Changing the color of atoms and molecules with light

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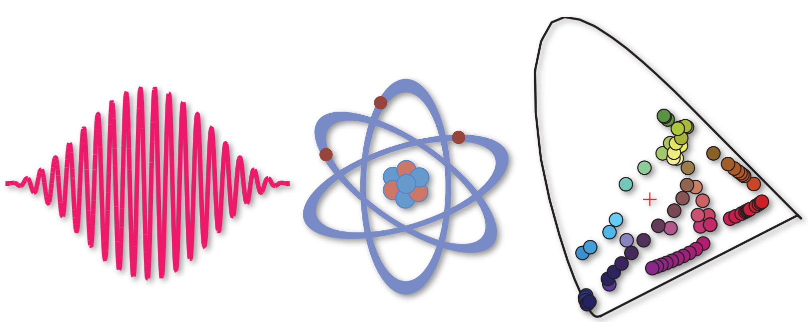


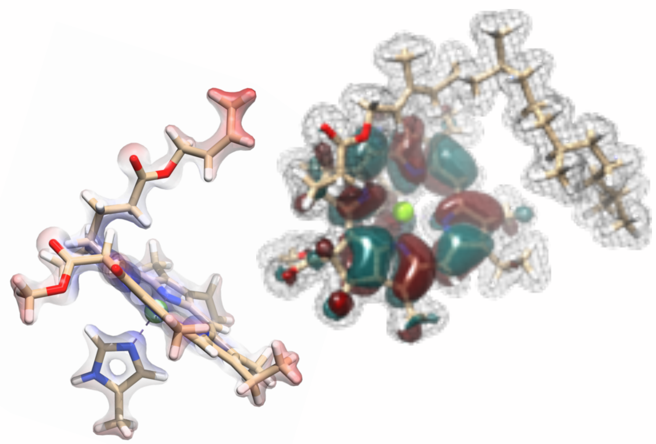
nano-bio spectroscopy group

eman ta zabal zazu
Universidad del País Vasco
Euskal Herriko Unibertsitatea

ETSF
European Theoretical Spectroscopy Facility

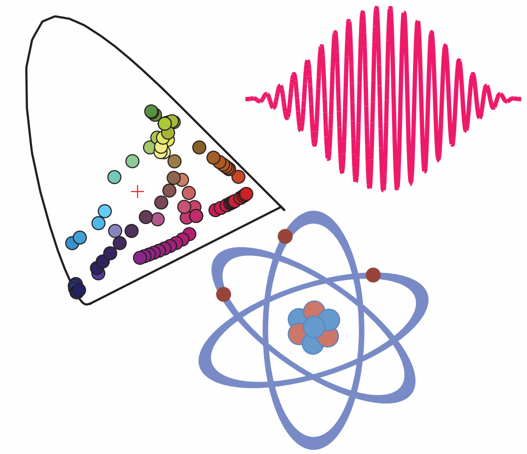
RES projects in the group (2013/2014)

Light harvesting complex LHCII + Octopus optimization



≈500 Khrs (x2 periods)

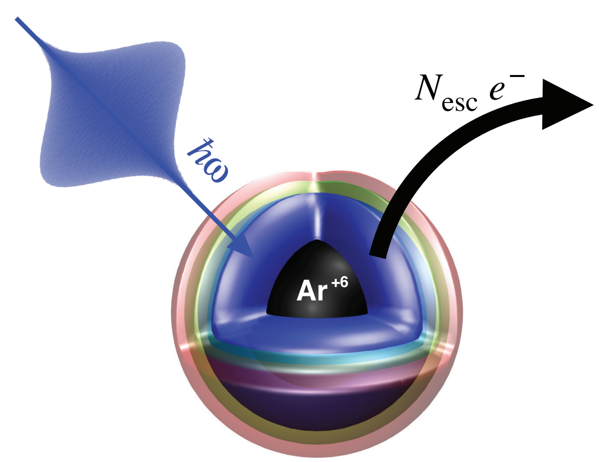
Light controlled optical properties of atoms and molecules



≈1000 Khrs (>x2 periods)

@ magerit

Ionization of noble gas atoms under strong X-ray radiation



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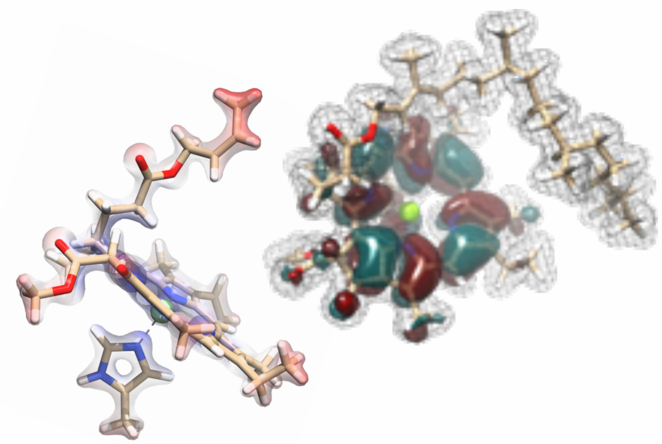

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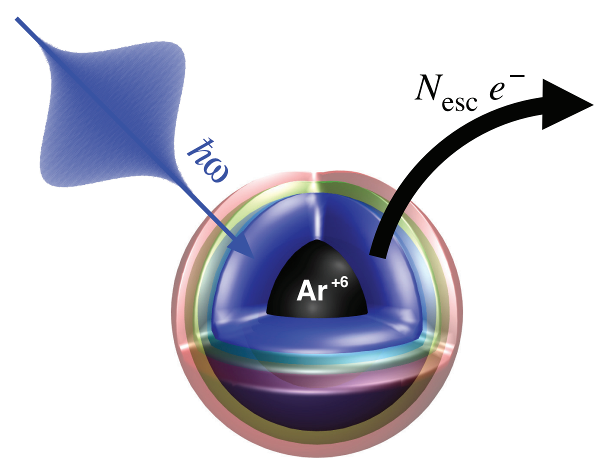

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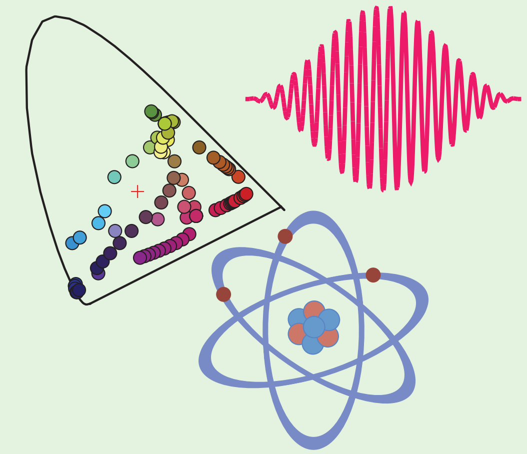

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@ magerit

People

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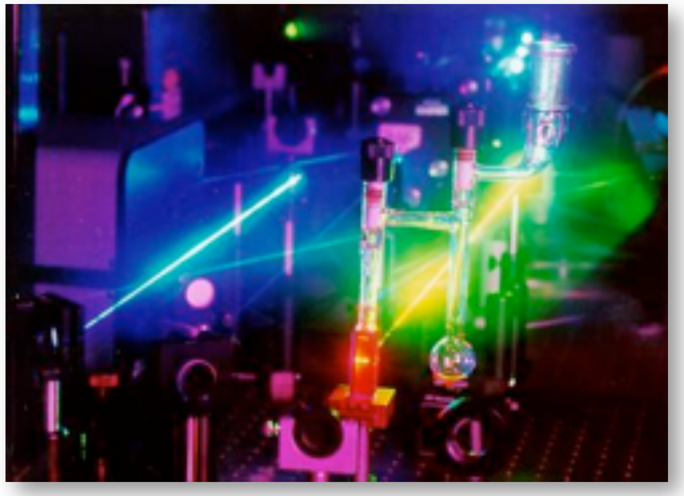
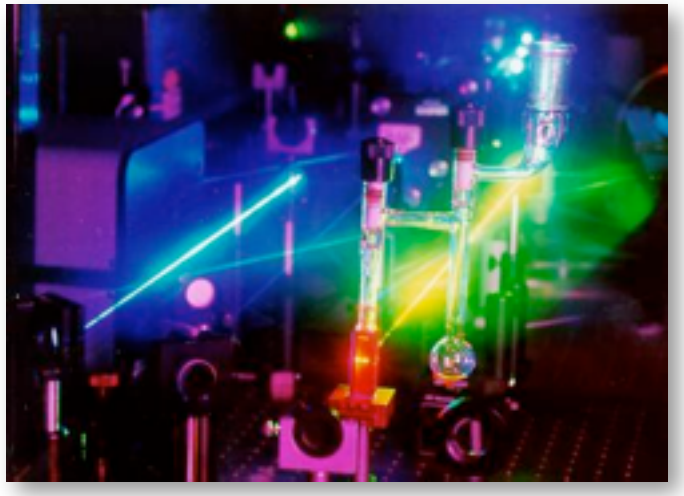
Motivation



To which extent it is possible to control the optical properties of matter with light?

Motivation

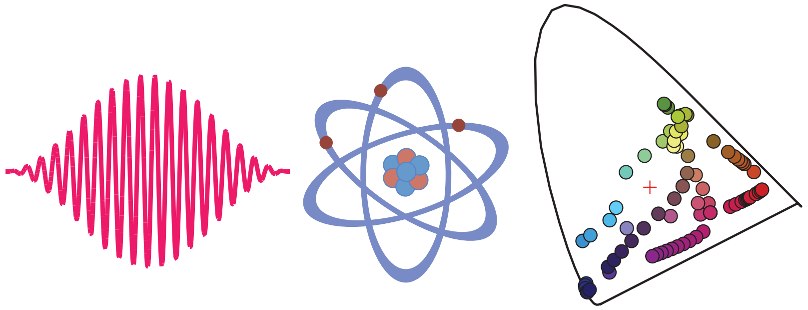


To which extent it is possible to control the optical properties of matter with light?

A specific case:

Show how it possible to turn visible transparent gases of atoms and molecules and control their color with lasers

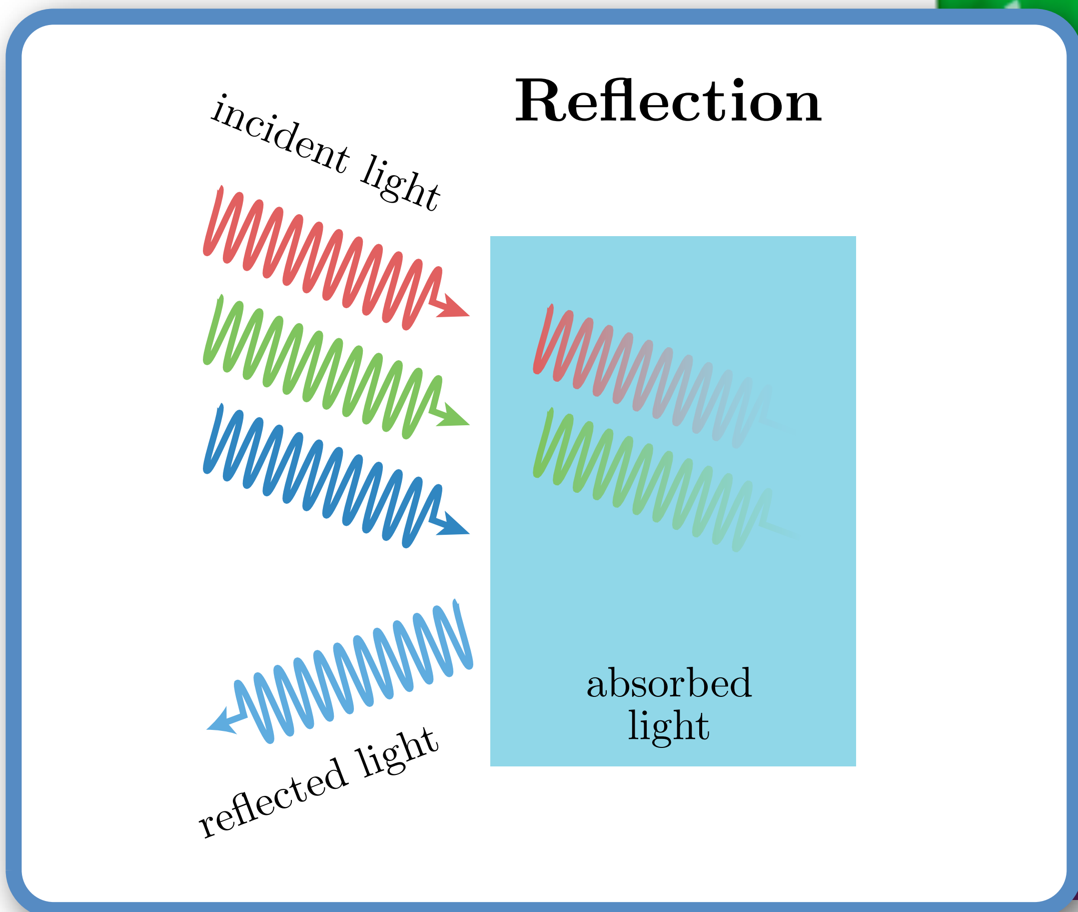
Outline

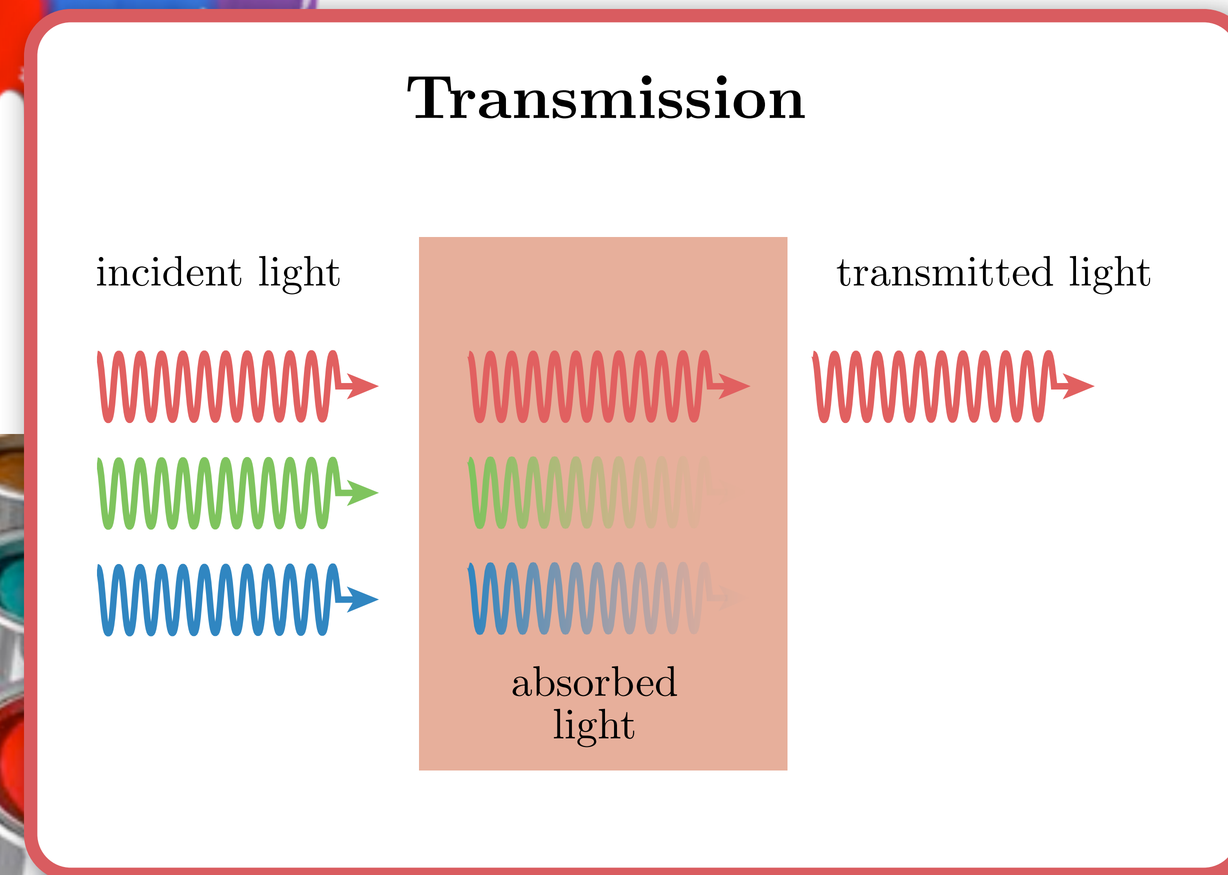


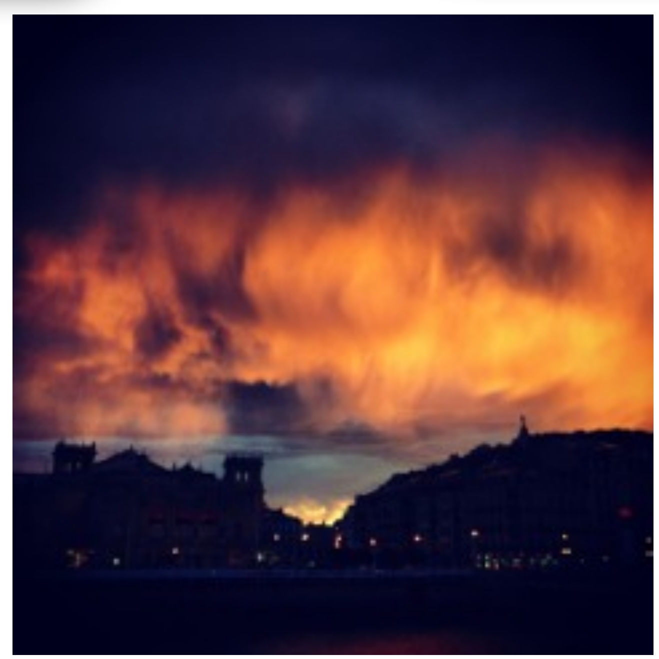
- **Overview:**
  - **color perception**
  - **idea**
- **Theory and tools:**
  - **TDDFT**
  - **OCT**
- **Applications:**
  - **hydrogen and methane**
- **Conclusions**

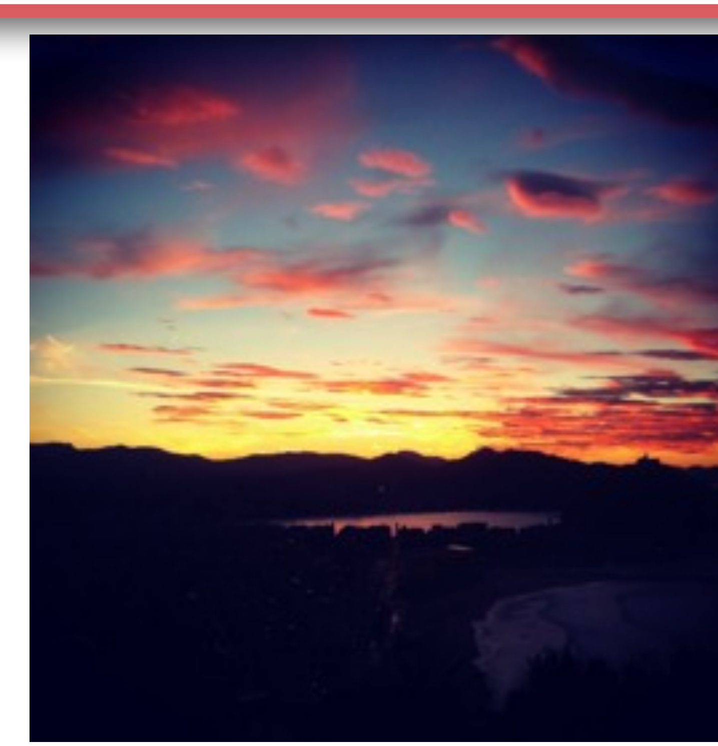
The perception of colors

The perception of colors









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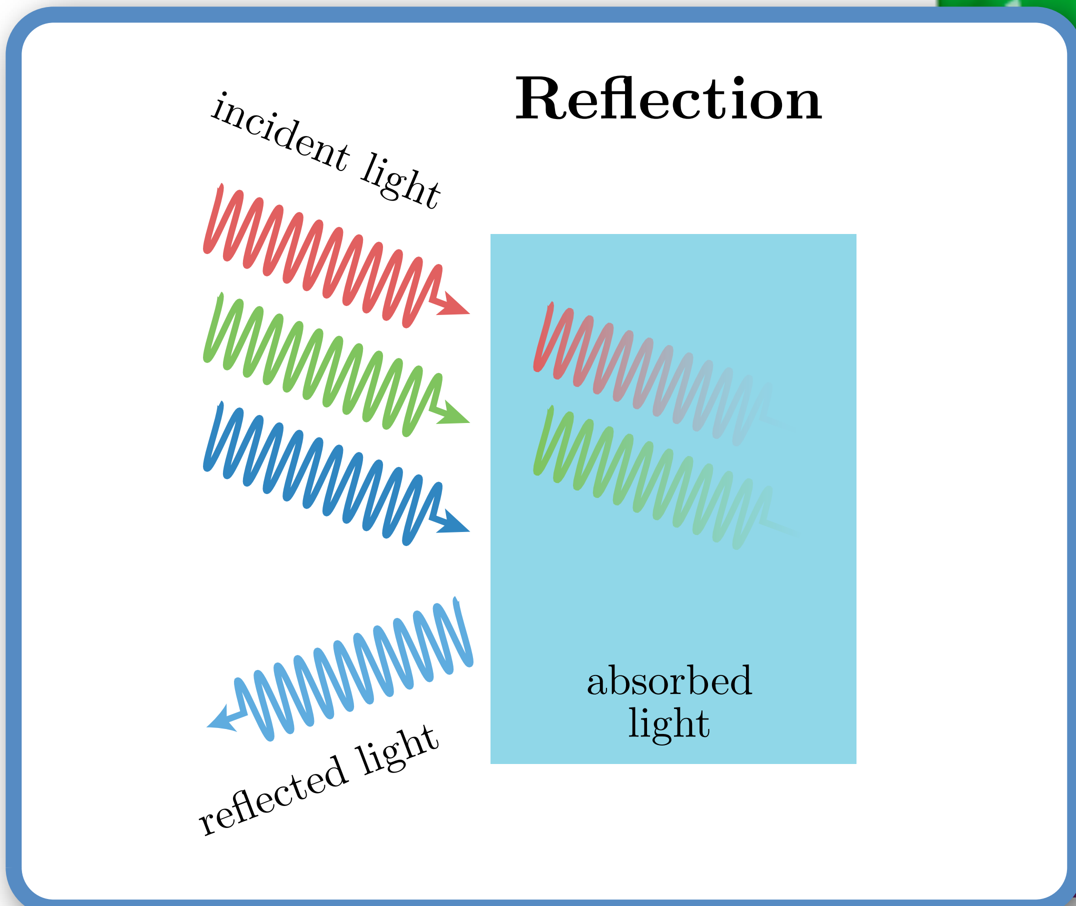

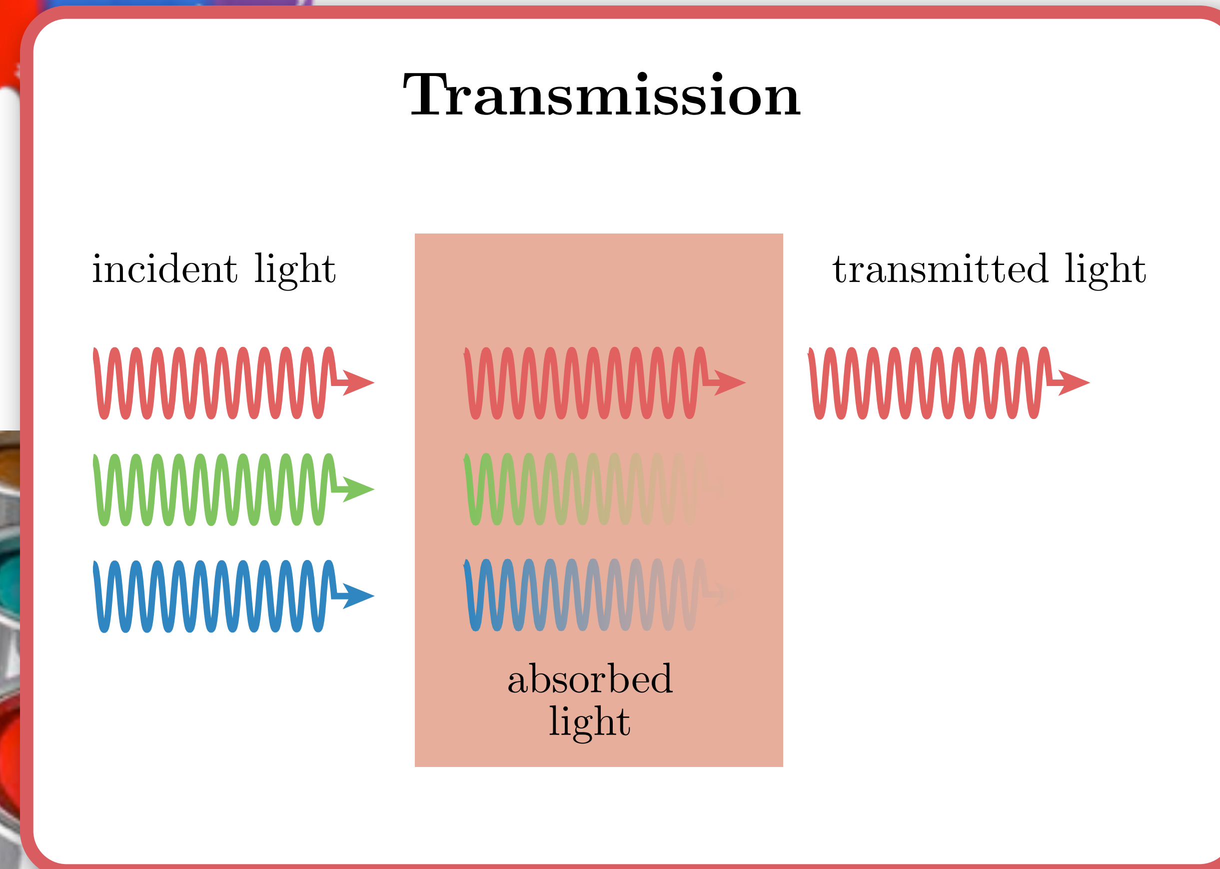

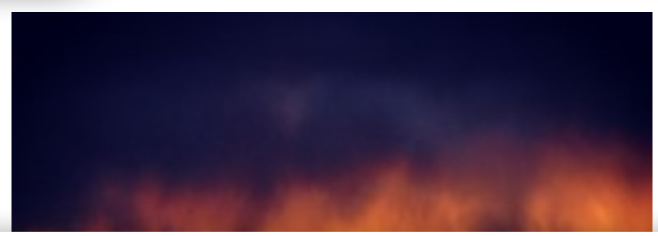

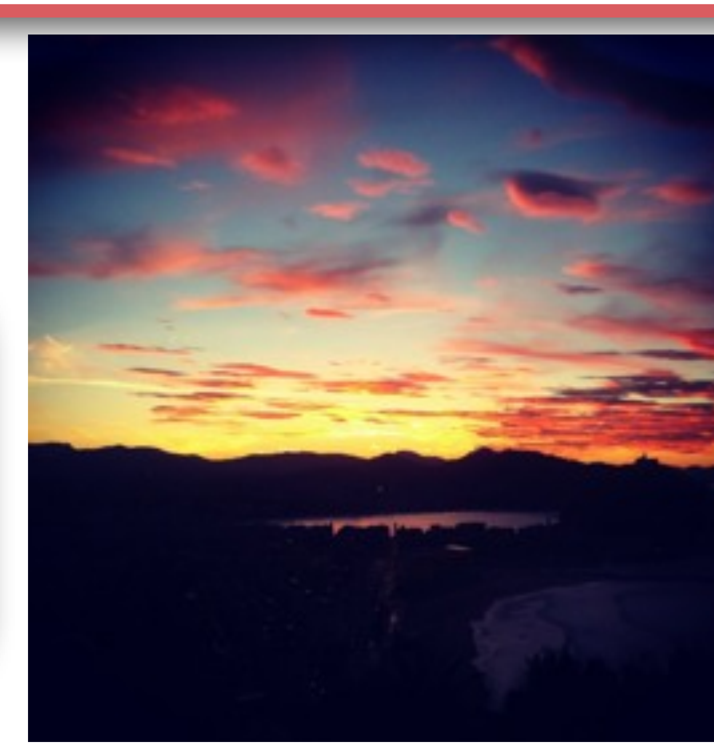

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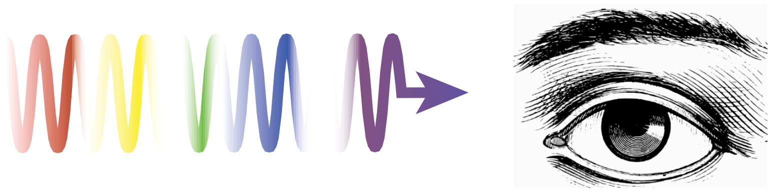

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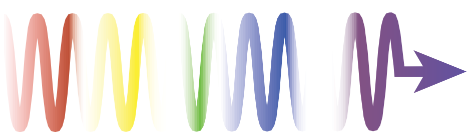

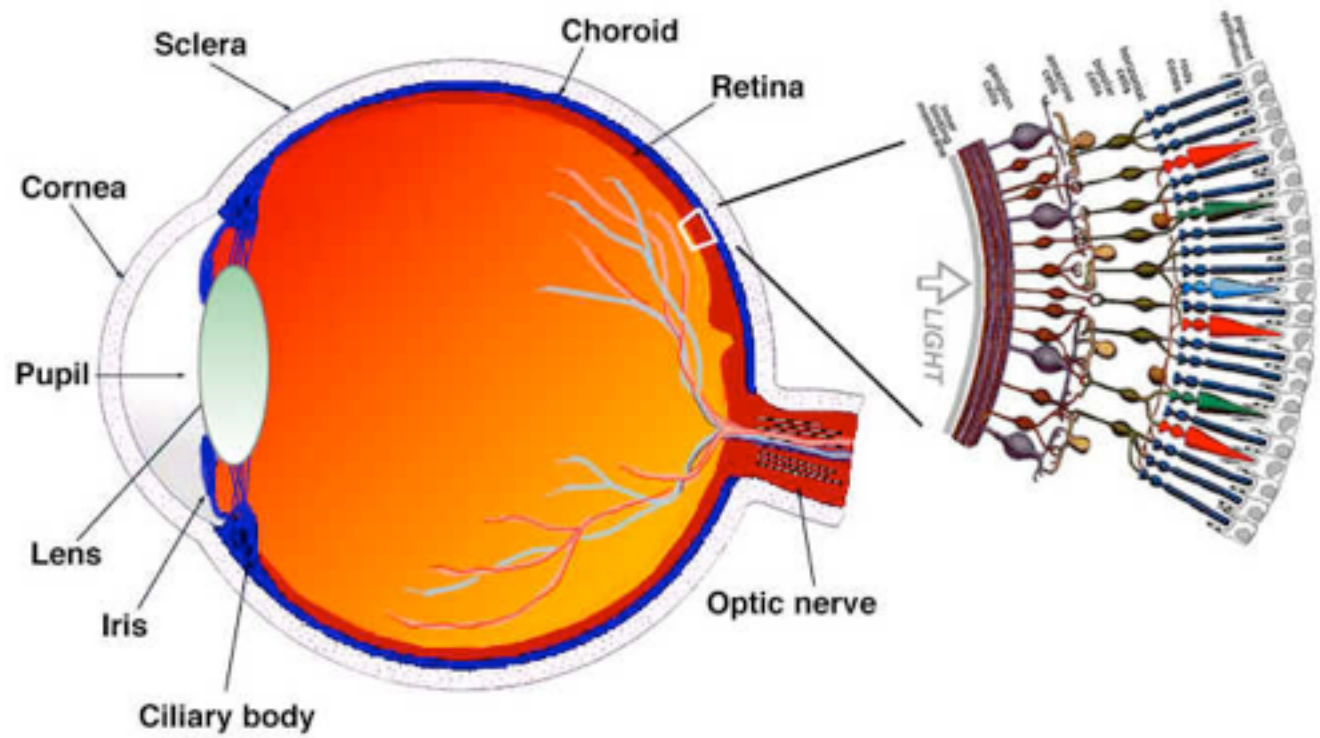

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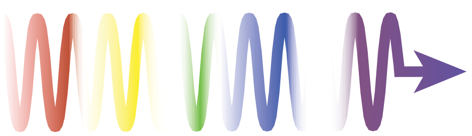
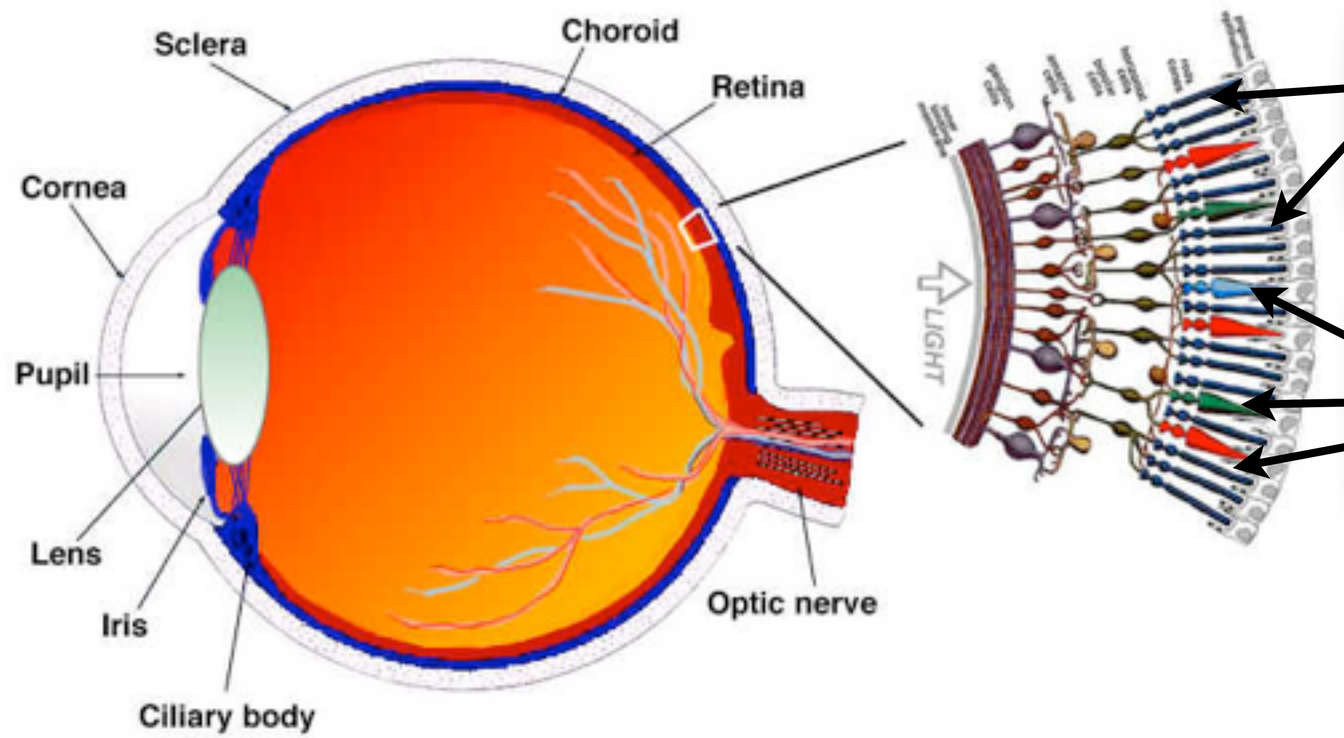
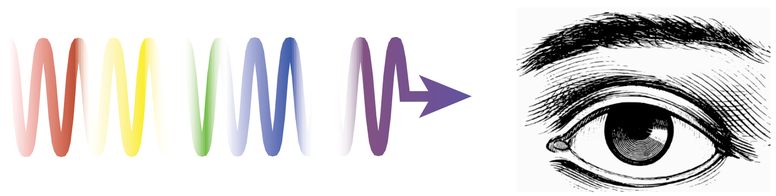


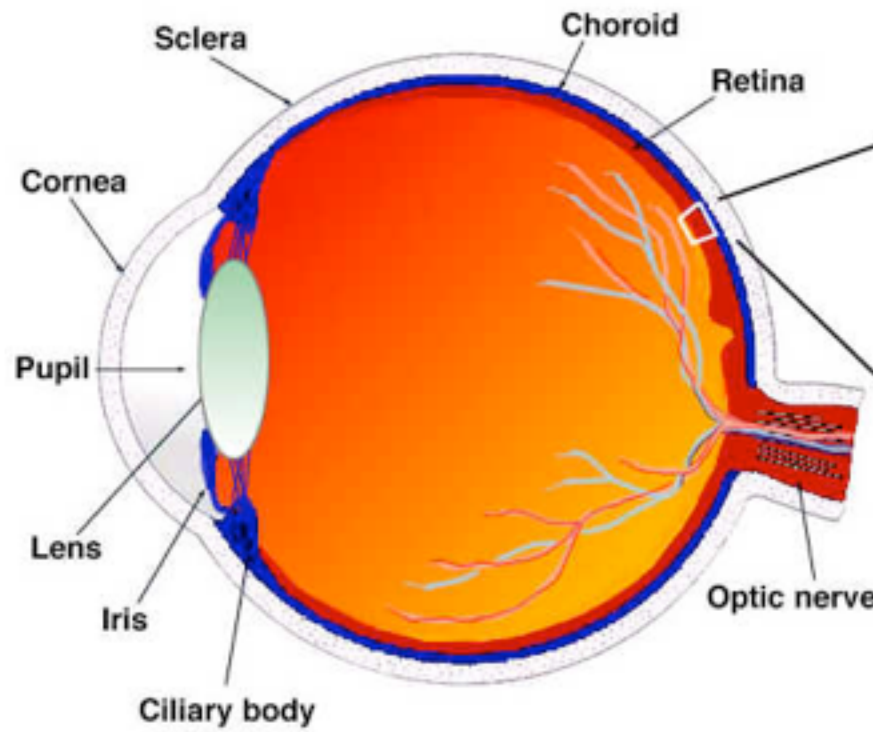


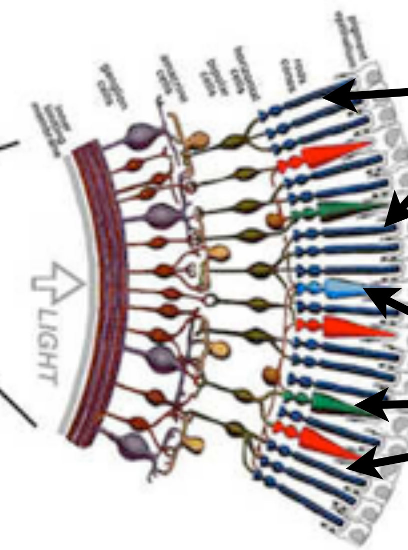
Rods:
scotopic vision
(i.e. night vision)

Cones (3 kinds):
photopic vision
(i.e. day vision)

The perception of colors







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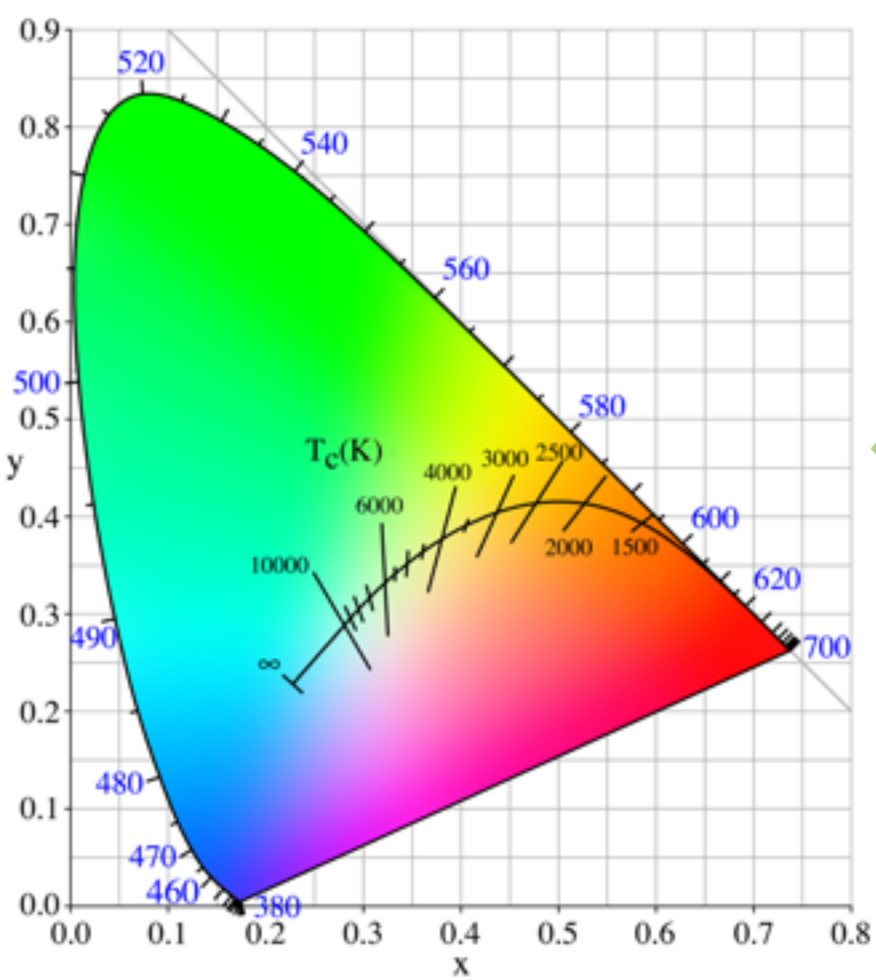
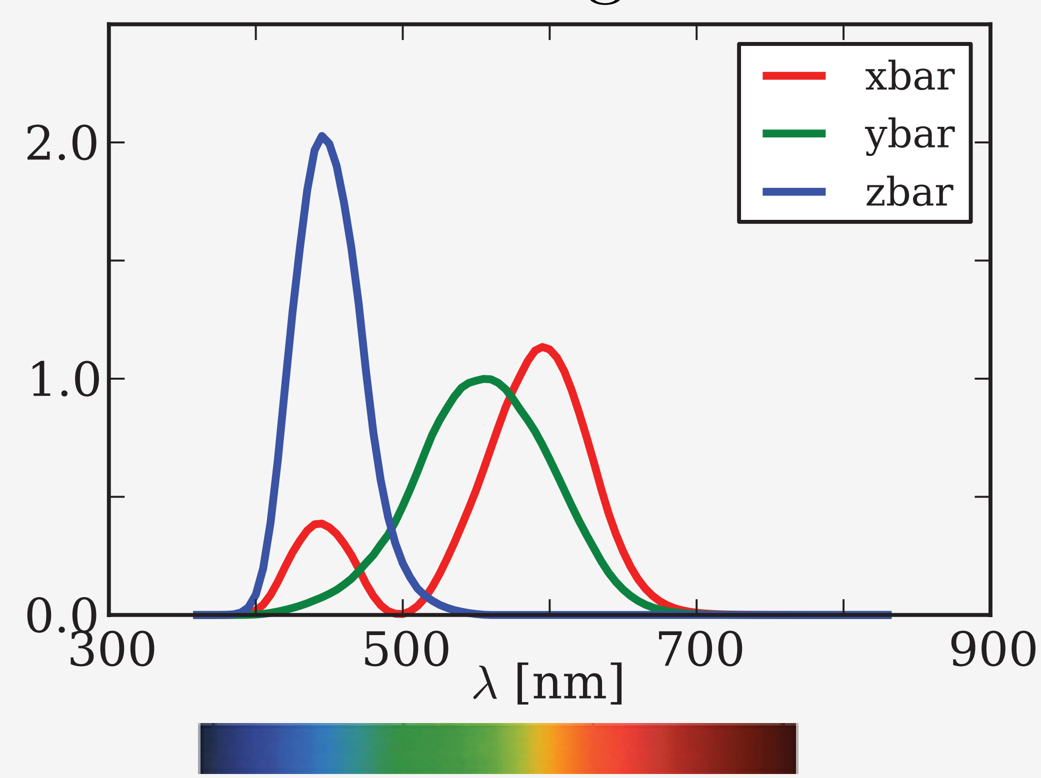
Chromaticity diagram



Color matching functions



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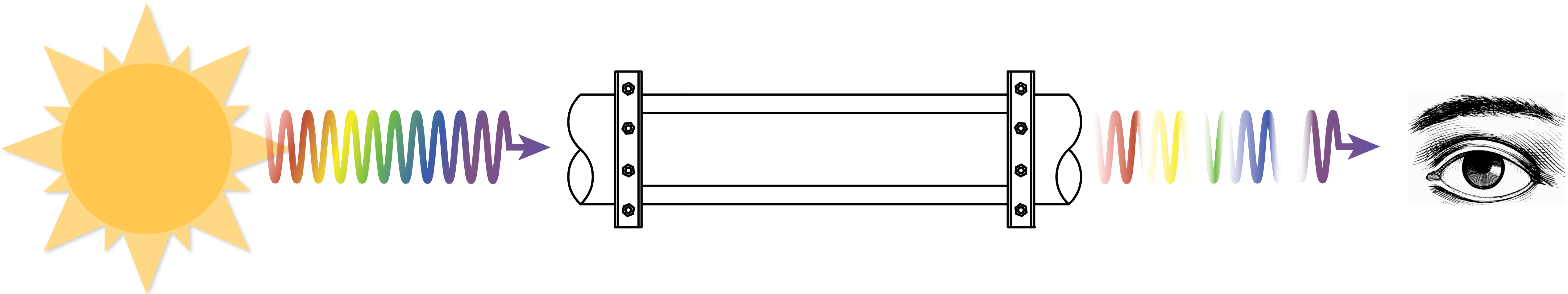

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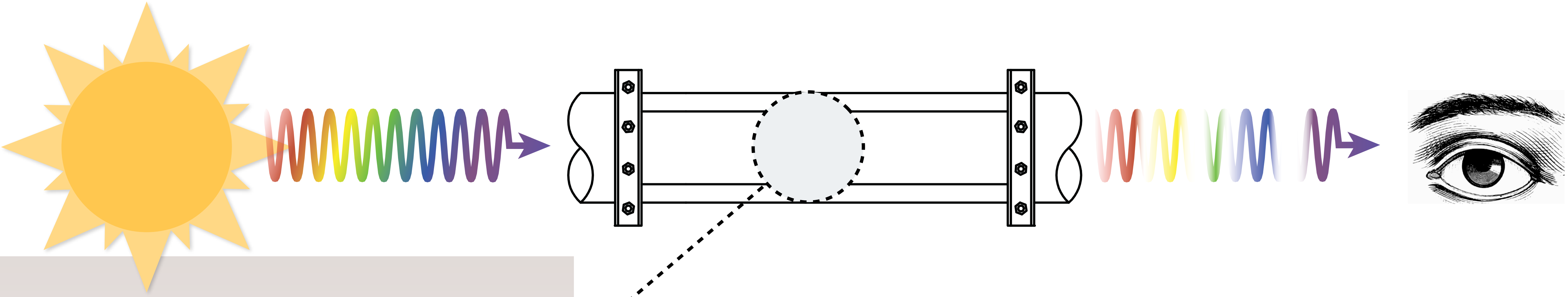
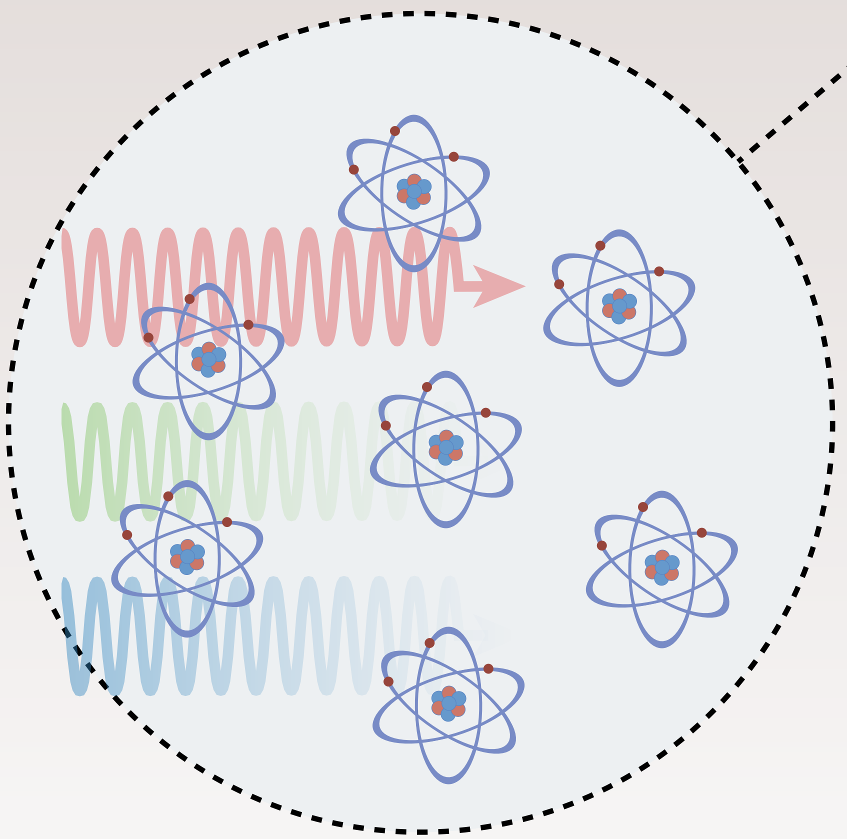


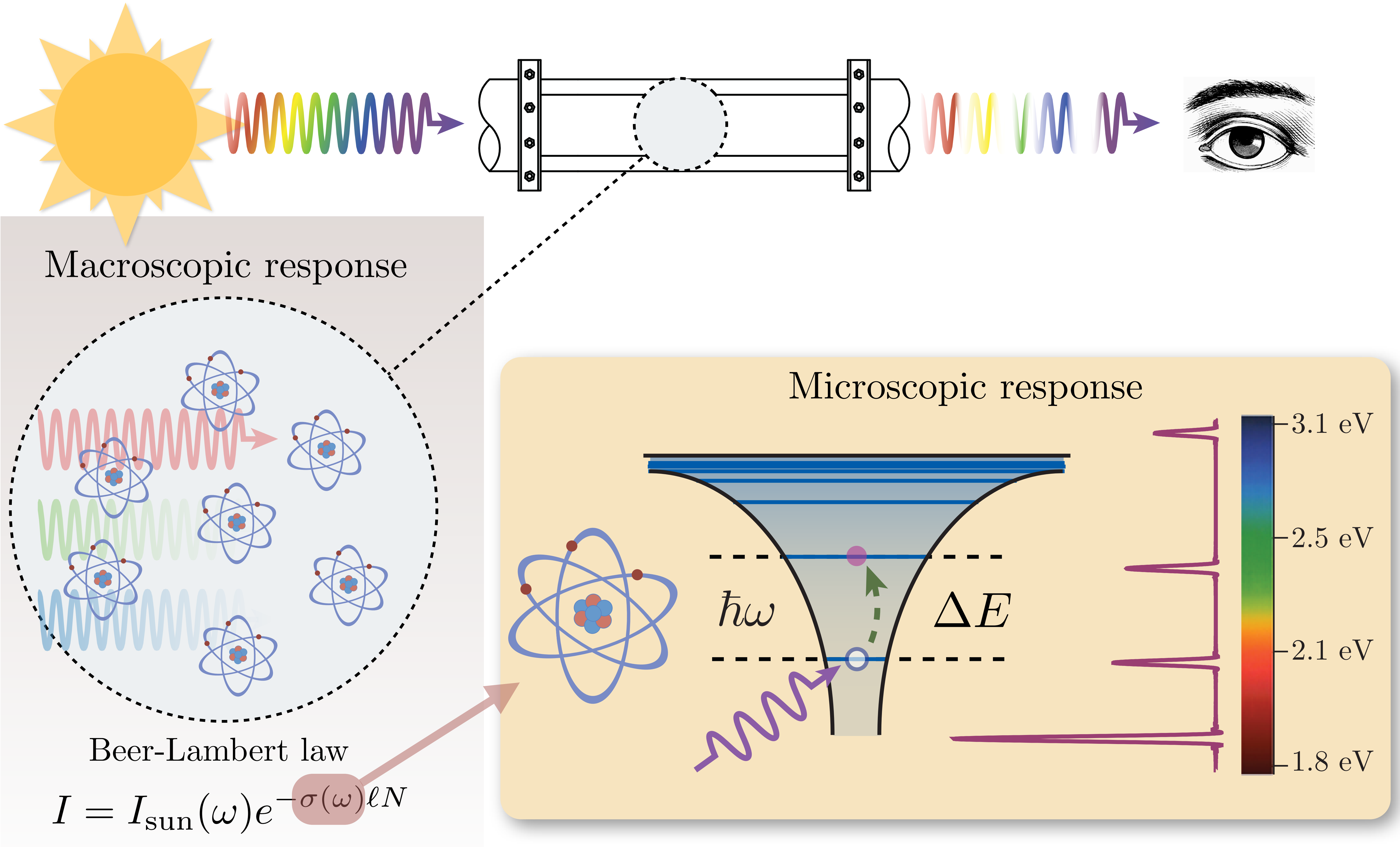
Macroscopic response



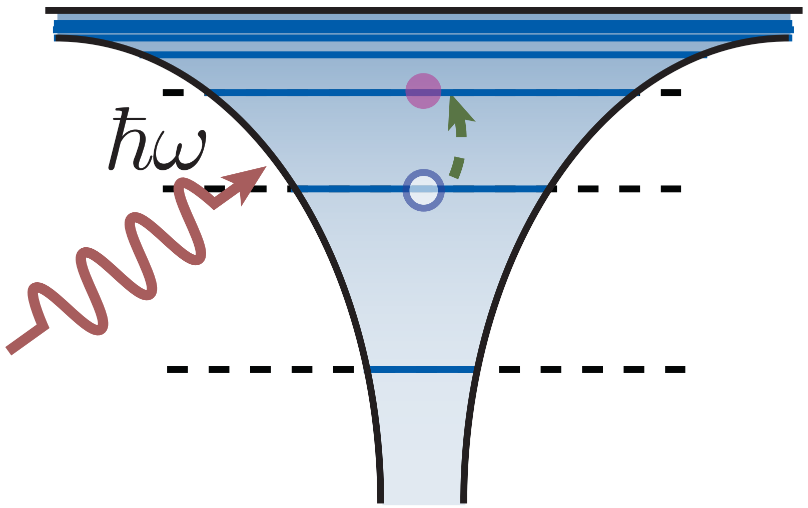
Beer-Lambert law

$$I = I_{\text{sun}}(\omega)e^{-\sigma(\omega)\ell N}$$

The perception of colors



Optical properties of excited states



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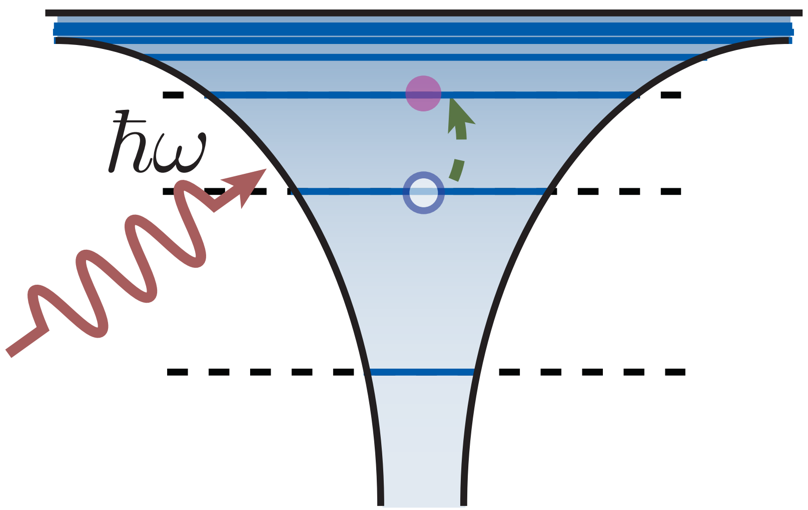

Hydrogen

$$\Delta E(n, N) = E_0 \left[\frac{1}{N^2} - \frac{1}{n^2} \right]$$

N=1 Lyman series (UV)

N=2 Balmer series (VIS)

N=3 Paschen series (IR)

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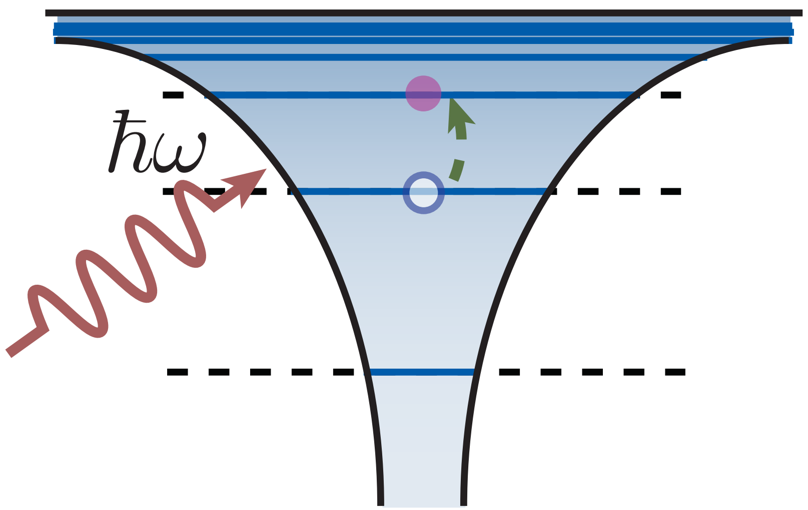

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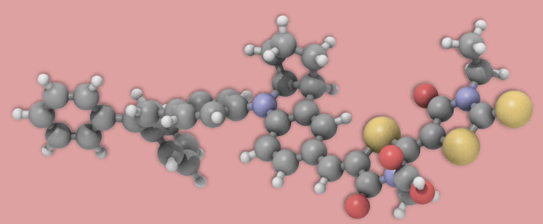
Larger systems have more complex excited-state structure



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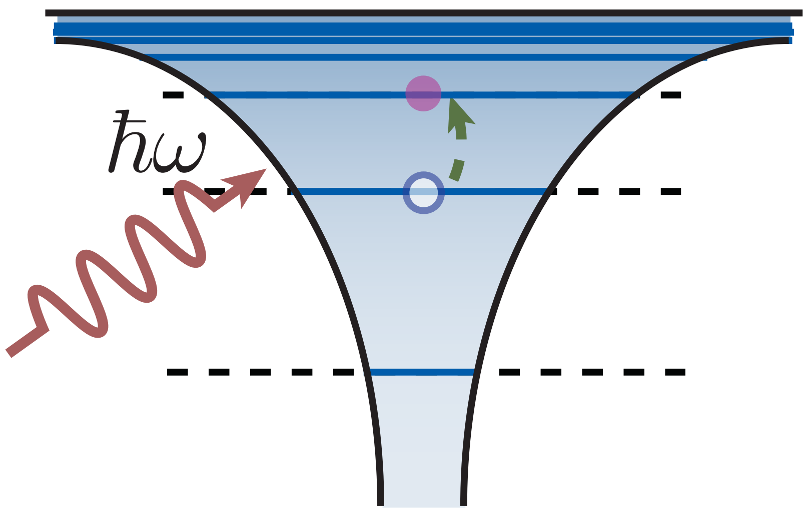

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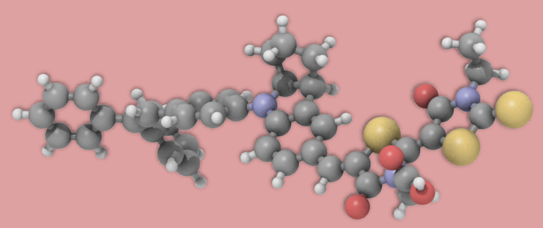
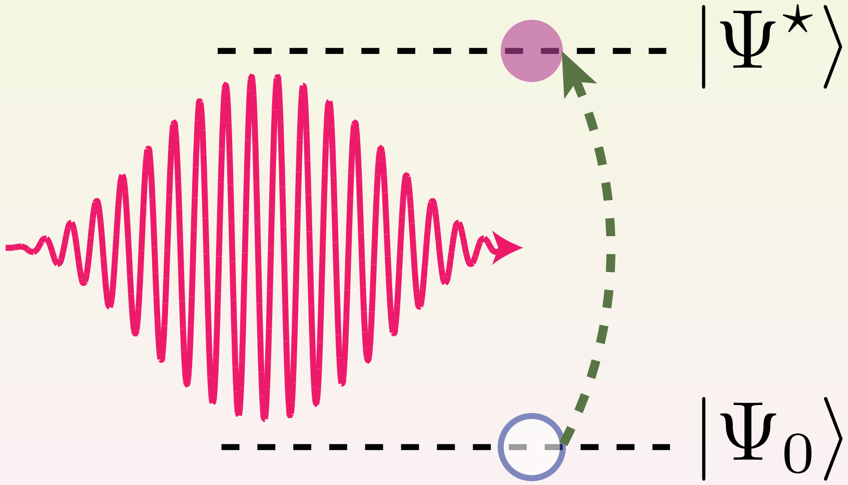


Present day laser sources can create tailored excited states



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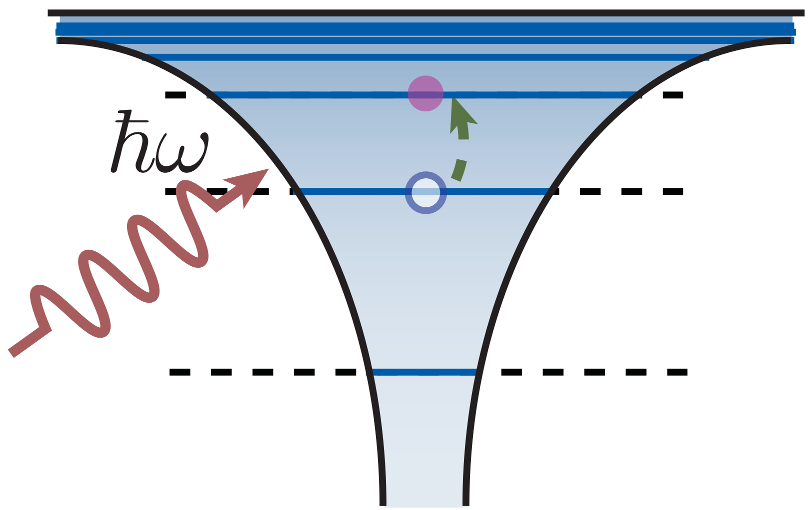

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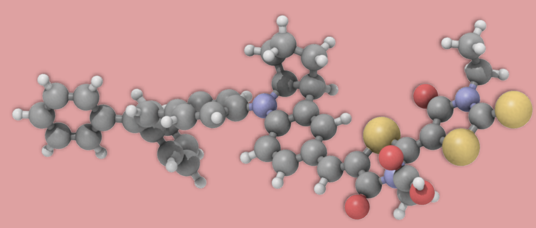

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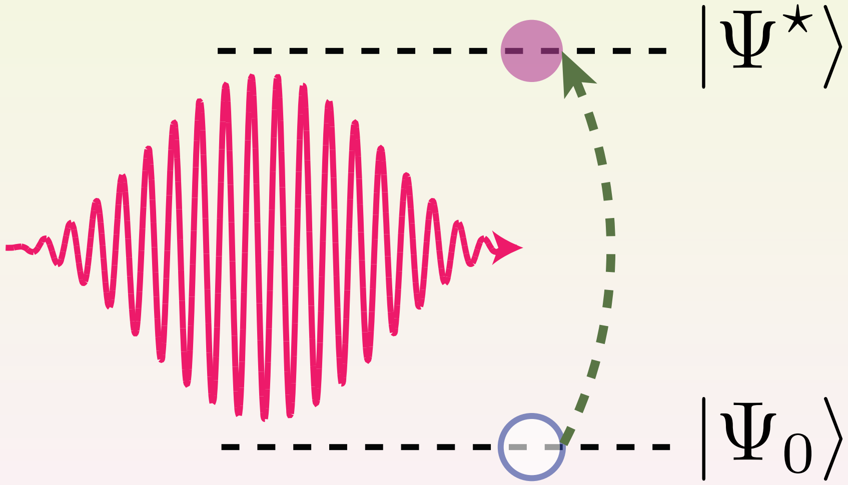
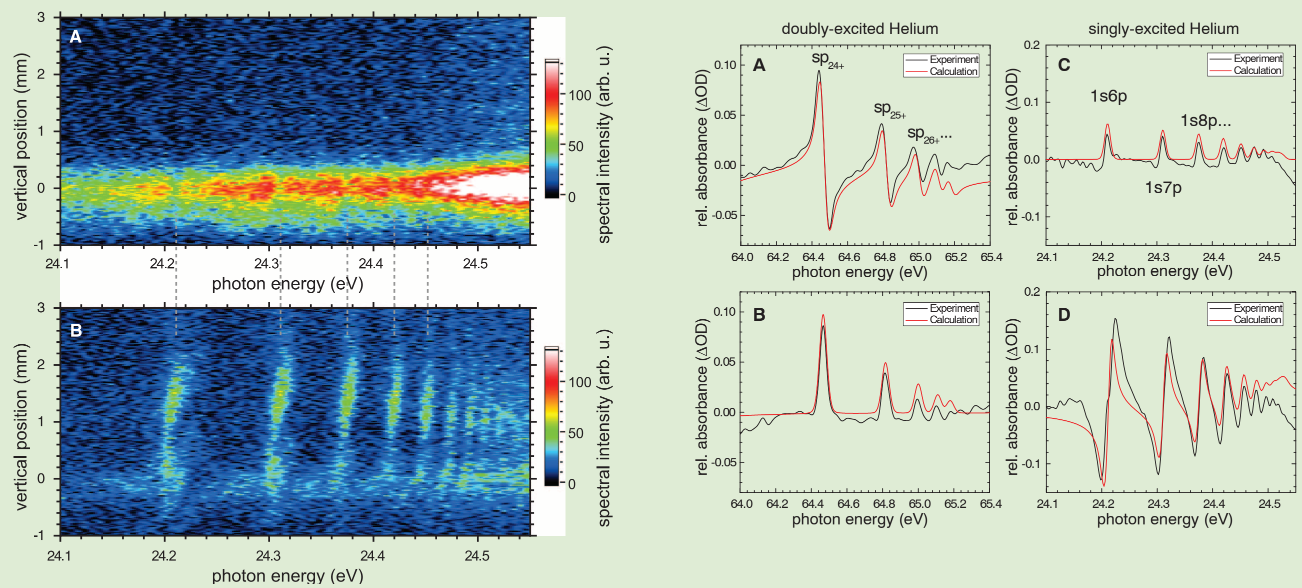


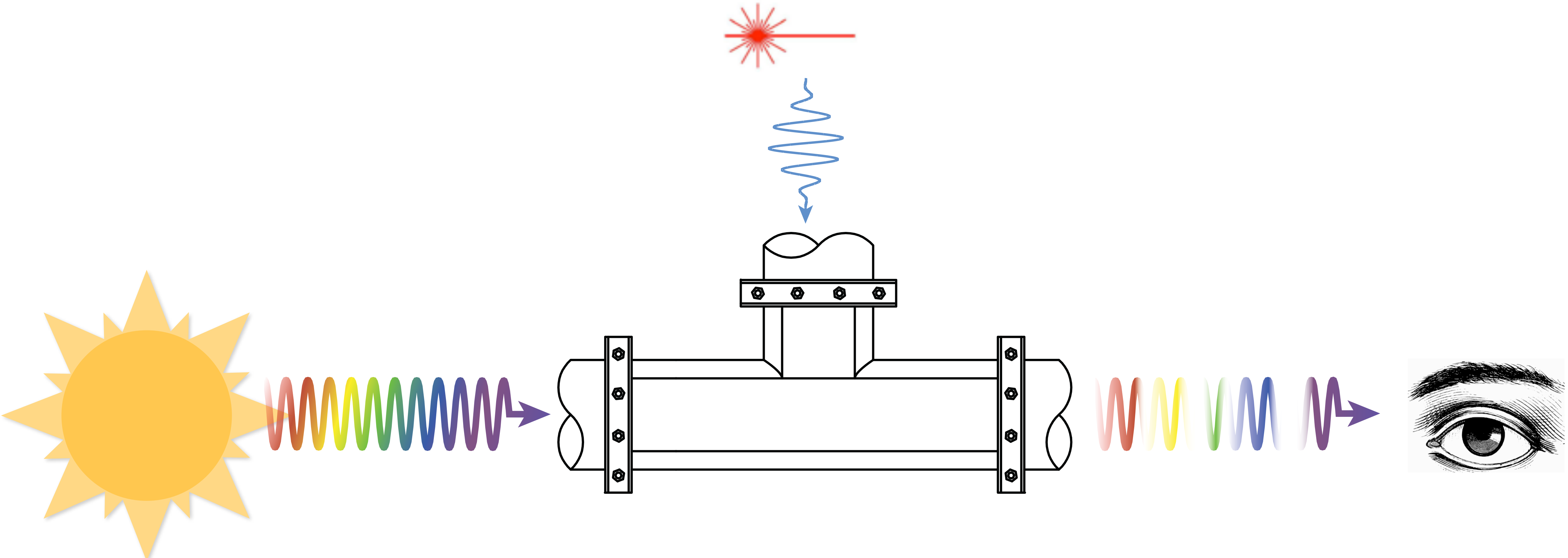
In principle we can do more

Fano - Lorentz transition



C. Ott, et al. *Science* **340**, 716 (2013).

The idea



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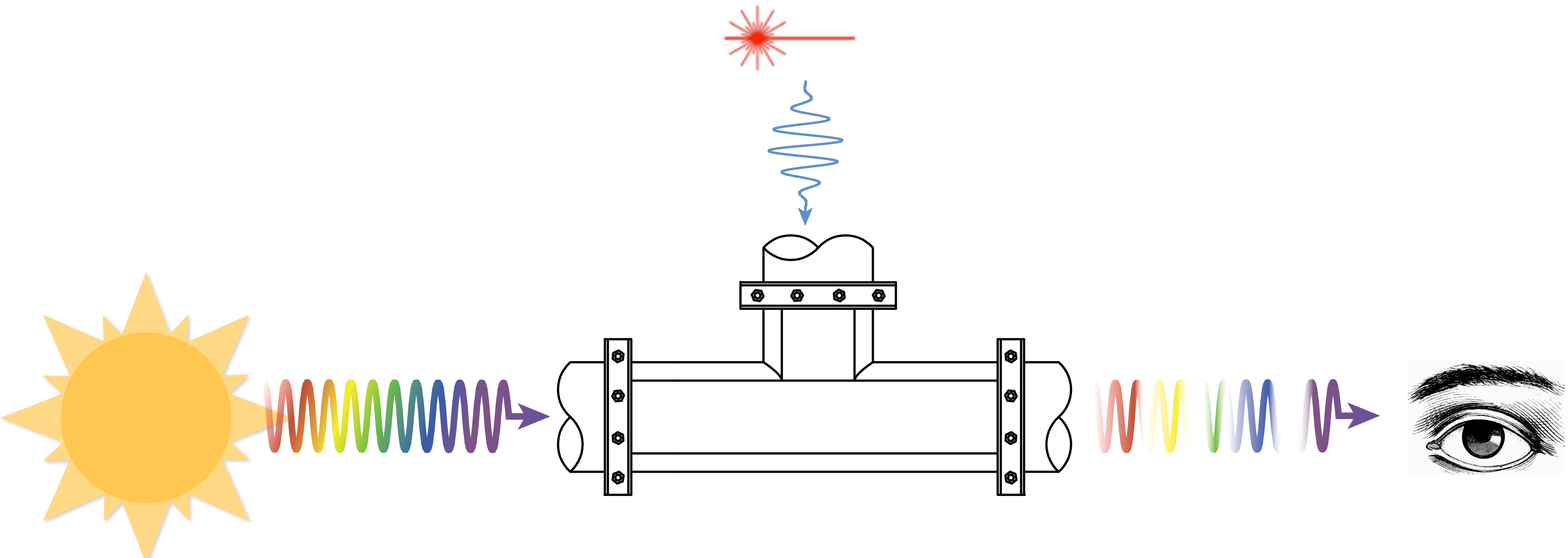
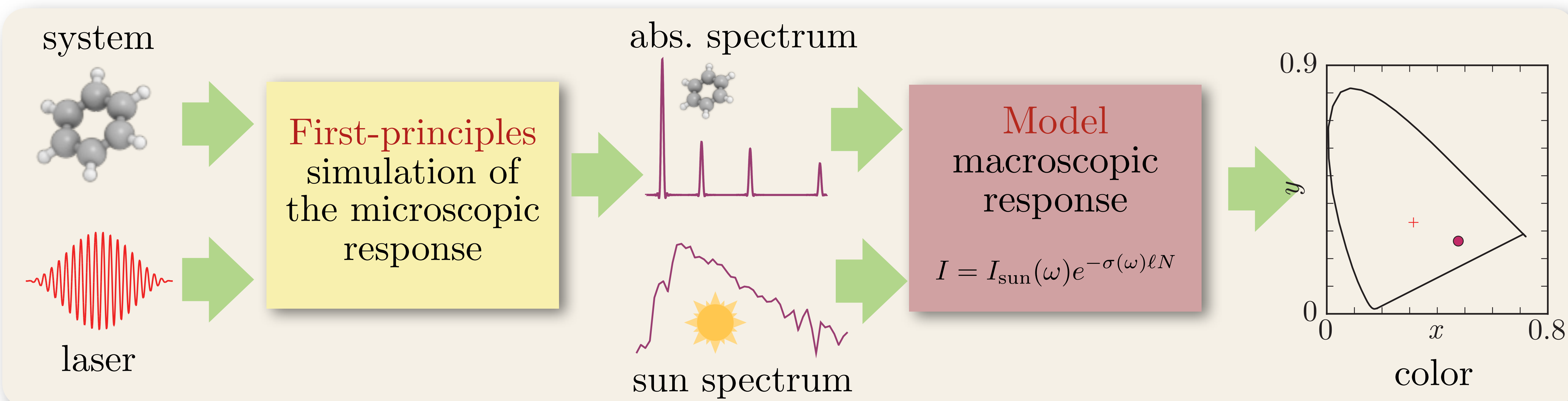


How do we simulate this process?



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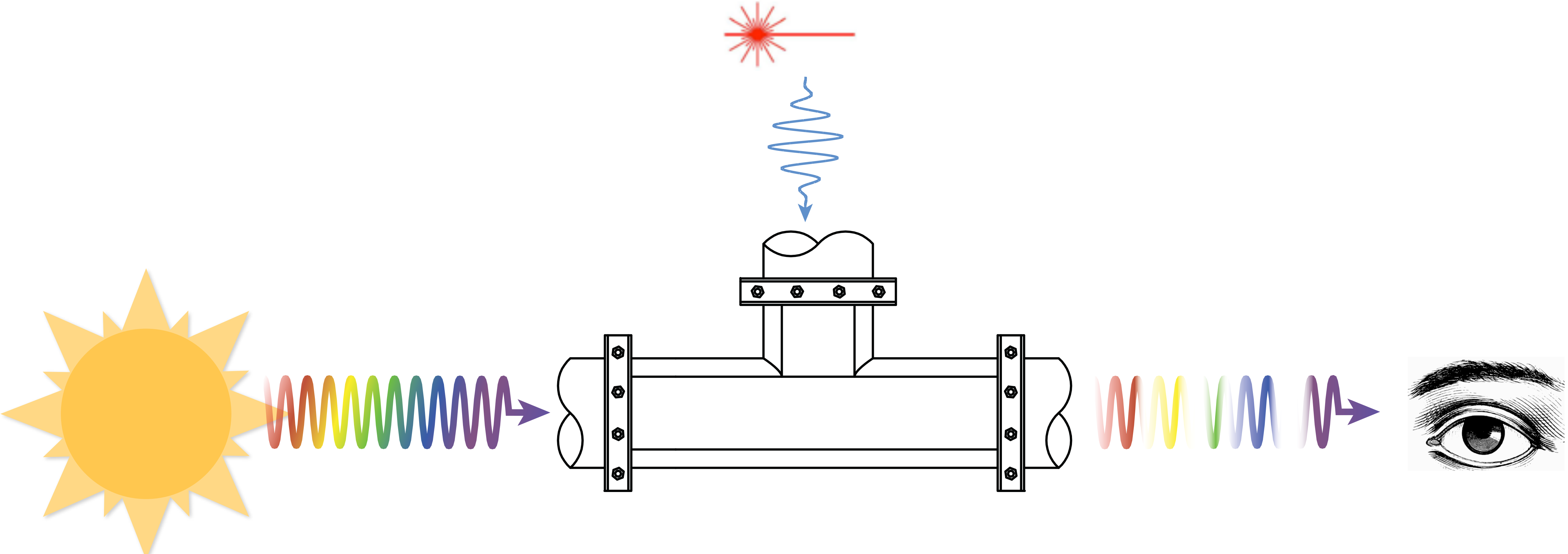

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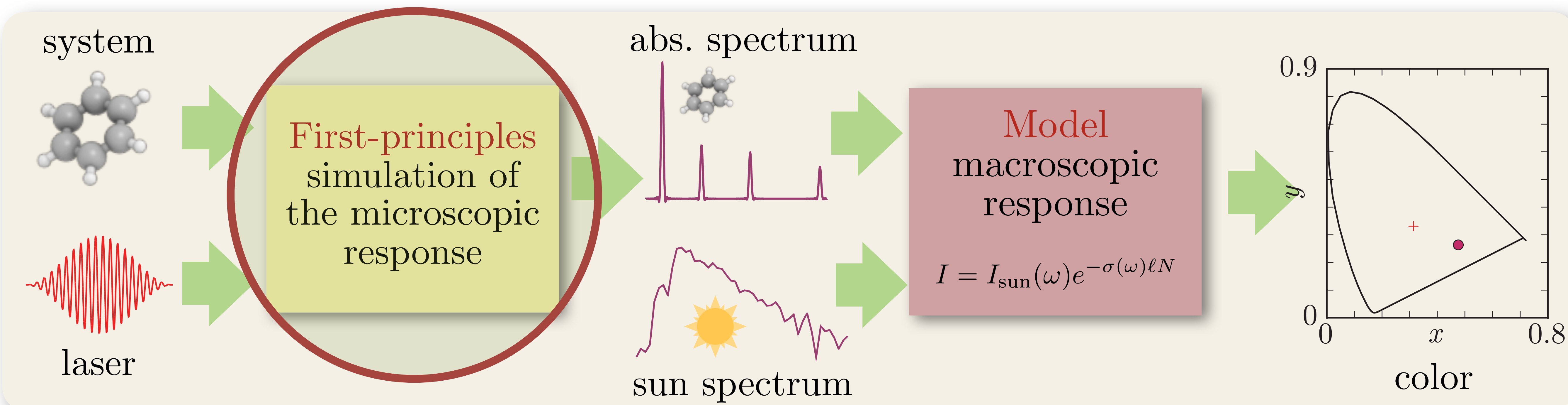

How do we find the laser? QOCT

Time-dependent density functional theory

OCTOPUS

real-space real-time FD

http://www.tddft.org/programs/octopus

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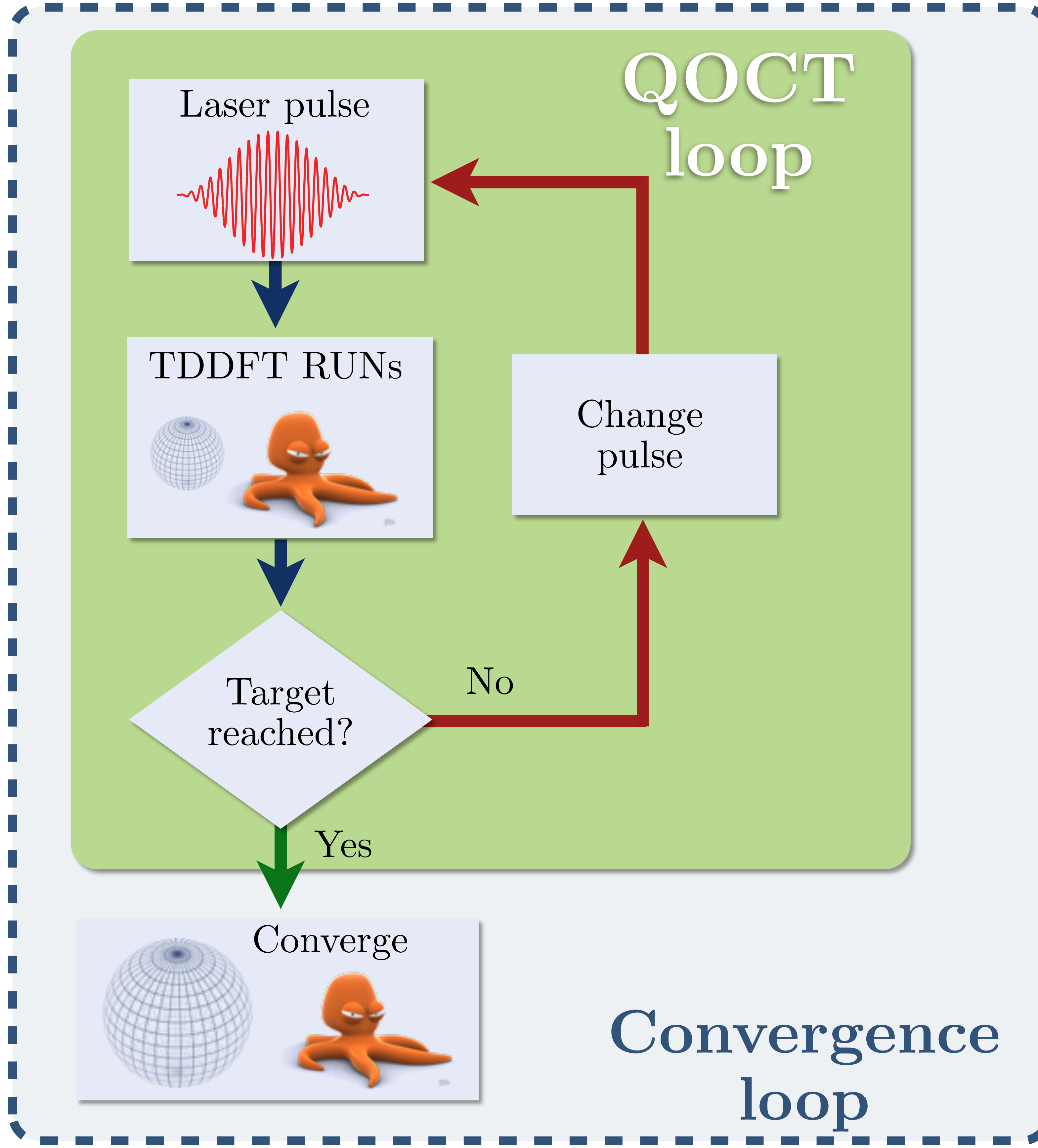

How do we find the laser? QOCT

Time-dependent density functional theory

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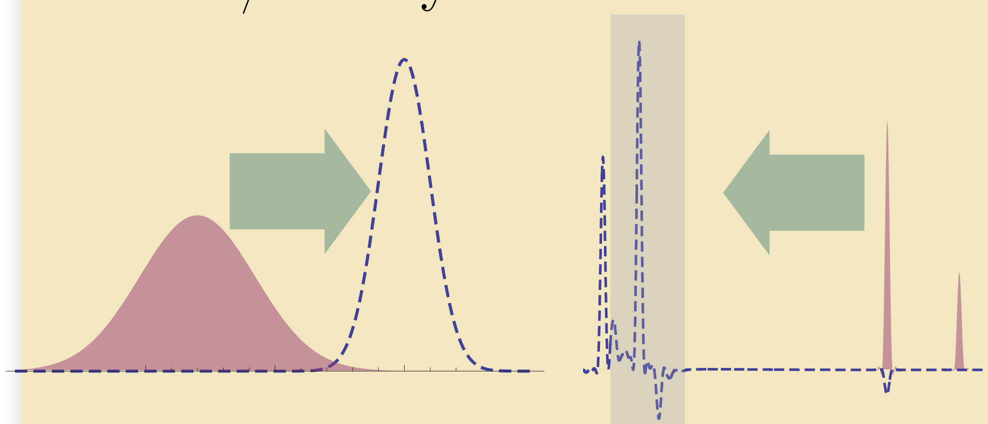
Target

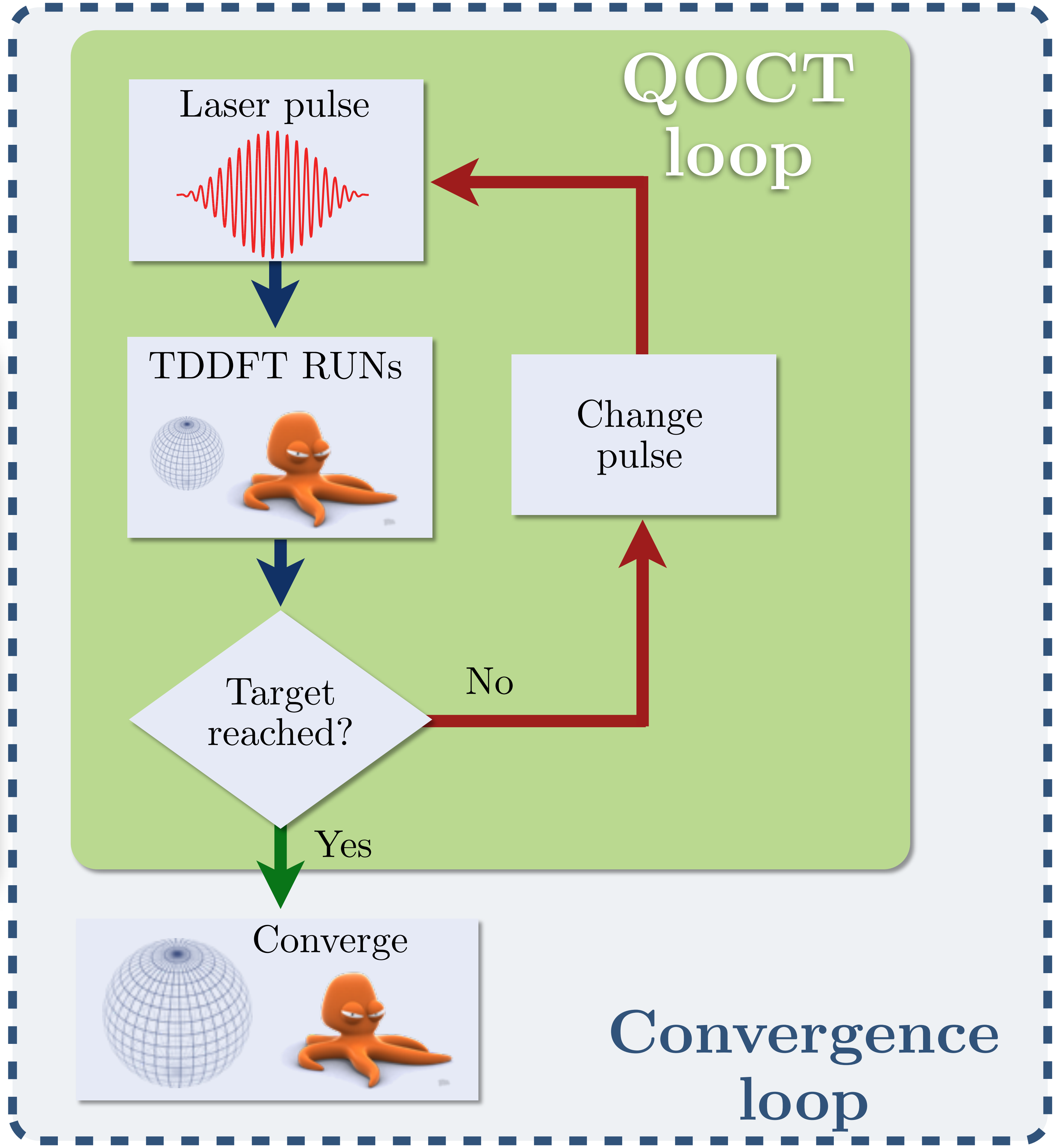
Excited state /density

Spectrum



large search space

small search space



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Time-dependent density functional theory

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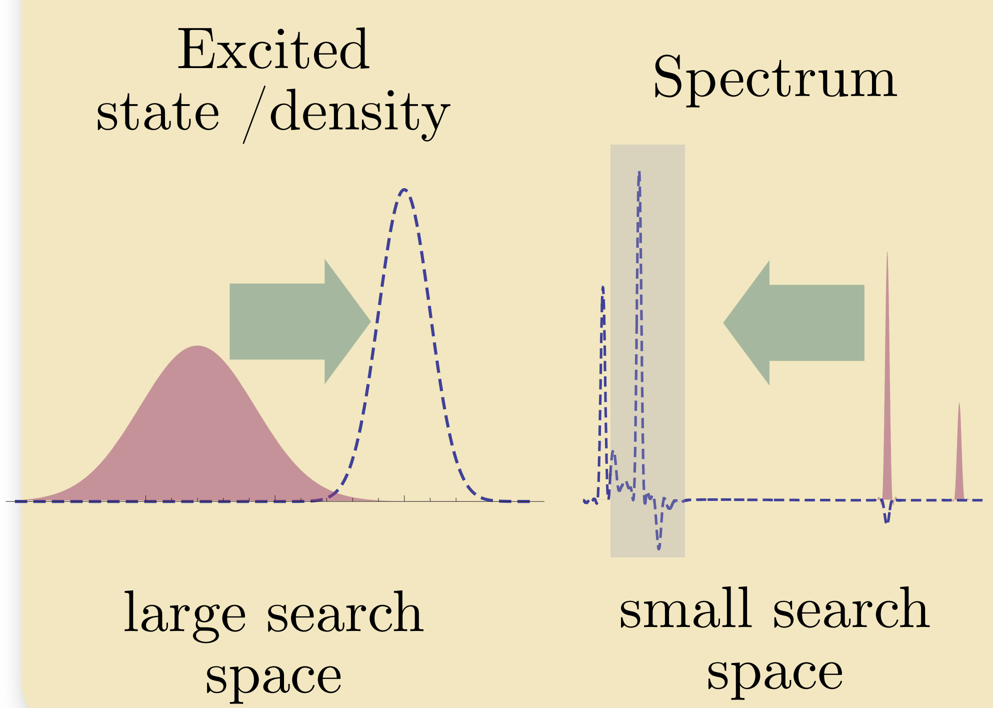
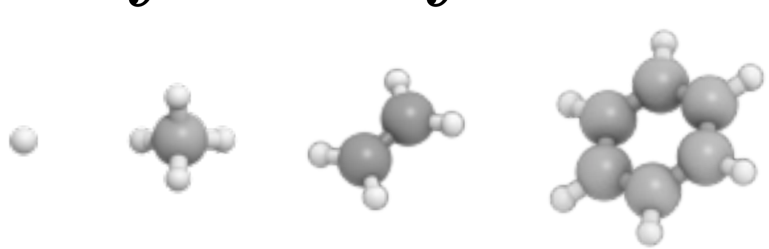
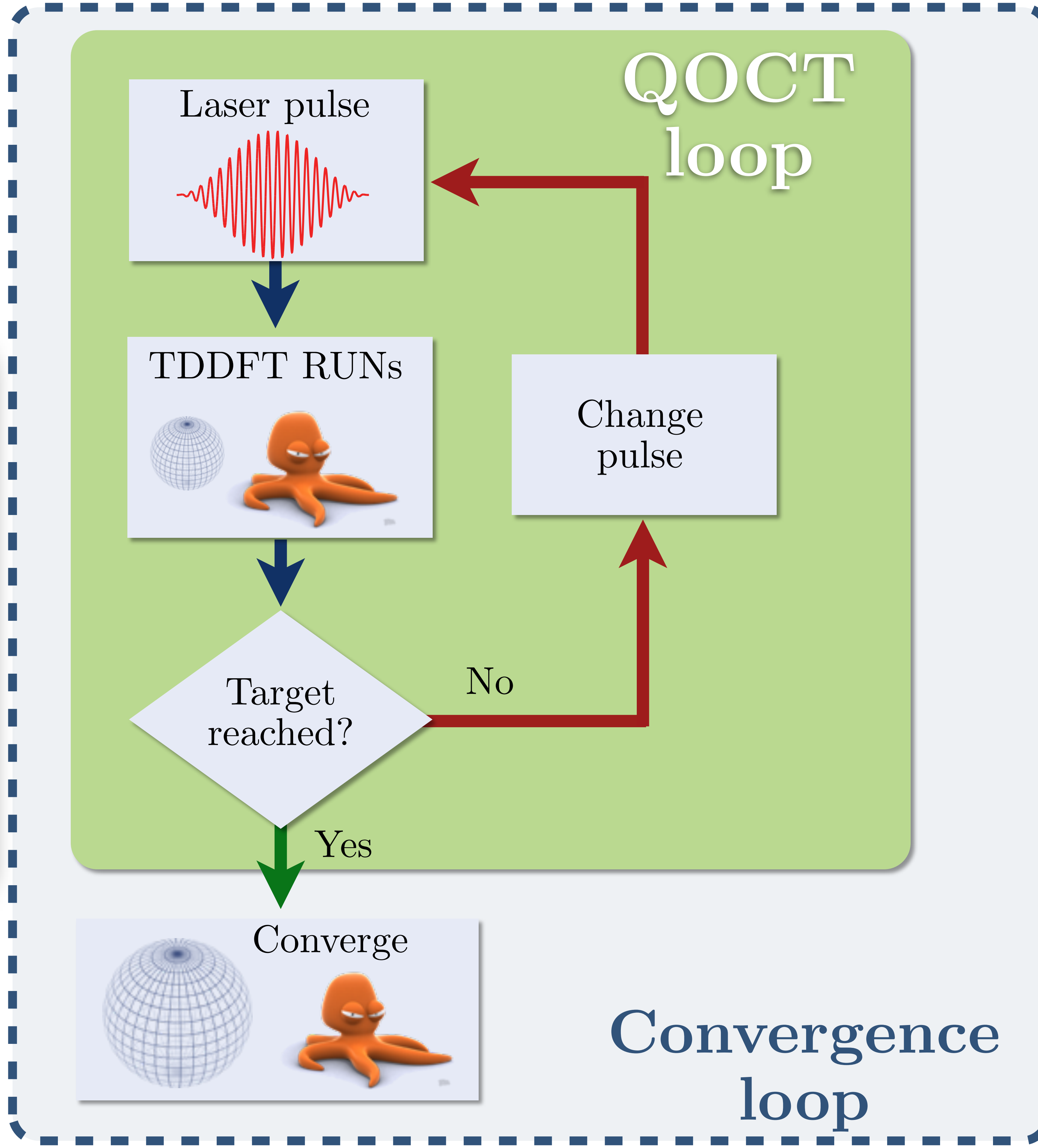
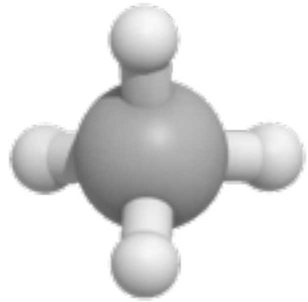


Physical systems



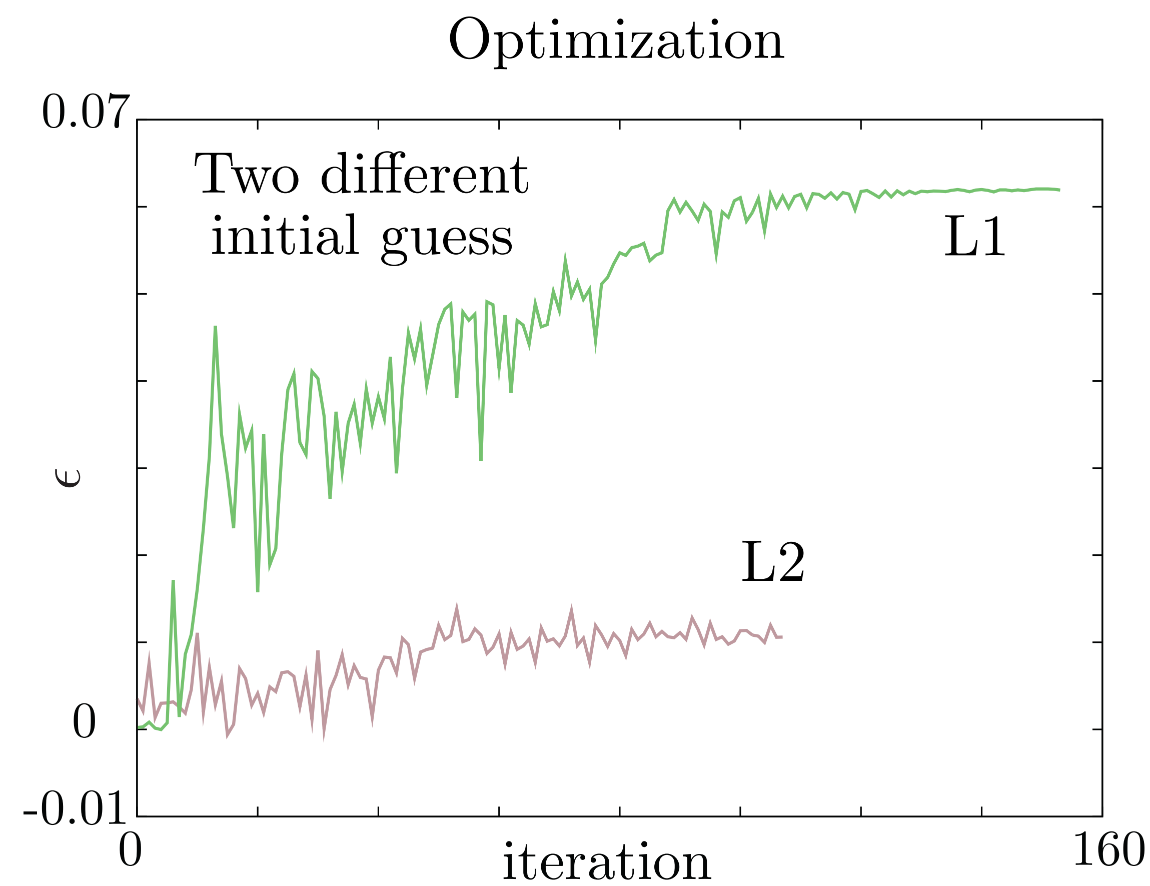


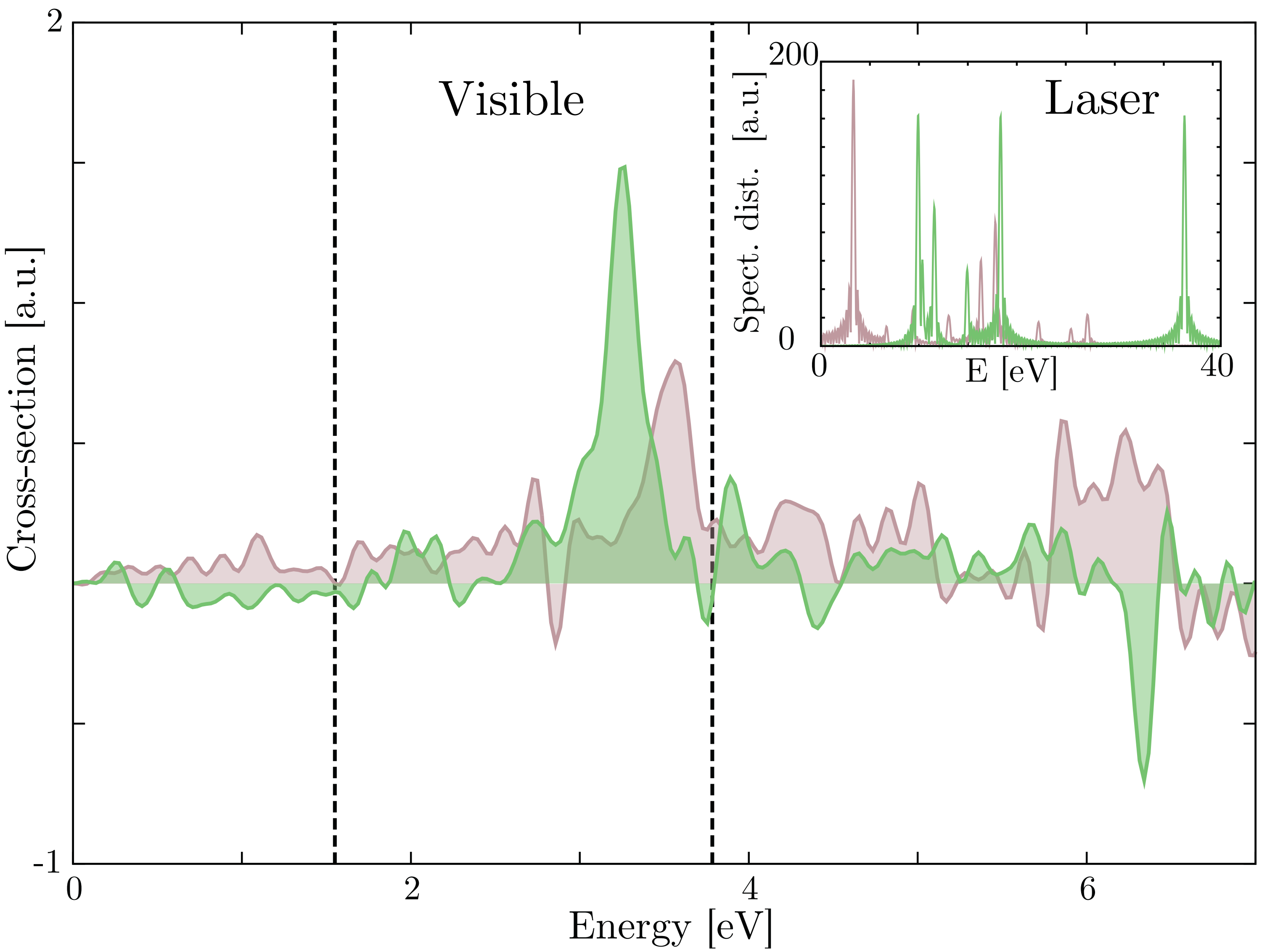
Doubly ionized methane(CH4-2e)

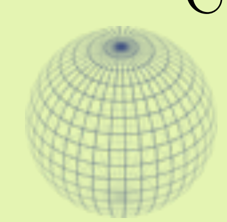


Target spectrum

$$\epsilon = \int_{\mathrm{VIS}} \mathrm{d}E\,\sigma(E)$$





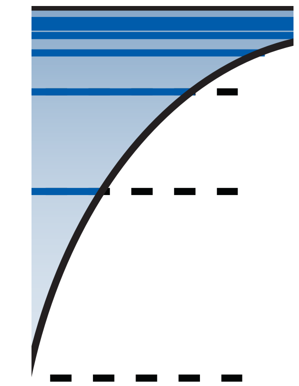


Computational cost
(@ R = 20 au)

L1 =18.4 Khrs

L2 =13.8 Khrs

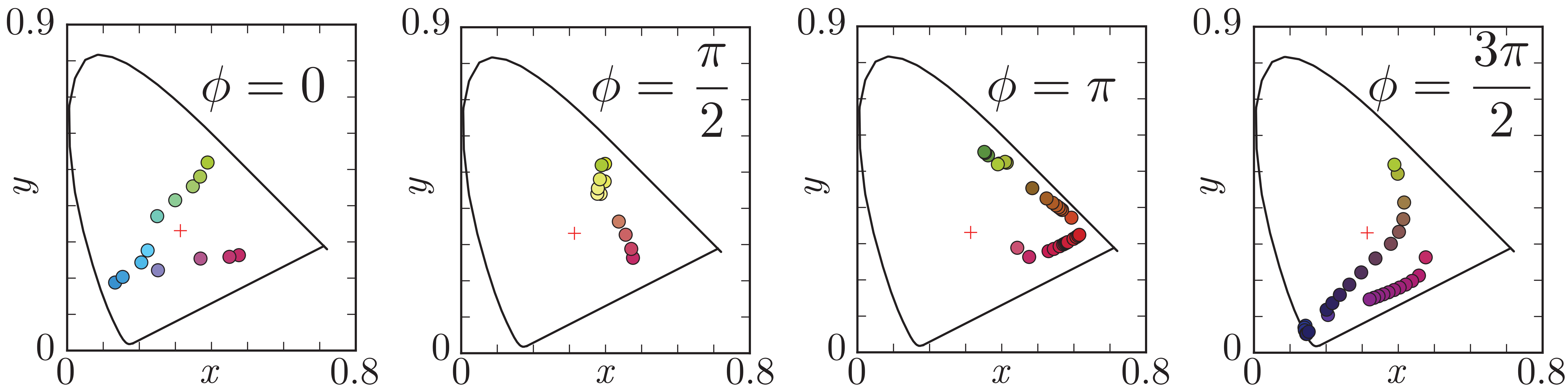
Hydrogen atom

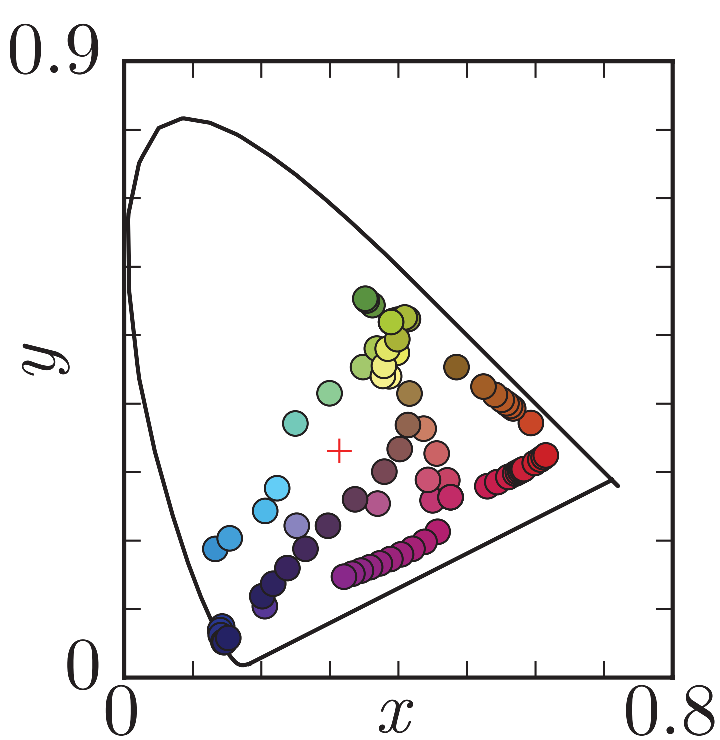


$$|\Psi(\alpha,\phi)\rangle = \sqrt{\alpha}|2\text{p}\rangle + e^{i\phi}\sqrt{1-\alpha}|3\text{p}\rangle$$

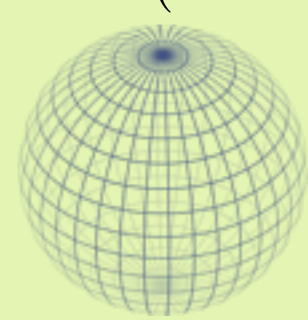
Balmer

Paschen (IR)





Computational cost
(@ R = 60 a.u. mesh≈ 11.8 Mpnts)



Single color ≈ 0.54 Khrs

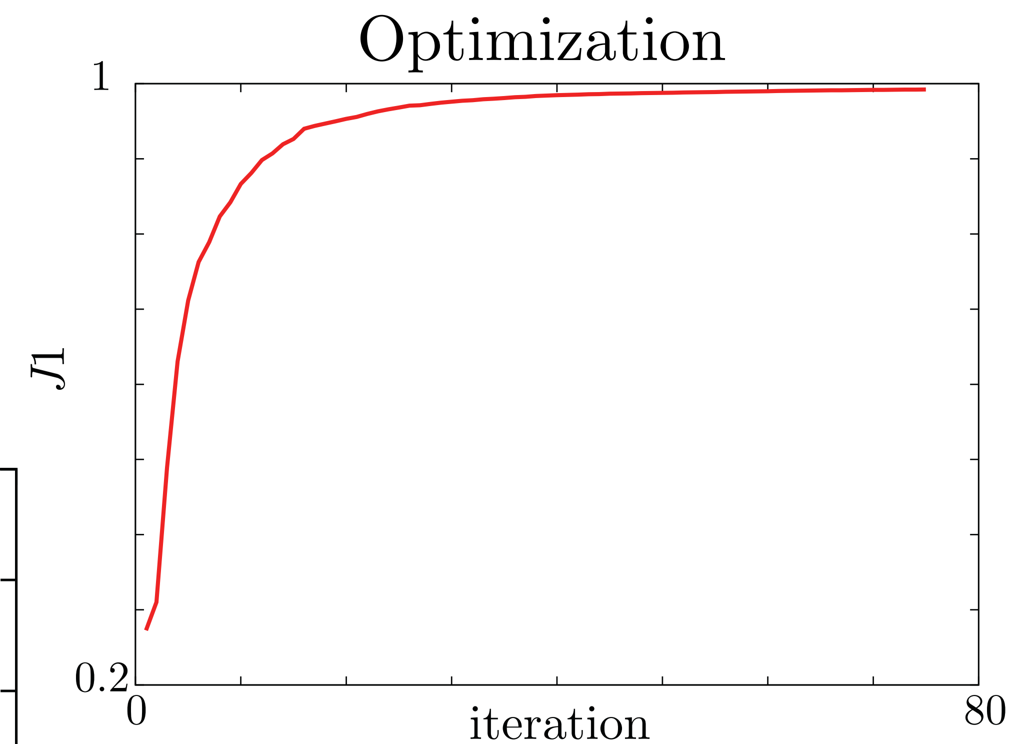
Total (x80) ≈ 43.3 Khrs

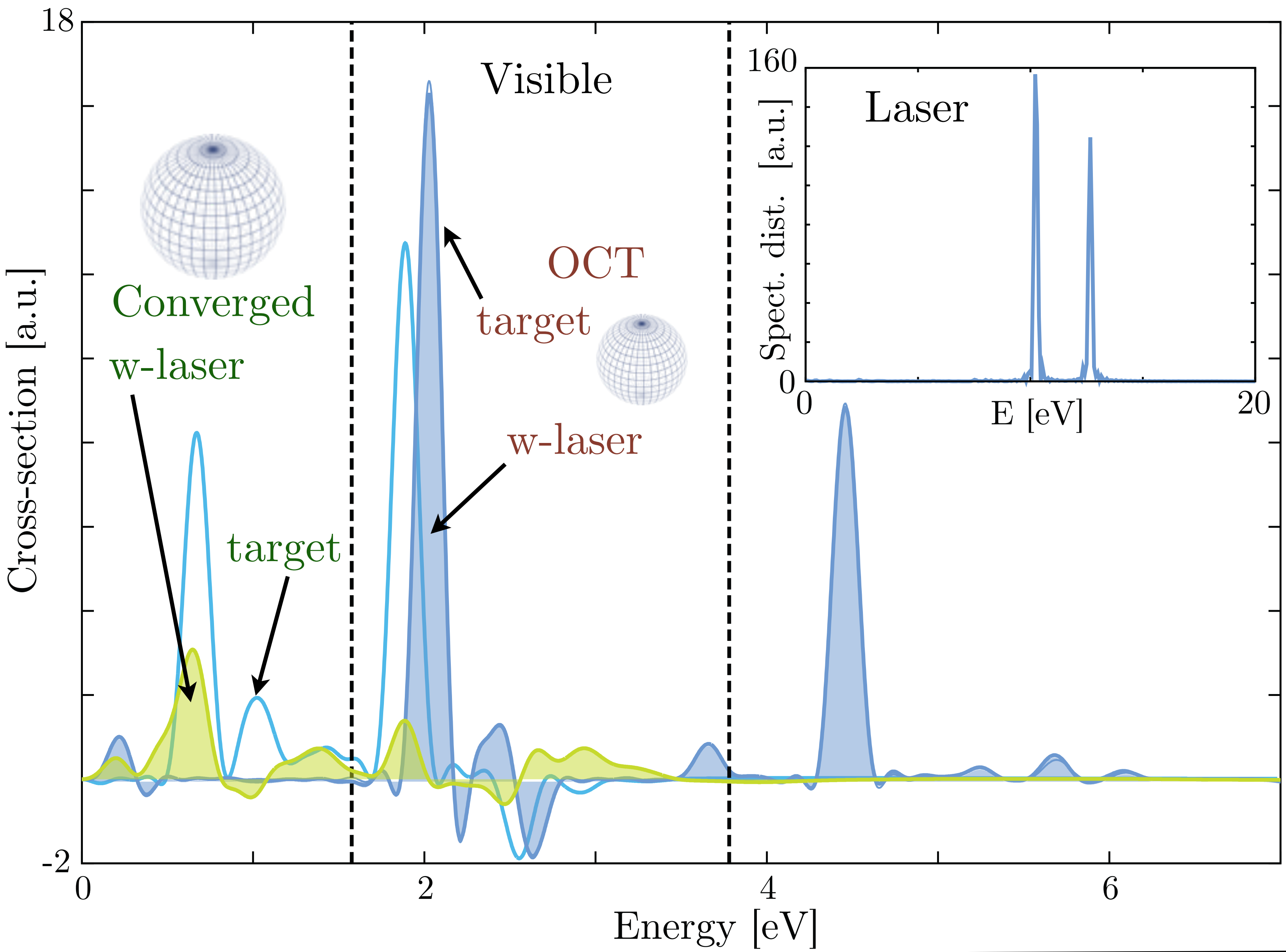
Hydrogen atom QOCT

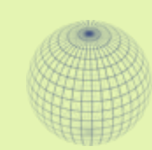
$$|\Psi(\alpha,\phi)\rangle = \sqrt{\alpha}|2\mathrm{p}\rangle + e^{i\phi}\sqrt{1-\alpha}|3\mathrm{p}\rangle$$

$\alpha = 0.5$
$\phi = 0$

Target state
$$J1[\Psi] = |\langle\Psi|\Psi_T(r)\rangle|^2$$

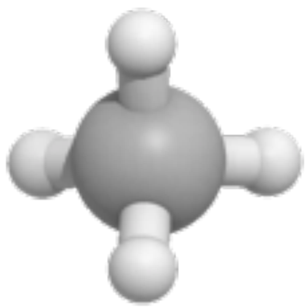


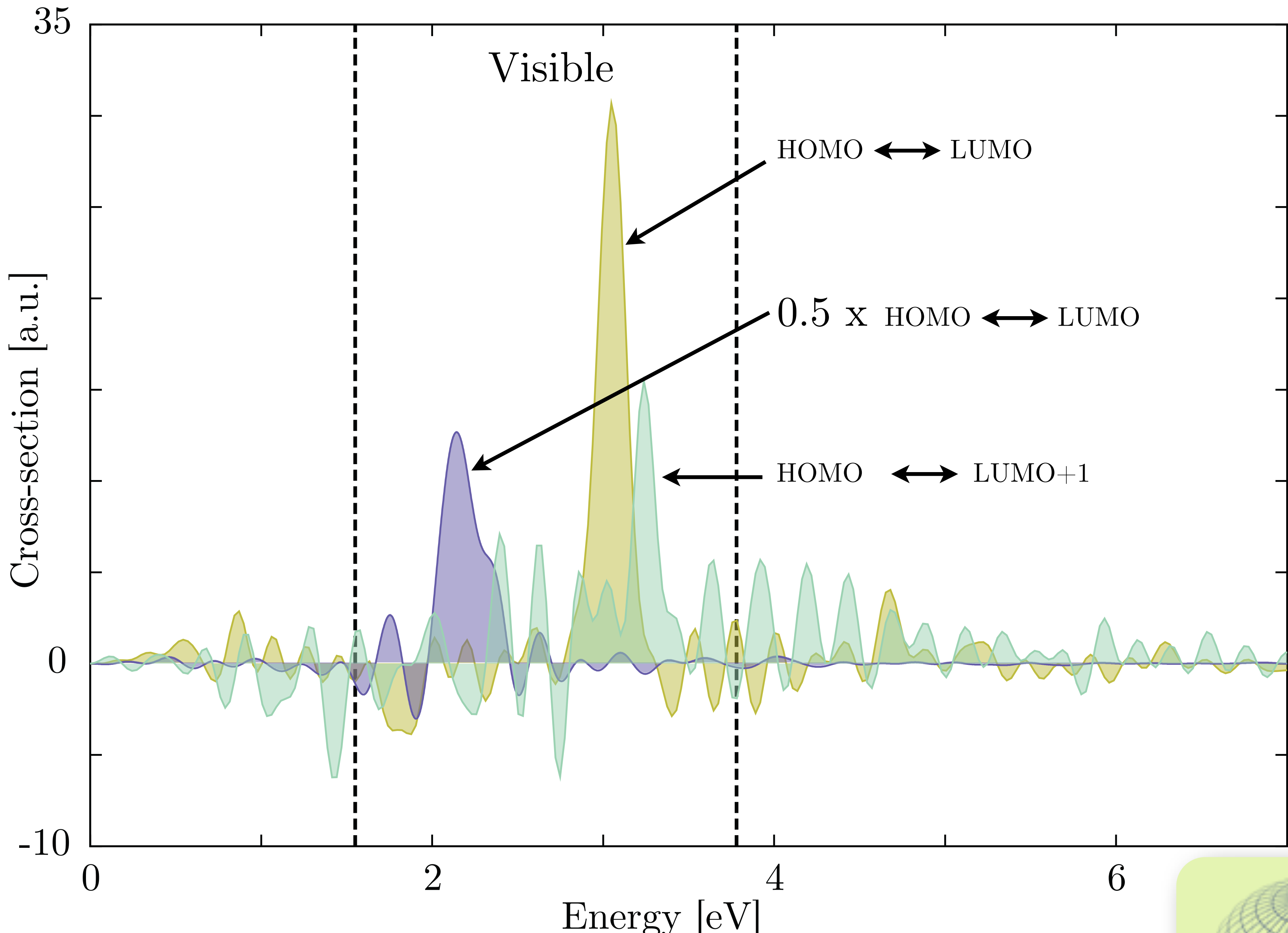


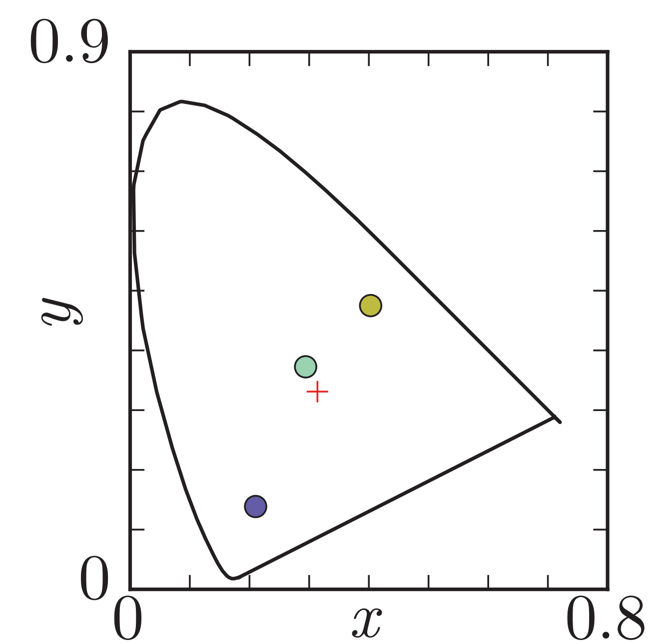


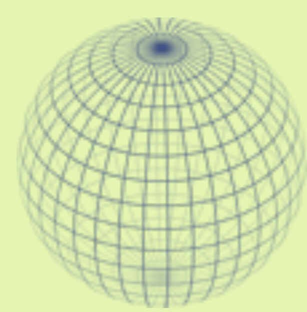
Computational cost
(@ R = 15 au)
QOCT =1.86 Khrs

Methane (CH4)



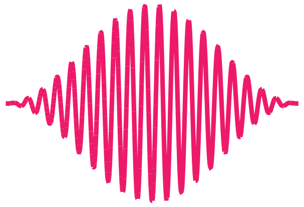


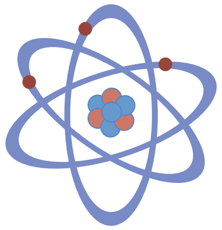


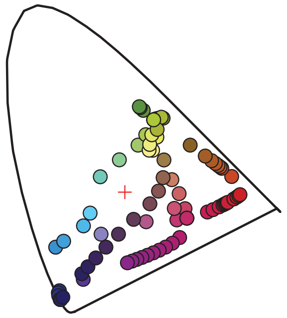


Computational cost
(@ R = 45 a.u.)

Single spect ≈ 5.2 Khrs







Conclusions

RES allowed us to:

- test OCT strategies
- search for interesting target states
- identify exciting fields
- investigate different systems

THANK YOU!!!