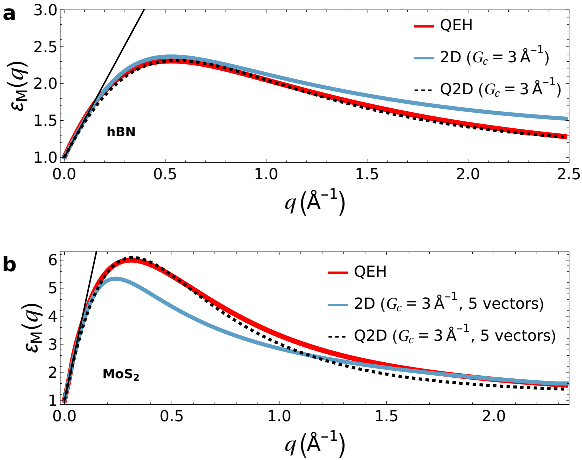

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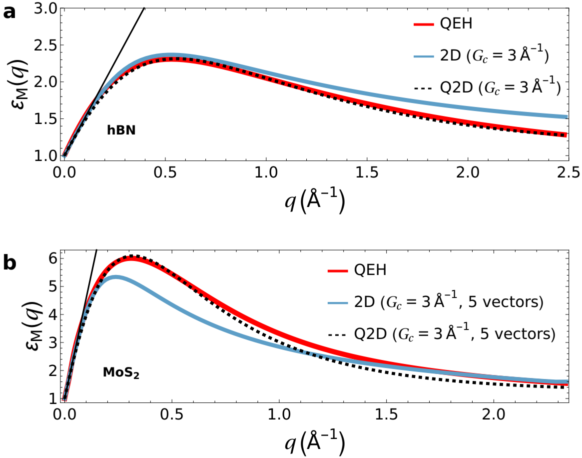

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- Very good agreement with the literature! For MoS_2 $r_0 \approx 32$ Å; for GeS $r_0 \approx 20$ Å

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Outline

1 Introduction to Excitons in 2D Materials

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

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

4 Conclusions

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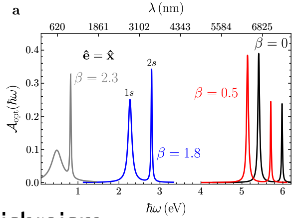
- hBN as a promising material for mid IR–UV polaritonics
- Tune the frequency of the optical resonances



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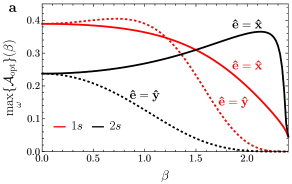

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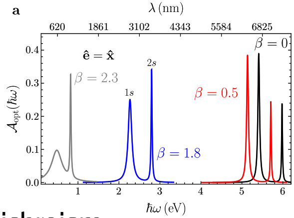

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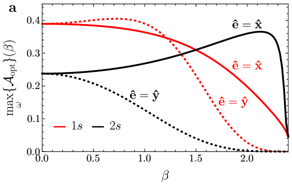

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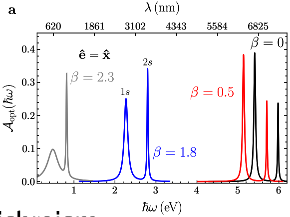

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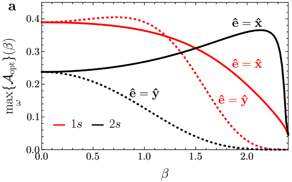

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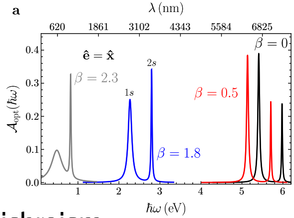

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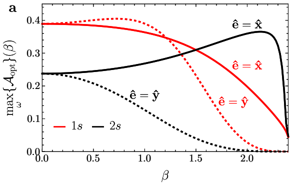

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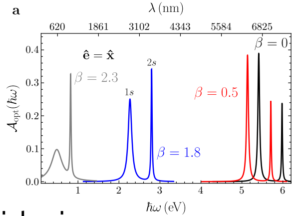

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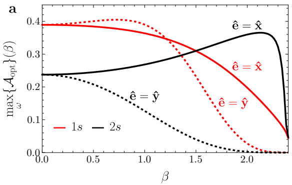

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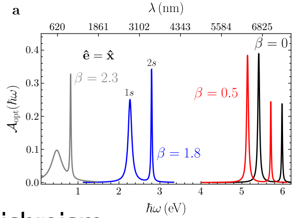

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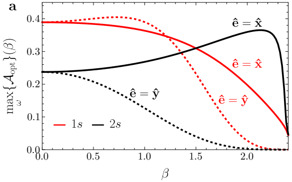

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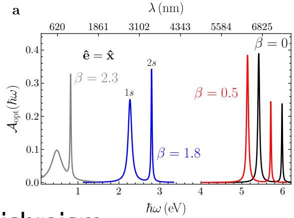

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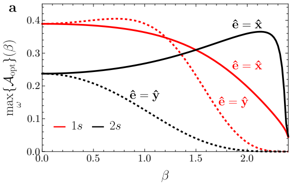

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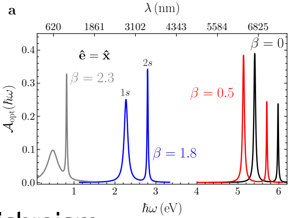

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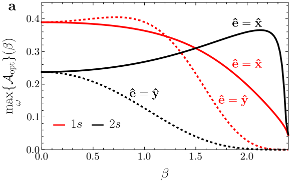

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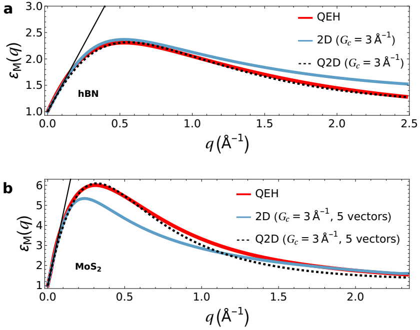

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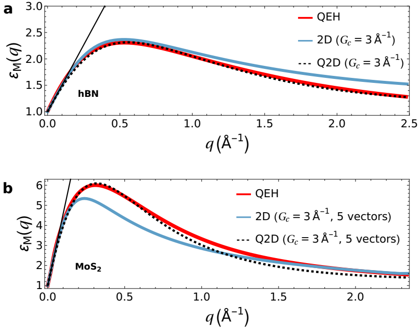

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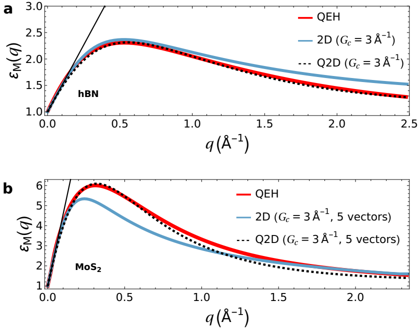

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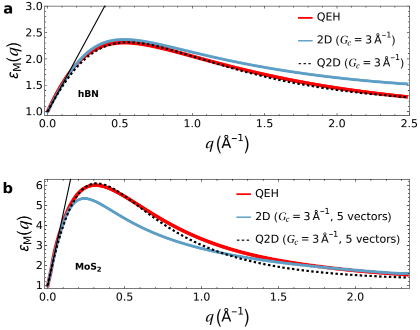
5. Panel **b** with 95 points:
   $\sim$ 20 mins for 2D, $\sim$ 30 mins for Q2D ⏱️



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DANMARKS FRIE FORSKNINGSFOND

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And the audience
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Screened potential matrix elements

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

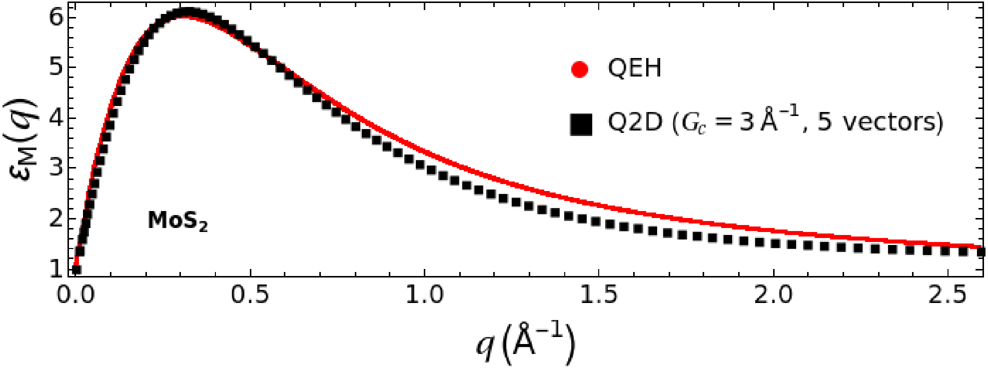
Regularizing the singular terms

$$W_{\mathbf{00}}(\mathbf{0}) = \frac{1}{\mathcal{A}_\Gamma}\int_{\mathcal{A}_\Gamma} \mathrm{d}\boldsymbol{q}\,\varepsilon^{-1}_{\mathbf{00}}(\boldsymbol{q})v_c(\boldsymbol{q}) \approx \frac{1}{\mathcal{A}_\Gamma}\int_{\mathcal{A}_\Gamma} \mathrm{d}\boldsymbol{q}\,v_c(\boldsymbol{q})\big(1 - r_0 q\big) \tag{2}$$

and for the wing terms

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

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

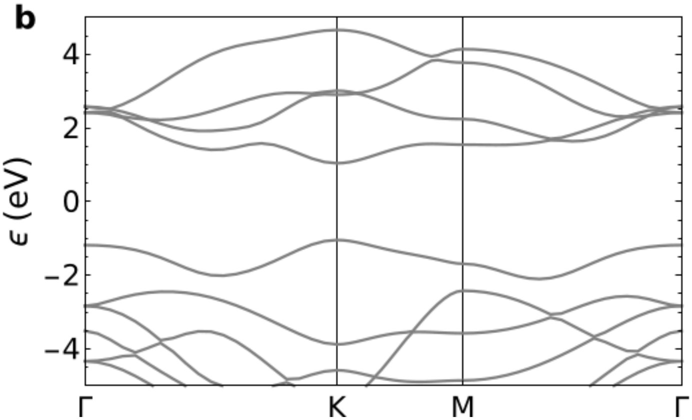


Figure: *Band structure of monolayer MoS_2 using CRYSTAL*

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