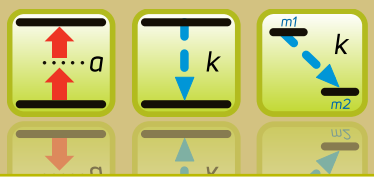
SimphoSOFT® Info+

Access to over 1,000 multi-photon materials and structures

Indispensible tool to compare and optimize photo-activated materials

Google-style search of parameters and structures

Best parameters source for SimphoSOFT modeling software

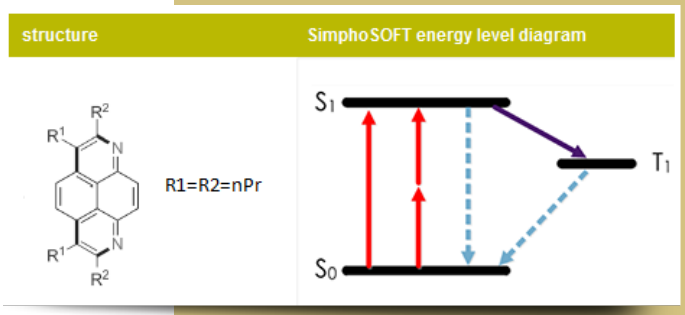


Main features

- Detailed photo-physical properties of over 1,000 MPA materials from peer-reviewed scientific papers
- Collected multi-photon absorption cross-section values and reconstructed energy level diagrams
- Proprietary, customizable search tool to localize materials with desired photo-physical parameters
- Indispensible information resource to determine the best published material with optimal parameters
- Enough supporting evidence to verify and to validate the material properties collected in database
- Continue validating and optimizing using SimphoSOFT with confidence

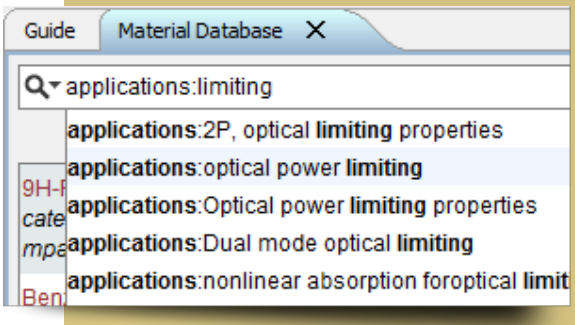
Imagine a task of finding an MPA material with the largest known absorption coefficient absorbing light within a desired wavelength. It can take hours, if not days, to find such a material shuffling stacks of papers and paid digital subscriptions. Use Info+ instead to speed up the process for a reasonable price.

- Over 12,000 collected values for an extensive set of photo-physical parameters
  - Material name
  - Chemical structure and energy level diagram
  - 1PA, 2PA, 3PA absorption spectrum and cross-sections
  - Decay time(s) of fluorescence and phosphorescence states
  - Intersystem crossing rate
  - Fluorescence and phosphorescence quantum yields
  - Fluorescence and phosphorescence emission spectrum
  - Nonlinear measurement method



Comprehensive search

- Desired materials can be searched by
  - Application, keywords, type of material
  - Numerical range
  - Author, country, type of measurement
- More advanced inquiries are also available
  - Find the largest cross-section
  - Find materials emitting light in a given wavelength range



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selected applications

- Bio-imaging
- Calcium imaging
- Cell imaging
- Confocal microscopy
- DNA detection
- Electron decay times
- Endoscopy
- Energy level diagram
- Energy transfer
- Excited state absorption
- Experimental methods
- Fluorescence imaging
- Fluorescence microscopy
- Fluorescence probes
- Fluorescence proteins
- Internal conversion
- Intersystem crossing
- Linear and nonlinear spectroscopy
- Micron and nano size fabrication
- Molecular structures
- Multi-photon absorption/emission
- Nonlinear transmission
- Nonlinear absorption probes
- Optical data storage
- Optical limiting
- Photodynamic therapy
- Photoluminescence
- Single photon absorption/emission
- Singlet oxygen
- Singlet/triplet states
- STED
- Synthesis and characterization
- Structure-property relationships
- Theoretical analysis
- TPEF
- Vascular bio-imaging
- Z-scan

sample materials

- Anthracene derivatives
- Azoaromatic moieties
- Azulenyl compounds
- Benzothiazoles derivatives
- Benzo[h]chromene-2 derivatives
- Bioconjugate probes
- Bis-Terpyridyl-stilbene derivatives
- Bis(styryl)benzene derivatives
- Branched conjugates
- Bromine substituted p-nitrostilbene drv
- Caged compounds
- Chromophores
- Cyanine dyes
- Cysteine derivatives
- Dendrimers
- Dendritic chromophores
- D-π-A-π-D, D-π-D, D-A chromophores
- Dipicolinic derivatives
- Dipolar chromophores
- Dithienocoronene Diimide
- Compounds containing europium (III)
- Fluorescent proteins
- Fluorophores
- Fluorene derivatives
- Heterafluorenes
- Graphene oxide
- Metalloporphyrins
- Multiporphyrins
- Octupolar molecules
- Orange/red fluorescent dyes
- Organoplatinum chromophores
- Paracyclophanes
- Phenylacetylene
- Phenylene-vinylene derivatives
- Phthalocyanine derivatives
- Platinum acetylide chromophores
- Polymeric materials
- Porphyrin dimers,oligomers,array
- Pyrrole derivatives
- Pyrene derivatives
- Ruthenium complexes
- Stilbene derivatives
- Squaraine dyes
- Star shaped octupolar triazatruxenes
- Styryl derivatives
- Tetraphenylporphycenes
- Triphenylamine derivatives
- Thiophene derivatives
- Triazine derivatives
- V-shaped organic complexes
- Zn(II) -fluorophores

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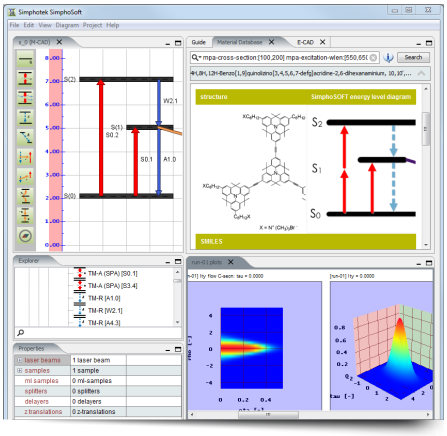
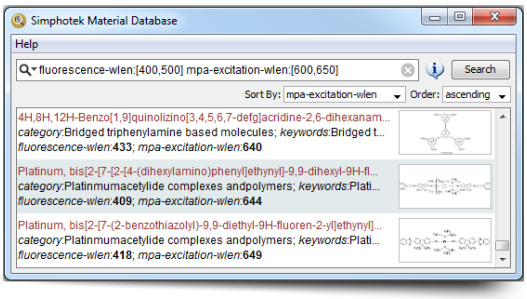


You now have a comprehensive collection of structure-property relationships.

The key parameters of the materials, such as its structure, its energy level diagram, its properties of absorption, relaxation, inter-system crossing, extinction coefficients, 1PA, 2PA or 3PA coefficients, wavelength, etc., can be quickly fetched from the database and passed to SimphoSOFT® for simulation. SimphoSOFT software can calculate the transmission characteristics of pulsed laser beam propagating in 1PA/2PA/3PA materials with or without taking into account the diffraction effects.

Identify material and prototype samples.

If an available laser has an intensity of 1GW/cm^2, what absorption coefficient is needed to limit the output at, for example, 0.5GW/cm^2? What concentration of the material is needed? What material host should be used so as not to absorb the light before it gets to the 2PA material? If too much laser intensity is used, will there be excitations to higher energy levels that affect the output intensity? Because these are nonlinear materials, the output power is not linearly related to the input power especially for organics that have both singlet and triplet states. SimphoSOFT calculates these more complicated cases. You will be able to estimate the excited state absorptions and relaxation times and use SimphoSOFT software to calculate/estimate the change in output intensity for high and low intensity lasers.

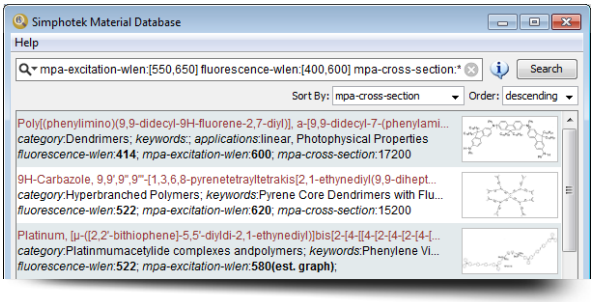


Find materials that absorb in your desired wavelength range.

Look for materials that absorb in a desired wavelength range (e.g. 600–650 nm) for 1PA, 2PA or 3PA and emit in a particular wavelength range (e.g. 400–500 nm) with large enough 2PA or 3PA coefficients for the laser power they are using.

Improve performance of materials you use now.

If you are a chemist/material scientist/engineer and you, for example, want to make a 2PA material that absorbs at 800–900 nm and has a low 1 photon absorption in this region, then what are the chemical structures and absorption parameters of other materials in this region? Our material database lists existing 2PA and 3PA materials absorbing in the UV, visible and IR spectral region. Using this information, the chemist can explore whether it makes sense to try to modify existing structures to obtain the required properties.



Choose the best material.

If you are a microscopist/biologist/industry applicant, having a choice of lasers at 600, 800, 2000 nm and you want to observe emission at 500, 800, 2100 nm, using 2PA/3PA material as a probe, then you can search for the best candidate material with the largest 2PA or 3PA cross-section.

Start collaboration.

If you want a published material that was made by a group, for example, in Spain over 3 years ago, Simphotek material database has the contact information of the group. Does that group still have the material? Can another group, for example, in Singapore get some of the material from that group in Spain?

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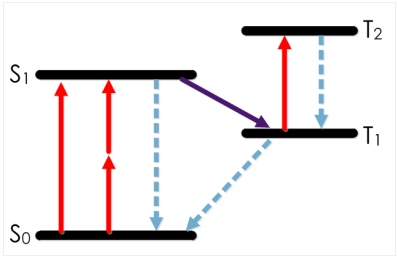
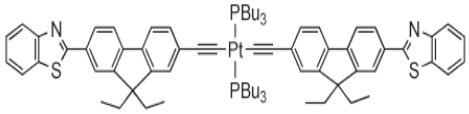
Organoplatinum chromophore (Info+ material set entry)

applications	category
High Performance Nonlinear Absorber	Platinmumacetylide complexes andpolymers

SMILES	chemical name
CCCCC[P-](CCCC)(CCCC)[Pt](C#CC1=CC2=C(C=C1)C1=CC=...	[bis({2-[7-(1,3-benzothiazol-2-yl)-9,9-diethyl-9H-fluoren-2-...

structure	simple energy level diagram
C77 H96 N2 P2 Pt S2	



2PA cross-section (GM)	2PA excitation wavelength (nm)
370	720

2PA measurement method	Solvent (TPA)
TPEF	benzene

2PA laser pulse width	decay time of phosphorescence state
fs	126 μs

1PA extinction coefficient (M^{-1} cm^{-1})	excited state absorption (ESA) wavelength (nm)
150×10^3	670 (T1-T2)

fluorescence emission wavelength (nm)	phosphorescence emission wavelength (nm)
418	565

year	country
2011	USA

Reference

Authors: Chen Liao, Abigail H. Shelton, Kye-Young Kim, and Kirk S. Schanze

Title: Organoplatinum Chromophores for Application in High-Performance Nonlinear Absorption Materials

Journal: ACS Appl. Mater. Interfaces, 3, 3225–3238 (2011)

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