Metal Nanoparticle Simulator 1.0

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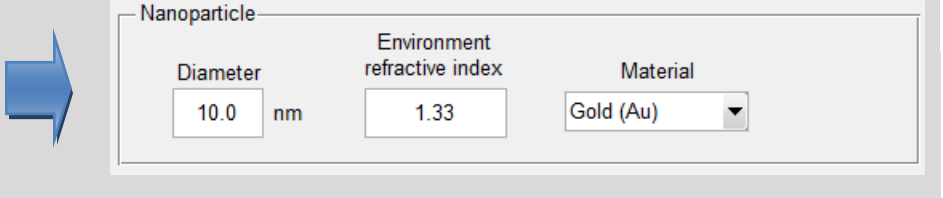
Introduction

The **Metal Nanoparticle (MNP)** simulator is a didactic software written as part of the NANOLAB project. **MNP** allows you to simulate the absorption, extinction and scattering spectra of metal nanoparticles dispersed in a solution. The material and size of the nanoparticles can be changed, as well as the type of solution, to highlight the size dependence of the optical properties of nano-materials, and their possible use, e.g., as sensors. **MNP** uses the Mie theory which allows to simulate spherical nanoparticles. **MNP** also tries to simulate the color of the solution as perceived by the human eye using colorimetric methods. The perceived color depends on the spectrum of the light source, which can also be changed.

Use of the software

This is where the target nanoparticle and its environment are defined.



Diameter The diameter of the nanoparticle in [nm]. Typical values range from a few to a hundred nanometers.

Environment refractive index The (real) refractive index of the solution where nanoparticles are dispersed. The refractive index of pure water is 1.33. Vacuum correspond to 1, so any value smaller than 1 is physically meaningless.

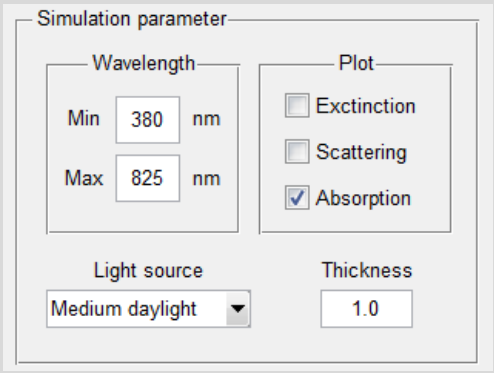
Material The material of the nanoparticles. The material is characterized by the complex dielectric function, which is taken from experiments. The dropdown menu allows to choose between Au and Ag, using corresponding datasets from Johnson, P. B.; Christy, R. W. “Optical Constants of the Noble Metals” Phys. Rev. B 1972, 6, 4370–4379. One can load the dielectric function for any other materials if this is available, choosing 'Load material...'. In this case the dielectric function must be tabulated in a text file with the following form

0.64 0.92 13.78

```
0.77    0.56    11.21
0.89    0.43    9.519
....    ....    .....
```

The 1st colum is the photon energy in [eV], and the 2nd and 3rd columns are the real and imaginary parts of the refractive index, *n* and *k*, respectively. An example file `example_material.dat` is provided with the distribution (which actually coincides with the Au dataset).

This is where the light source is defined and the type and range of graphs are chosen



Wavelength The minimum and maximum wavelength to calculate the spectra. The visible range correspond to the range [380 nm, 825 nm], approximately. You can choose larger values of `min` or smaller values of `max` for plots. However, if the calculation does not cover the whole visible range, the simulated colors calculation might be inaccurate. A warning is issued in the **Hint** section in this case.

Plot Choose which functions will be plot the next time you hit **Run simulation**.

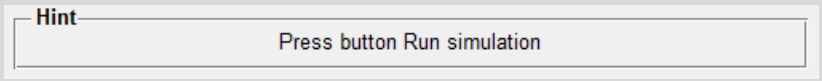
Light source Choose the type of light source. Possible choices are the sun medium daylight emission using the D65 Medium daylight with UV component (6500K) dataset (see cvrl.ioo.ucl.ac.uk) , the standart tungsten filament emission (2856K), and the equal energy illuminant, an ideal white source emitting at any wavelength with the same intensity. The user can also load the illuminant from an external file choosing 'Load illuminant...'. The file must contain illuminant intensity in the form

```
300  0.930483
301  0.967643
302  1.005970
....  ........
```

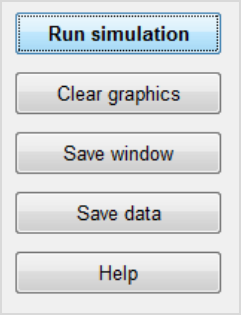
The 1st colum is the wavelength in [nm]. An example file `example_illuminant.dat` is provided with the distribution (it actually coincides with the tungsten filament dataset).

Thickness The thickness of the sample traversed by light. It has no dimension. Typical values are around 1, and should be adjusted by comparison with the experiment. To some extent, changing the thickness mostly affects intensity but not much the color.

This is where messages on what to do next or warnings are given to the user.



These buttons allow to run the simulation, clear the graphs, save results as images or datasets, output this help file.



Run simulation Hit this button to run the simulation, after you have set all parameters. When you start the application, all parameters are set to reasonable default values, and you can just hit this button (as suggested by the **Hint** box) to see a typical result. If you change any parameter and hit this button again, the old results will be kept, so spectra and perceived colors will accumulate in the respective panels. In this way, you can easily compare different cases to an experiment, analyze trends and so on.

Clear graphics Hit this button when you want to clear all graphic panels and start over again.

Save window Hit this button to save a picture of the entire window in the current status of the simulator for later processing or printing.

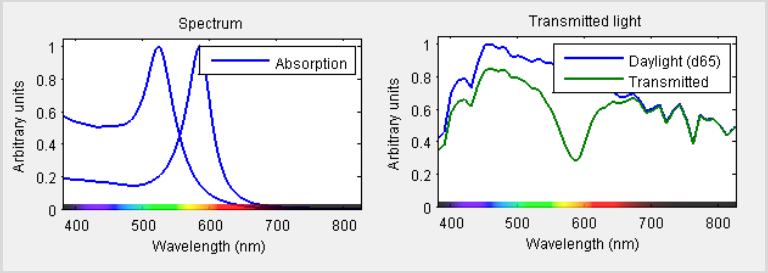
Sava data Hit this button to save the calculated extinction, absoprtion and scattering spectra in a text file. Only the last calculated spectra are saved. If you want the spectra corresponding to different parameters, you need to hit **Run simulation** and **Save data** subsequently several times. Data are saved in the following format:

380.000000 0.060979 0.060810 0.000169
381.000000 0.060938 0.060770 0.000168
382.000000 0.060884 0.060717 0.000167
... ...

The 1st column contains wavelengths in [nm], the 2nd, 3rd and 4th column contain extinction, absorption, and scattering intensities in arbitrary units.

Help Hit this button to show this file of instructions.

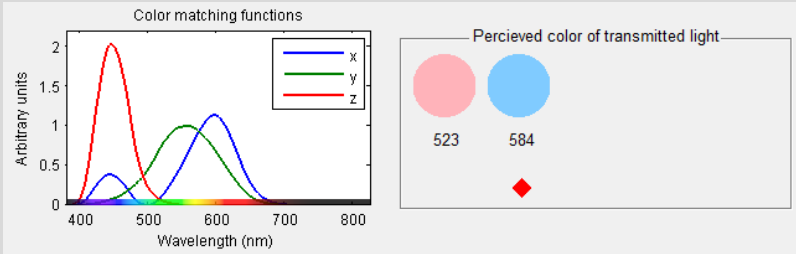
This is where the calculated spectra and the illuminant energy distribution are shown. The color spectrum is shown on the wavelength scale.



Spectrum This plot shows the calculated spectra. Extinction, absorption and scattering spectra will be shown, according to the choices made in **Plot**. When you hit **Run simulation,** the new spectra is rendered with the previous ones. If want to avoid this, you can clear this panel with Clear graphics. The spectra are calculated according to the Mie theory, using a Matlab library written by C. Mätzler.

Transmitted light The light intensity emitted by the selected light source and light transmitted through the sample are shown here. The transmitted light is exponentially weaker at the wavelength where absorption is larger. The amount of absorbed light is controlled by **Thickness**.

This is where the color matching functions and the percieved color are shown. The color spectrum is shown on the wavelength scale.



Color matching functions The three functions which define the human eye sensitivity named x, y, z are shown, using the CIE 1964 dataset (see cvrl.ioo.ucl.ac.uk) . These define the human eye perception and, although they are re-plot each time you hit **Run simulation,** they do not depend on any parameter of the simulation and are always the same .

Perceived color This is the apparent color of the nanoparticle in a given solution. It depends on the material type and diameter, solution, light source. Each time you hit **Run simulation** a new color is added and the wavelength corresponding to maximum absorption is shown in [nm]. A red diamond indicated the last calculated color. You can clear this panel with **Clear graphics**.

Installation details, terms of use, credits

Download The **MNP** simulator can be freely downloaded at www.nanolab.unimore.it. **MNP** is written in MATLAB, a proprietary software. However, **MNP** is a standalone application which runs on any PC, even if not featuring a MATLAB license, if the *free* MATLAB Compiler Runtime (MCR) has been installed on that PC. The *MCR can be installed using an application which we distribute together*

*with **MNP**.*

Two different kinds of files are freely available for download at www.nanolab.unimore.it:

MNP_pkg.exe	Includes the installation file of MCR.
MNP_pkg_noMCR.exe	It **does not** include the installation file of MCR.

If you know that the MCR had been already installed on your PC (for example when using another standalone application written in MATLAB), you should download the much smaller file MPN_pkg_noMCR.exe. However, if you are unsure/don't know, it is always fine to download MNP_pkg.exe.

Install The downloaded files are of the auto-installer kind. To install **MNP** you must:

1) Download one of the two installation files in an empty directory.

2) Execute the downloaded file (*double click* or *right mouse button | open*).

The file MNP_pkg_noMCR creates the required files into the same directory. To run the **MNP** software it's enough to execute the MNP.exe file (*double click* or *right mouse button | open*)

The MNP_pkg file initially requests to install the MCR software. The whole process runs automatically. Once you've launched MNP_pkg, choose the language (it refers to MCR language and has nothing to do with **MNP**, whose interface is in English). Then click on Install/Next as many times as needed throughout the installation process. The procedure is slightly different whether MCR is already installed or not. The file MNP_pkg creates the required files in the same directory. To run the **MNP** software just execute the MNP.exe file (*double click* or *right mouse button | open*)

Requirements At the moment **MNP** runs on Windows systems only. If you want to contribute the executables for different systems, we welcome your collaboration. The source MATLAB files are available from the author. Depending on the resolution of your screen, the graphic interface may not show correctly. Try to resize the window with your mouse until all graphics shows correctly (sometimes axis get blurred, but this does not affect the functioning).

Contacts & info Please, contact the author for any suggestion or comment on the **MNP** software or its use in a didactic context. See www.nanolab.unimore.it for more details on the use of **MNP** and the NANOLAB project.

License The **MNP** simulator is distributed under the Creative Commons 3.0 licence.

Disclaimer The **MNP** simulator is for didactic use only. No responsibility is taken by the author or NANOLAB project for inappropriate use and errors.

Credits The author wishes to acknowledge discussions with S. Corni and A. Calzolari (CNR-NANO, Italy) and with A. Lisotti and V. De Renzi (University of Modena and Reggio E., Italy), co-authors of the NANOLAB project.

Files included in the distribution

The following files are distributed with the **MNP** software and will be found in the installation directory after the installation process:

`MNP_pkg_noMCR.exe/MNP_pkg.exe`	Self-extracting installation files
`MNP.exe`	**MNP** executable file
`MNPHelp.pdf`	Help file in english, similare to the present file. This is the file which is shown hitting the Help button in the **MNP** interface.
`MCRInstaller.exe (*)`	Self-extracting installation file for MCR
`Readme.txt`	Text file with installation details. On normal succesfull installation, there should be no need to refer to this file.
`example_illuminant.dat`	An example dataset for the illuminant energy distribution (it actually coincides with the medium daylight dataset, see instructions for **Illuminant**)
`example_material.dat`	An example dataset for the material dielectric function (it actually coincides with the Gold dataset, see instructions for **Material**)
`example_spectra.dat`	An example dataset for the calculated spectra (it actually coincides with the spectra calculated with the default parameters, see instructions for **Save data**)

(*) Not present if you download the `MNP_pkg_noMCR file.`