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LayerOptics: Microscopic modeling of optical coefficients in layered materials

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Reference

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LayerOptics: Microscopic modeling of optical coefficients in layered materials

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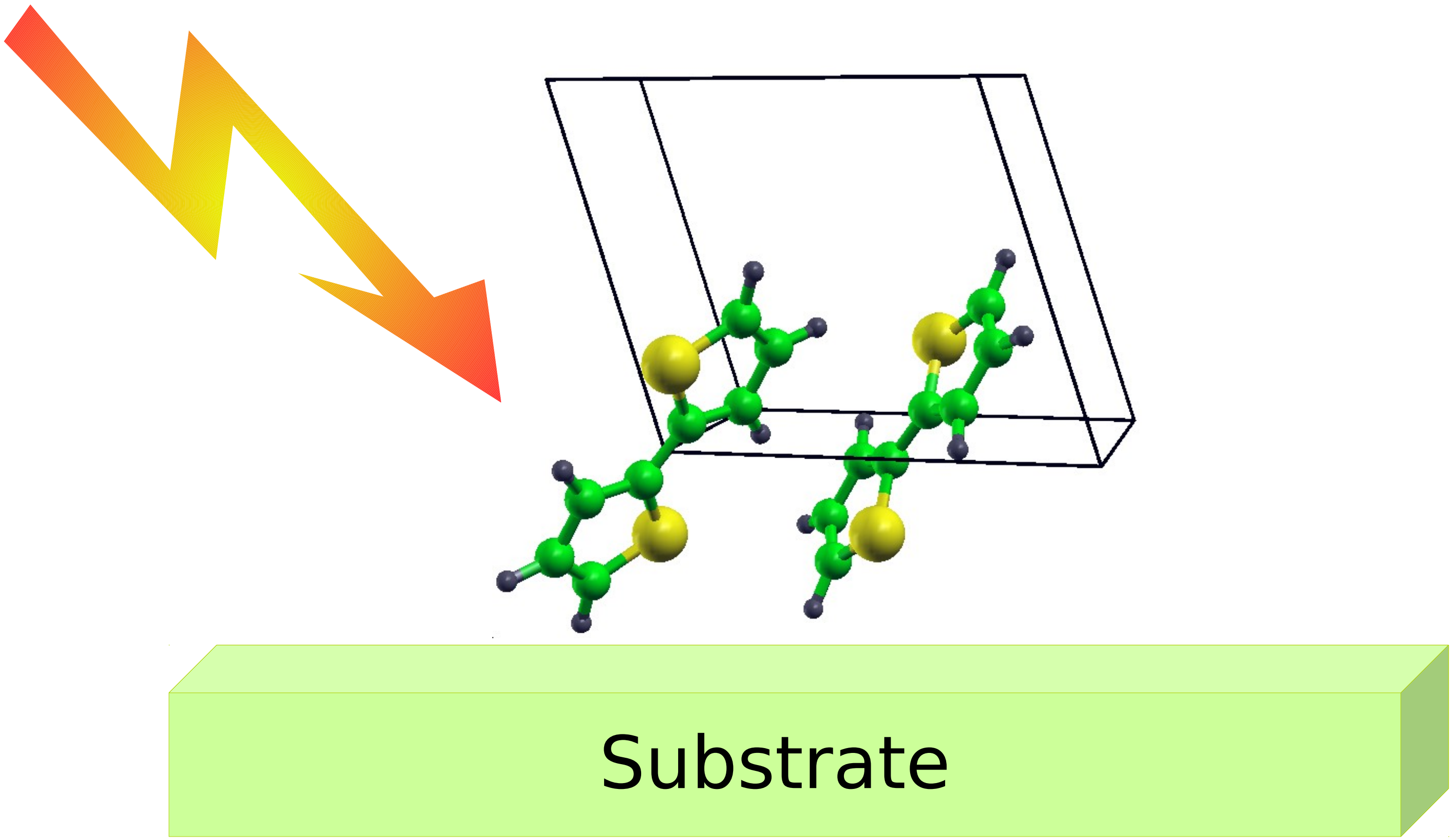
ABSTRACT

Theoretical spectroscopy is a powerful tool to describe and predict optical properties of materials. While nowadays routinely performed, first-principles calculations only provide bulk dielectric tensors in Carte-

Introduction



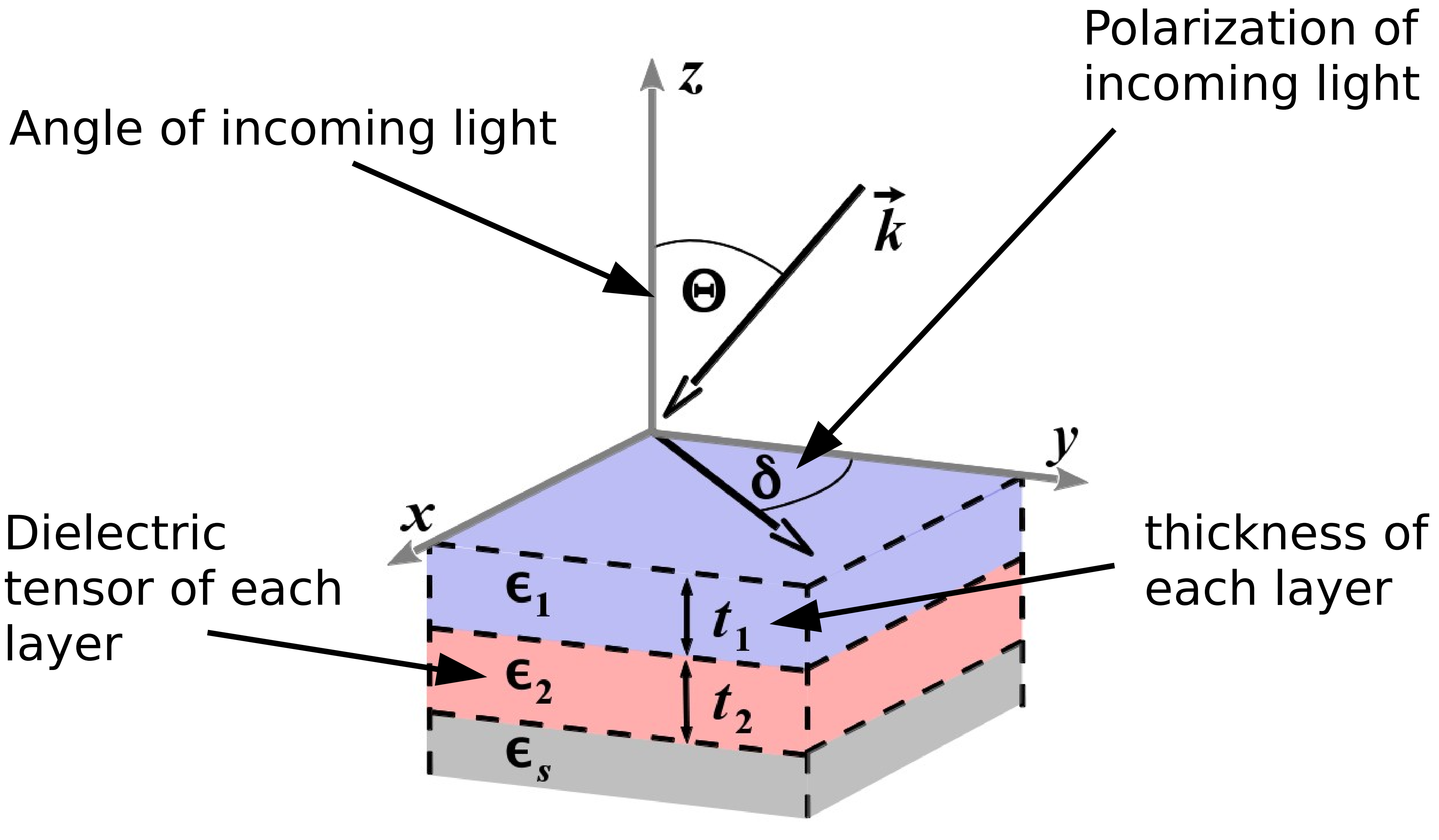
- Layered structures are technologically relevant field of study
- Response to light not fully determined by dielectric tensor of constituting layer materials

Introduction

- What is response of layered system to light?
- What is the absorption/ reflection/ transmission spectrum?
- What is the influence of anisotropy?
- What is the influence of experimental parameters (beam angle, light polarization)?

➡ Tool to obtain optical coefficients of layered systems of anisotropic materials from dielectric tensor of components

Setup



Angle of incoming light
Polarization of incoming light
Dielectric tensor of each layer
thickness of each layer
z
x
y
k
Θ
δ
ϵ1
ϵ2
ϵs
t1
t2

Formalism

$$\mathbf{E} = \sum_{\sigma=1}^{4} A_\sigma \mathbf{p}_\sigma \exp \mathrm{i} \left[k_x x + k_y y + k_{z,\sigma} z - \omega t \right]$$

$$\mathbf{A} = \begin{cases} A_1 & \leftarrow \quad \text{downwards perpendicular component} \\ A_2 & \leftarrow \quad \text{upwards perpendicular component} \\ A_3 & \leftarrow \quad \text{downwards parallel component} \\ A_4 & \leftarrow \quad \text{upwards perpendicular component.} \end{cases}$$

Boundary Condition of electric and magnetic field at layer boundaries

Matrix formulism for the amplitudes

Matrix equation

$$\mathbf{A}(0) = \underbrace{\mathbb{D}^{-1}(0)\mathbb{T}(1)\mathbb{T}(2)\ldots\mathbb{T}(N-1)\mathbb{T}(N)\mathbb{D}(s)}_{=\mathbb{T}}\mathbf{A}(S).$$

Amplitude
In vacuum

Transfer matrix
of layer 1

Amplitude
In substrate

Final output

$$\mathcal{T}_p = c\mu_0|A_3(S)|^2|\mathbf{p}_3(S) \times \mathbf{q}_3(S)|,$$

$$\mathcal{T}_s = c\mu_0|A_1(S)|^2|\mathbf{p}_1(S) \times \mathbf{q}_1(S)|,$$

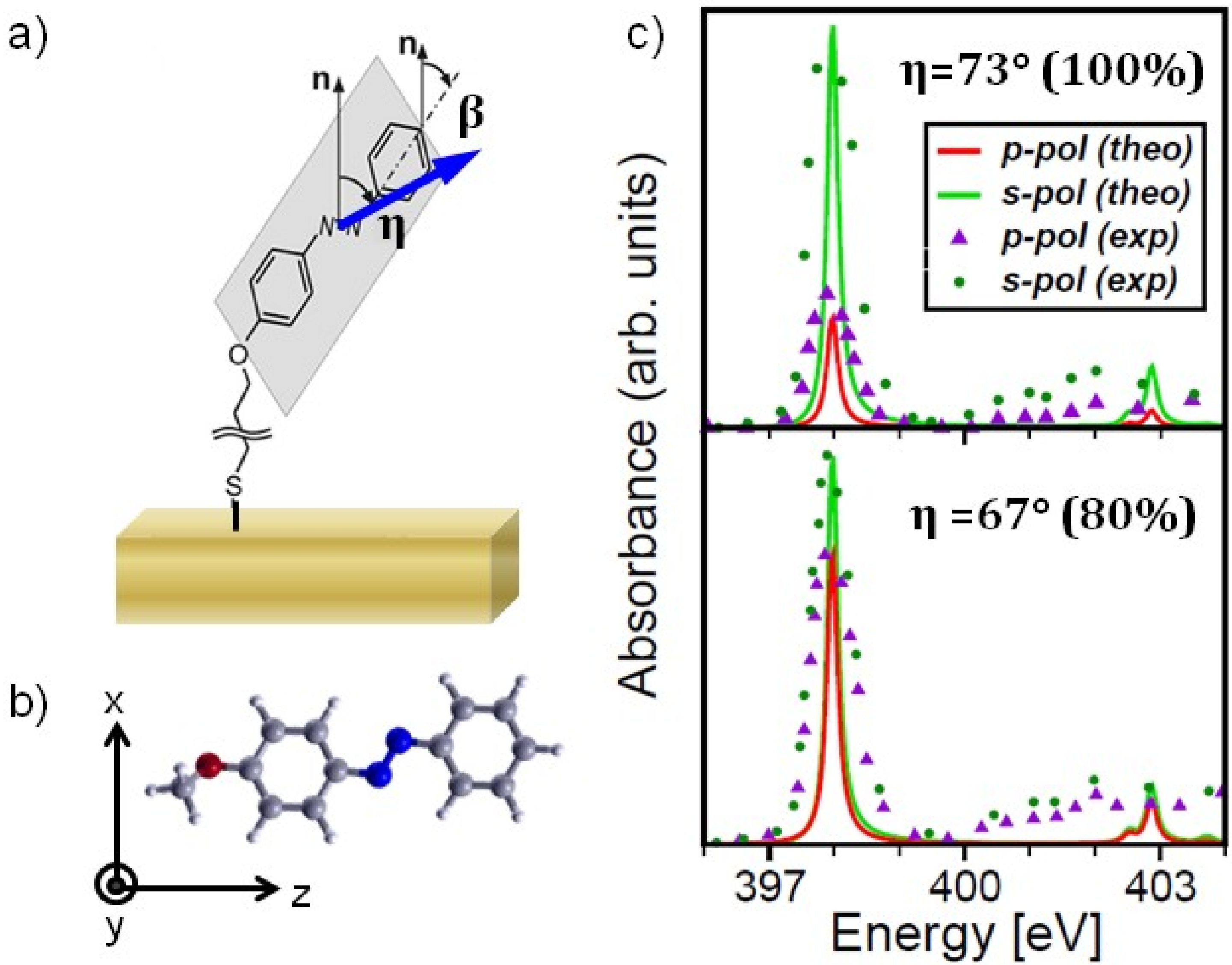
Transmission coefficients

$$\mathcal{R}_p = |A_4(0)|^2,$$

$$\mathcal{R}_s = |A_2(0)|^2$$

Reflection coefficients

Selected Examples: Azobenzene SAM



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LayerOptics Tutorial

by Christian Vorwerk & Caterina Cocchi for exciting *carbon*

Purpose: This tutorial demonstrates the usage of the **LayerOptics** package, which allows for the determination of optical coefficients of layered systems. We will demonstrate the functionality of the package on the example of bithiophene thin films.

Fold

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