Impact of hBN-encapsulation on light absorption in 2D-TMD based photodetectors

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hBN encapsulation helps preserving desired properties. But, how relevant are vdW (van der Waals) gaps in the propagation and absorption of light at the device level?

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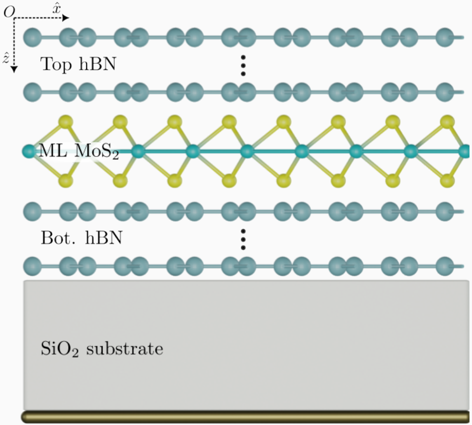
Test structure



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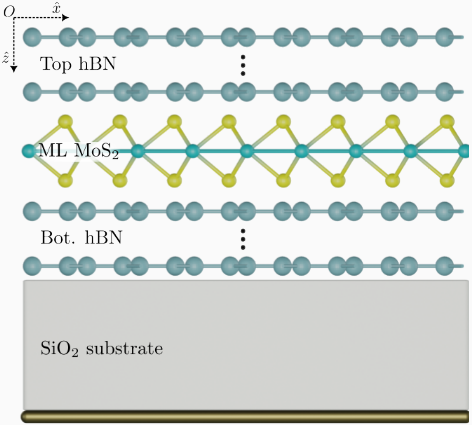

Macroscopic modeling of layers:

- Large in-plane (*XY*) spatial extension compared to vertical thickness.

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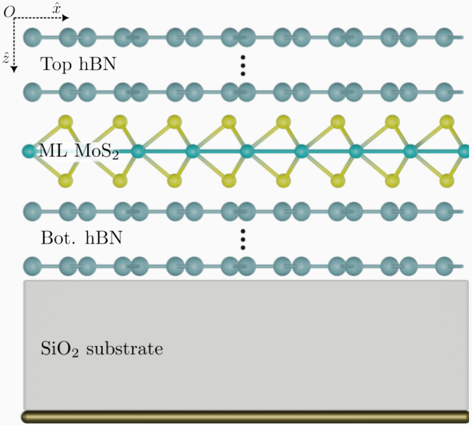

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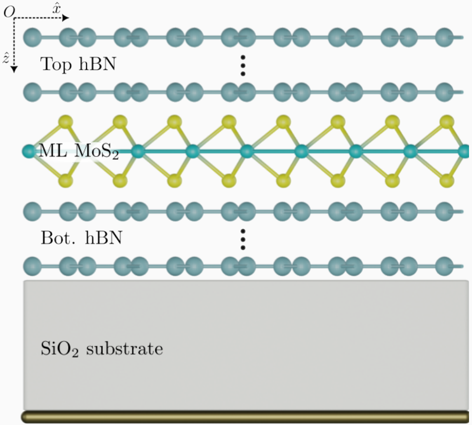

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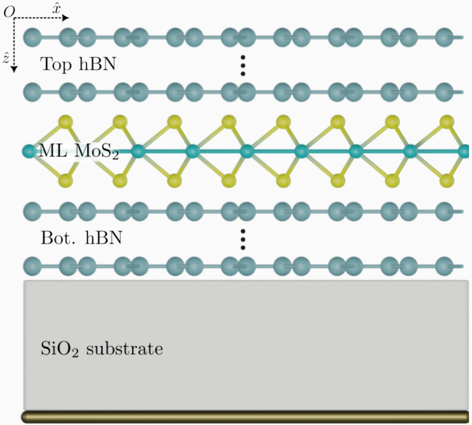

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- Optical properties fully described by $n = \eta - i\kappa$. Normal incidence is assumed.
- vdW gaps represented as thin "vacuum" between adjacent 2D material layers.

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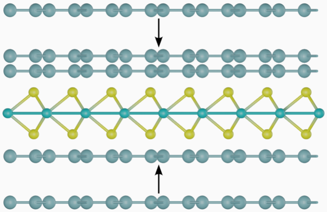

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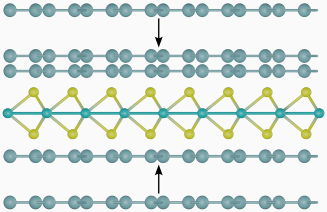
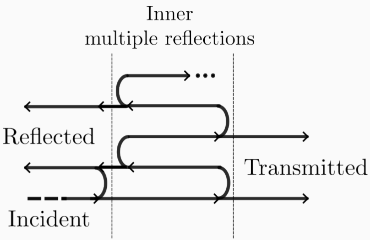


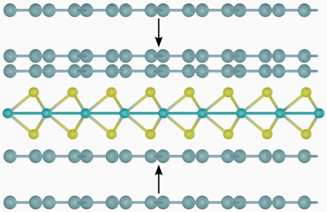


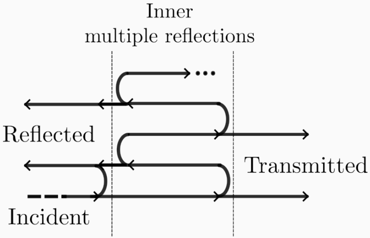
Classical analytical models for light absorption

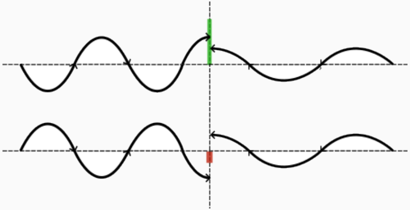
Standard models allow to evaluate the importance of

- layer thickness and number,
- multiple reflections,
- interference effects

among others with negligible computational cost.







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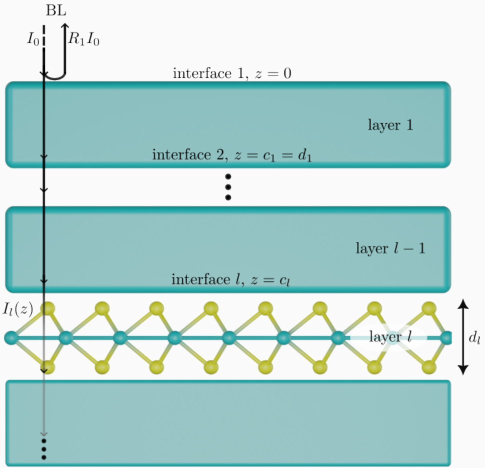


Beer-Lambert

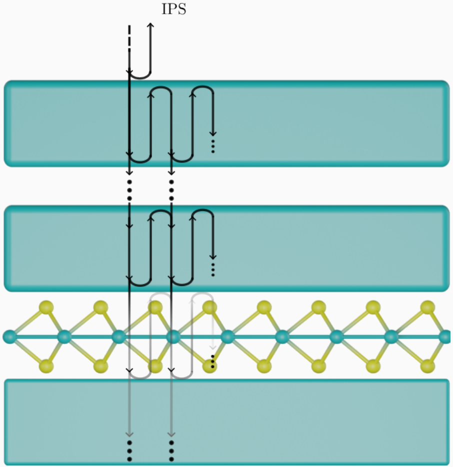
$$Q_l = I_0 T_l^{\mathrm{BL}} (1 - \omega_l), \qquad T_l^{\mathrm{BL}} = \omega_{l-1} T_{l-1}^{\mathrm{BL}}$$

$$T_1^{\mathrm{BL}} = 1 - R_1, \qquad \omega_l \equiv e^{-\alpha_l d_l}$$

No reflections but on the uppermost interface.

$Q_l \equiv$ energy absorption rate per unit surface for layer l.

Classical light absorption



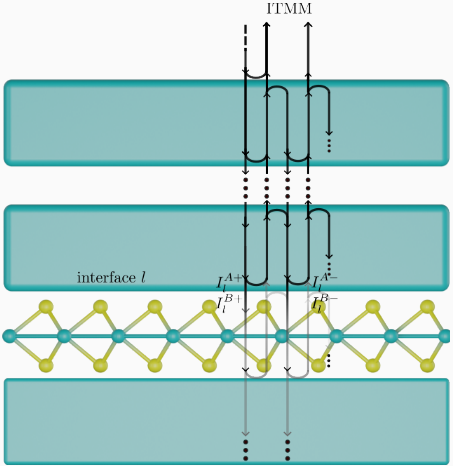
Incoherent Path Sum (IPS)

$$Q_l = I_0\, T_l^{\mathrm{IPS}} \frac{(1-\omega_l)(1+\omega_l R_{l+1})}{(1-R_l R_{l+1}\omega_l^2)},$$

$$T_l^{\mathrm{IPS}} = T_{l-1}^{\mathrm{IPS}} \frac{(1-R_l)\omega_{l-1}}{1-R_{l-1}R_l\omega_{l-1}^2},$$

Multiple reflections inside each layer, but no upwards transmission through interfaces.

Classical light absorption



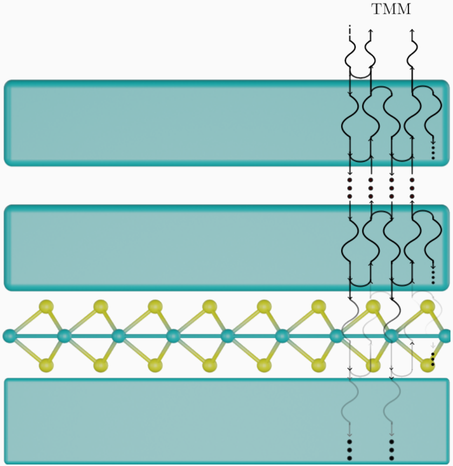
Incoherent Transfer Matrix Method (ITMM)

$$Q_l = \left(I_{l+1}^{A-} + I_l^{B+}\right)(1 - \omega_l)$$

Reflections of all orders are included, but spatial coherence and hence spatial interference is still neglected[4].

[4] J. S. C. Prentice. J. Phys. D: Appl. Phys. 32 (1999) 2146.

Classical light absorption



Transfer Matrix Method (TMM)

$$Q_l(z) = \alpha_l I_0 \frac{\eta_l}{\eta_0} \frac{|\boldsymbol{E}_l(z)|^2}{|\boldsymbol{E}_0^+|^2}$$

Propagation of normal E.M. fields.
Spatial coherence $\Rightarrow$ interference effects[5].

[5] K. Ohta, H. Ishida. Applied Optics 29(13) (1990), 1952.

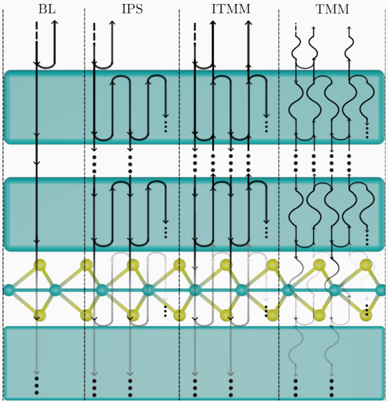
Comparison of the models

BL

No reflections but on the uppermost interface.

IPS

Multiple reflection of arbitrary order inside each layer, but no upwards transmission across interfaces.



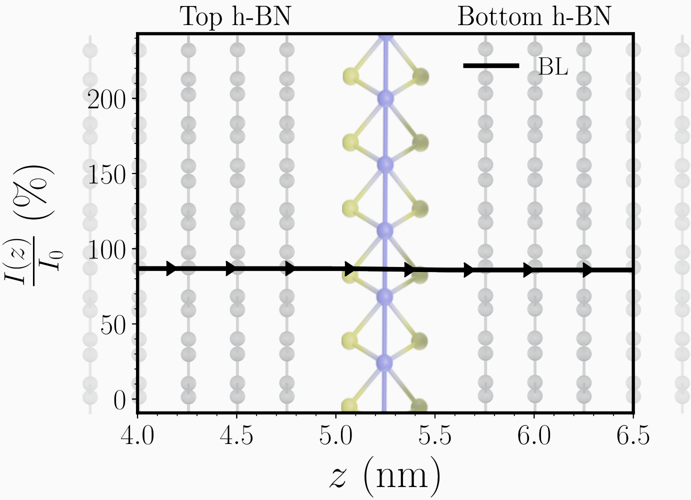
ITMM

Accounts for all reflections and paths.

TMM

Wave-like propagation of normal E.M. fields $\Rightarrow$ spatial coherence.

Comparison of the models



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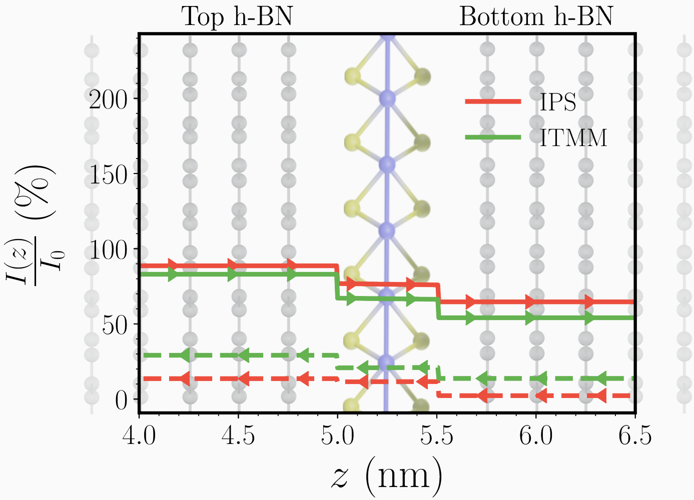

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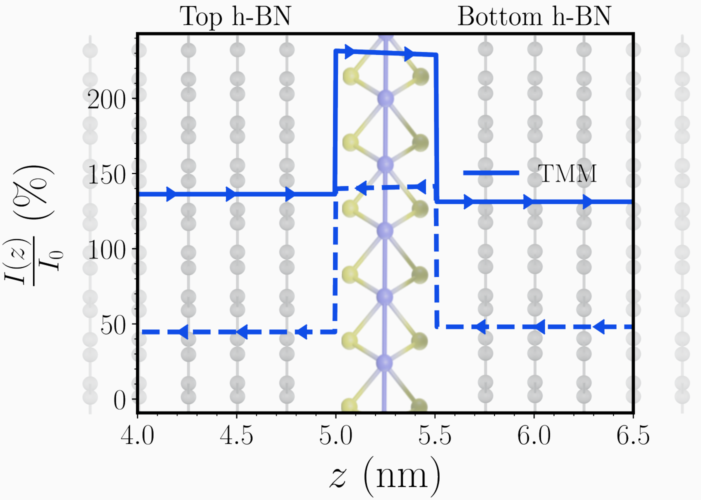

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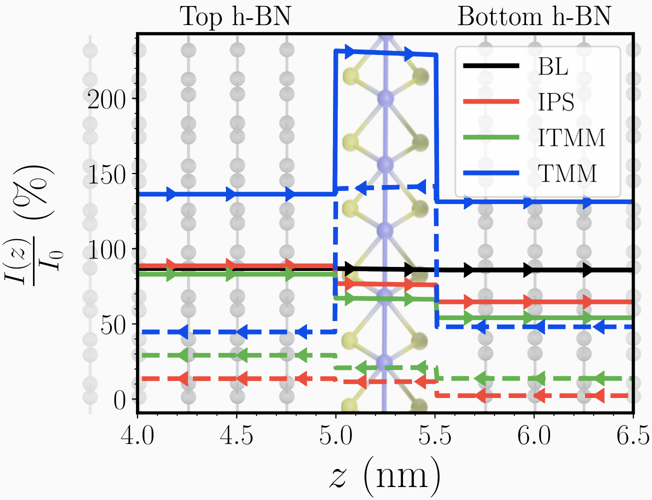

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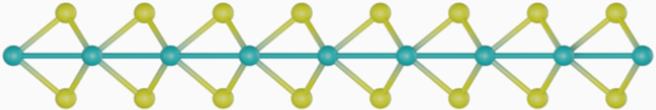

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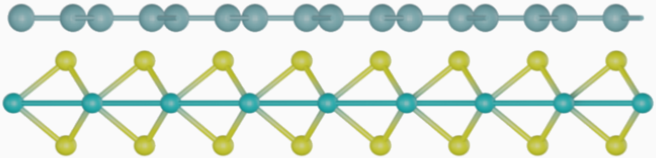

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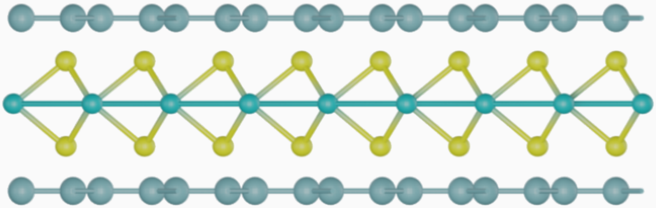

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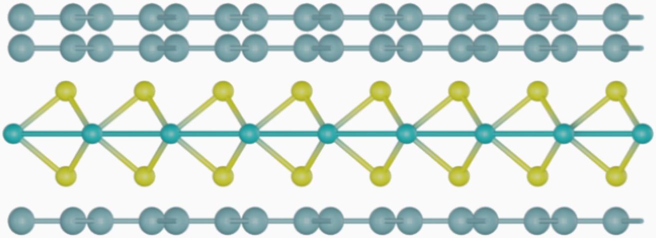

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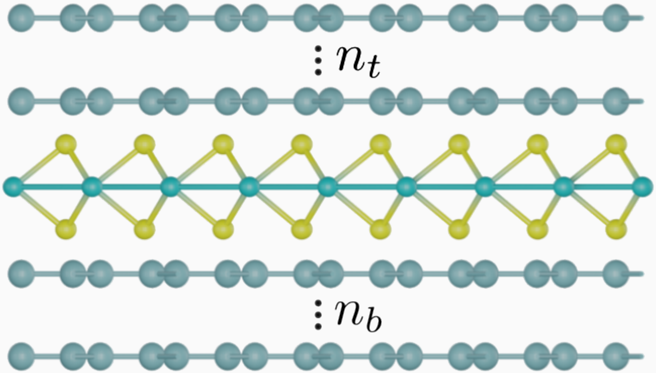

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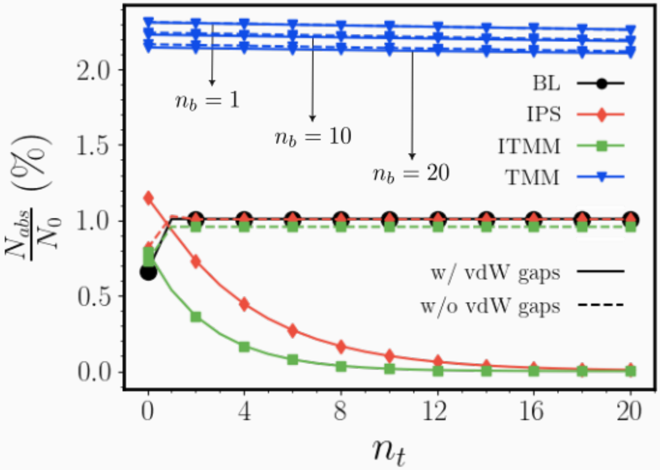

Substrate thickness $t_s = 270$ nm.

- For **BL**, independent of n_t, n_b.
- Top layer enhances optical coupling.

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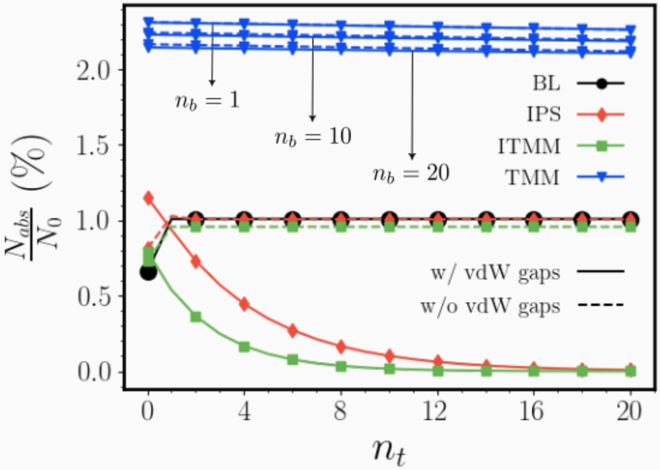

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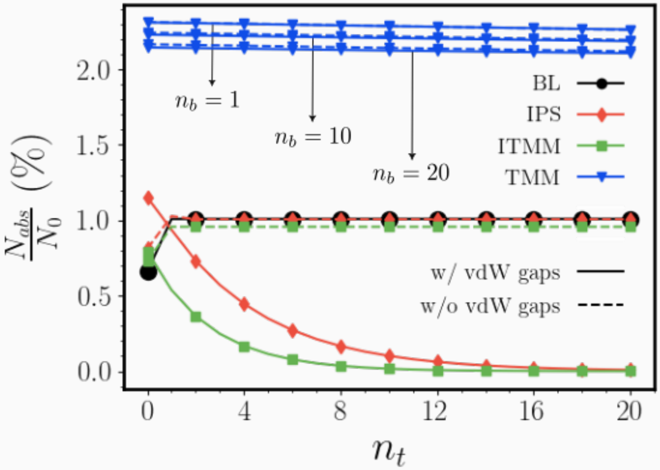

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- For **BL**, independent of n_t, n_b. Top layer enhances optical coupling.
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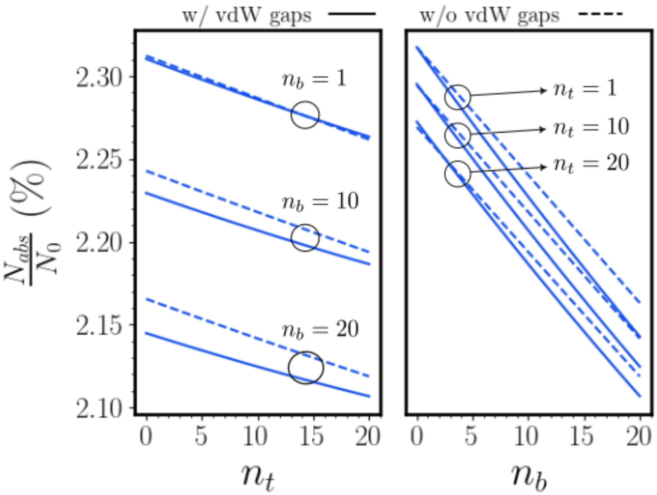
- TMM makes evident the importance of interference.

Effect of layer number and vdW gaps: TMM



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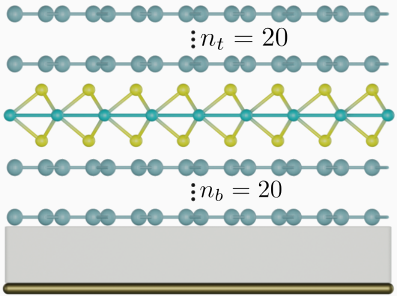

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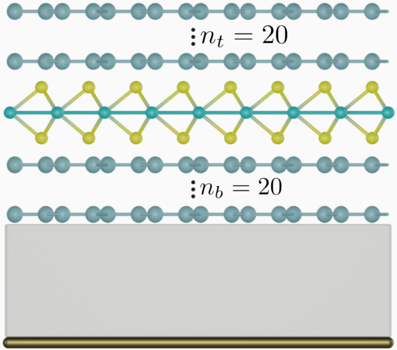

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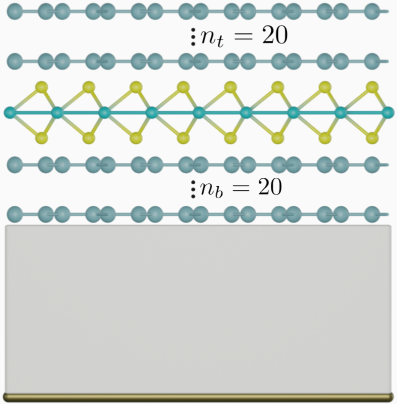
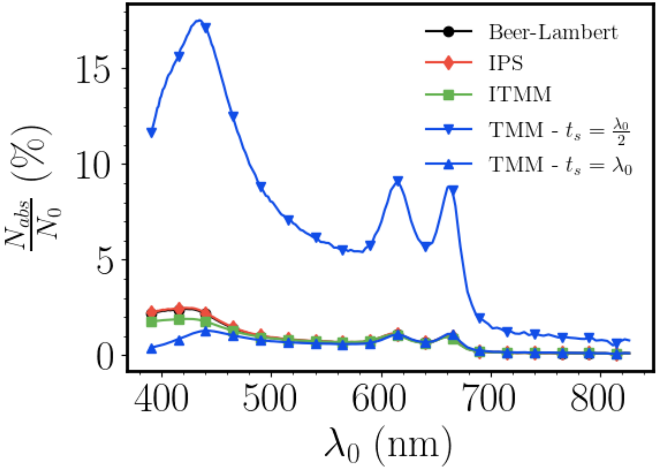


Effect of spatial coherence: resonances



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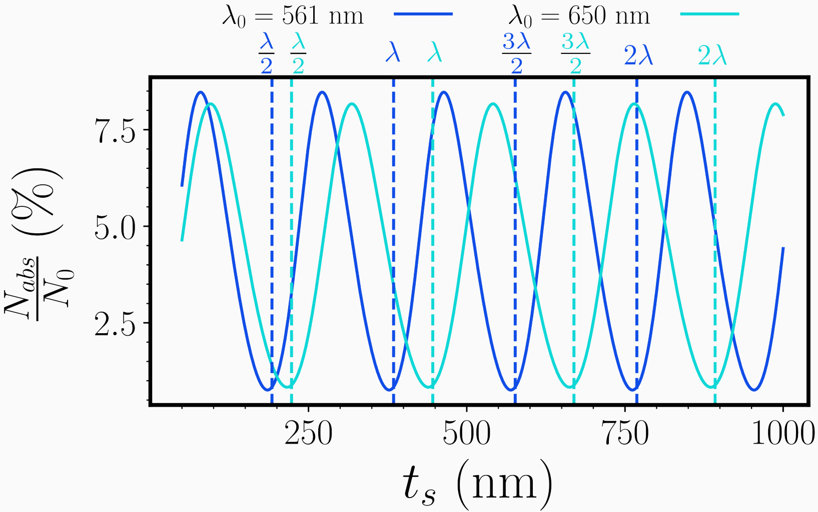

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- **encapsulating layers have little effect** on the result predicted by more realistic **TMM** model,
- comparison of the models reveals the **capital relevance of interference in thin-layer stacked structures**,
- **resonances must be investigated numerically** in order to **maximize absorption** at active region.

Appendix

- Thickness ML hBN $t_{\mathrm{hBN}} = 0.25$ nm. [10.1021/acsami.8b08609].
- Thickness of vdW gaps between hBN monolayers $d_{\mathrm{IL\ hBN}} = 0.08$ nm. [10.1021/ct200880m].
- S-S distance in ML MoS_2 $t_{\mathrm{MoS_2}} = 0.5$ nm.
- Thickness of vdW gaps between hBN and MoS_2 monolayers is an averaged value $d = 0.05$ nm.
- Input wavelength at vacuum $\lambda_0 = 561$ nm and substrate thickness $t_s = 270$ nm unless stated otherwise.
- Refractive indices: SiO_2 [10.1364/JOSA.55.001205], hBN [10.1002/pssb.201800417], ML MoS_2 [10.1515/nanoph-2018-0120], doped Si [10.1103/PhysRevB.27.985].