MAN
Modal Analysis
of Nanoresonators

QNMtoolbox_alpha: an openly available toolbox for computing the excitation coefficients of QuasiNormal Modes expansions

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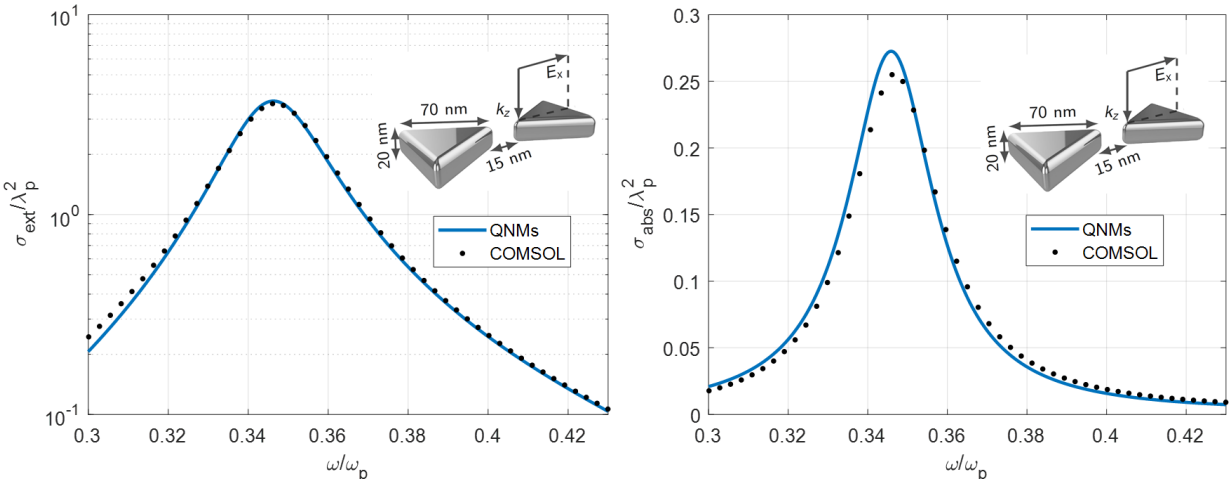


Figure 1. Scattering(left) and absorption(right) cross sections of a bowtie antenna.

QNMtoolbox_alpha is an openly available toolbox; you can redistribute it and/or modify it under the terms of the GNU General PublicLicense as published by the Free Software Foundation, either version 3 of the License, or (at your option) any later version. It is composed of

- the present user guide document,
- **QNMtoolbox_alpha.m**, a Matlab open-source script of the freeware package **MAN** (Modal Analysis of Nanoresonators) [1], built for extracting the normalized resonance modes (also called the quasinormal modes or QNMs) of plasmonic and photonic resonators, and computing the excitation coefficients of QNM expansions at real frequencies. It also computes the absorption and scattering cross-sections of nanoresonators, using the QNMs. The script preferentially operates on the Matlab-COMSOL Livelink environment with the solver **QNMEig** of the package **MAN**; however, the code would also work with QNMs computed with other software,

- **QNMEig_bowtie.mph**, a COMSOL model for operation with the **QNMEig** solver.

Content

1. INTRODUCTION TO QNMTOOLBOX_ALPHA.M

QNMtoolbox_alpha.m extracts the normalized QNMs of electromagnetic resonators computed with the QNM solvers of the **MAN** package and computes the excitation coefficients associated to each QNM at real frequencies. The example is provided for a bowtie antenna excited by a plane-wave polarized along the x-axis propagating along the z-axis (TM polarization).

In this section, basic information about **QNMtoolbox_alpha.m** is provided.

1.1 Download & Installation

QNMtoolbox_alpha.m is a Matlab script to be used with the Matlab-COMSOL livelink environment, in conjunction with the solver **QNMEig** and the model **QNMEig_bowtie.mph**. The script needs to be placed in your Matlab folder to be run.

1.2 How to acknowledge and cite

We kindly ask that you reference the **MAN** package from IOGS-CNRS and its authors in any publication/report for which you used it. The preferred citation for **QNMtoolbox_alpha.m** is the following paper:

[ref] W. Yan, R. Faggiani, and P. Lalanne, "Rigorous modal analysis of plasmonic resonators", Phys. Rev. B **97**, 205422 (2018).

A brief description of the algorithm might be:

"The modal excitation coefficients are obtained analytically from the quasinormal modes computed with the solver QNMEig software of the freeware MAN (Modal Analysis of Resonators) under the COMSOL Multiphysics environment [ref]."

1.3 Units and conventions of input/output data for QNMtoolbox_alpha

Unit. All the input information is required to be in the **SI unit** (e.g., volts per meter for electric field **E**, amperes per meter for magnetic field **H**, …). Accordingly, the output information is given in **SI unit** as well.
Convention. The time dependent terms $\exp(i\omega t)$ used by COMSOL is adopted.

1.4 Outline of the theory and related key issues

QNMtoolbox_alpha is particularly useful for designing micro or nanoresonators, or optical nanoantennas, since analytical solutions and simulation provide great insights into how these devices operate. Since nanoresonators are essentially made of metal and can have different shapes, their simulation should rely on a software that can represent their geometry and model their electromagnetic properties accurately. **QNMtoolbox_alpha** relies on COMSOL Multiphysics®, its RF Module, and MATLAB®.

Classically, to solve Maxwell's equations, one uses a particular excitation, i.e. a given incidence, wavelength, and polarization of an incident light beam. However, the whole numerical simulation has to be redone each time the excitation field changes, in particular the wavelength. Then the numerical load may be heavy, and, above all, the computed results may still hide a great deal of knowledge about the physical

mechanisms at play. Modes represent a powerful characteristic of the resonator. If one is able to find these modes (they are called quasinormal modes) and understand how they are excited, then it is possible to describe the interactions between the resonator and its environment much more easily and intuitively.

The approach adopted by **QNMtoolbox_alpha** is exactly this one. It permits allow one to compute the excitation coefficients of the normalized modes computed by **QNMEig**, simply by evaluating a volume integral [1]. This part is crucial as it results in a rapid and analytical method to calculate the electromagnetic field scattered by the resonator, and all the associated physical quantities, such as the scattering and absorption cross sections and the radiation diagram depicted in figure 3.

In more mathematical terms, we consider a field $\mathbf{E}_b(\mathbf{r},\omega)$ that is incident on the nanoresonator. $\mathbf{E}_b(\mathbf{r},\omega)$ can be a plane wave (to calculate cross-sections) or the field radiated by a dipole source (to calculate the mode volume or the Purcell factor). The optical response of the resonator (e.g. the scattered field) $\mathbf{E}_S(\mathbf{r},\omega,e)$ can be written with a modal expansion of the form

$$\mathbf{E}_\mathrm{S}(\mathbf{r},\omega,\mathbf{E}_\mathrm{b}) = \sum_\mathrm{m} \alpha_m(\omega,\mathbf{E}_\mathrm{b})\,\tilde{\mathbf{E}}_\mathrm{m}(\mathbf{r},\tilde{\omega}_\mathrm{m}), \tag{1}$$

where $\tilde{\mathbf{E}}_m$ denotes the electric-field map of the normalized QNM m, $\tilde{\omega}_m$ is the mode complex frequency, $2Q = \mathrm{Re}(\tilde{\omega}_m)\,/\,\mathrm{Im}(\tilde{\omega}_m)$, and the α_m's are the excitation coefficients that **analytically** depend on the incident field. This implies that, once the resonant modes of a nanostructure are calculated, the optical response is known analytically (i.e. by numerical computation of simple overlap integrals between the incident field $\mathbf{E}_b(\mathbf{r},\omega)$ and the QNM field $\tilde{\mathbf{E}}_m$ [1]) for any instance of the excitation field and the physical understanding is immediate and unambiguous since the mode expansion explicitly depends on the excitation parameters.

For plasmonic resonators whose permittivity follows a single Lorentz pole model, $\varepsilon(\omega) = \varepsilon_\infty\left(1 - \frac{\omega_p^2}{\omega^2-\omega_0^2+i\gamma\omega}\right)$, the modal excitation coefficient can be written:

$$\alpha_m(\omega) = \left(\varepsilon_b - \varepsilon_\infty - \Delta\varepsilon(\tilde{\omega}_m)\frac{\tilde{\omega}_m}{\tilde{\omega}_m-\omega}\right)\iiint_{V_{res}} \mathbf{E}_b\cdot\tilde{\mathbf{E}}_m d^3\mathbf{r}. \tag{2}$$

Note that if dispersion is not considered ($\omega_p = 0$), Eq. 2 becomes $\alpha_m(\omega) = (\varepsilon_\infty - \varepsilon_\mathrm{b})\,\frac{\omega}{\tilde{\omega}_m-\omega}\iiint_{V_{res}} \mathbf{E}_b\cdot\tilde{\mathbf{E}}_m d^3\mathbf{r}$. The derivation of Eq. 2 can be found in section 3.5 of the supplementary material of [1]. The extinction cross-section σ_{ext} and the absorption cross section σ_{abs} at frequency ω are plotted using the scattered field calculated with the QNM expansion

$$\sigma_{ext} = -\frac{1}{2S_0}\iiint_{V_{res}} \mathrm{Im}\left[\omega\big(\varepsilon_\infty(\mathbf{r}) - \varepsilon_b(\mathbf{r},\omega)\big)\mathbf{E}_S(\mathbf{r},\omega)\cdot\mathbf{E}_b^*(\mathbf{r},\omega) - i\mathbf{J}_S\cdot\mathbf{E}_b^*(\mathbf{r},\omega)\right]d^3\mathbf{r}\,, \tag{3}$$

$$\sigma_{abs} = \frac{1}{2S_0}\iiint_{V_{res}} \left[\frac{\gamma}{\varepsilon_\infty\omega_p^2}\right]|\mathbf{J}_S|^2 d^3\mathbf{r}\,, \tag{4}$$

where S_0 is the time-averaged power of the incident plane wave onto the system and $\mathbf{J}_s = \sum_m \alpha_m(\omega)\big(-i\tilde{\omega}_m(\varepsilon(\tilde{\omega}_m) - \varepsilon_\infty)\tilde{\mathbf{E}}_m\big)$. The details for these formulations can be found in sections 2.2 and 3.6 of the supplementary material of [1] and in [2]. If dispersion is neglected, Eqs. (3) and (4) becomes

$$\sigma_{ext} = -\frac{\omega}{2S_0}\iiint_{V_{res}} \mathrm{Im}\big\{(\varepsilon_\infty(\mathbf{r}) - \varepsilon_\mathrm{b})\big(\mathbf{E}_S(\mathbf{r},\omega) + \mathbf{E}_b(\mathbf{r},\omega)\big)\cdot\mathbf{E}_b^*(\mathbf{r},\omega)\big\}d^3\mathbf{r} \tag{5}$$

$\sigma_{abs} = -\frac{\omega}{2S_0}\iiint_{V_{res}} \mathrm{Im}\big(\varepsilon_\infty(\mathbf{r})\big)|\mathbf{E}_S(\mathbf{r},\omega)+\mathbf{E}_b(\mathbf{r},\omega)|^2 d^3\mathbf{r}$.

To summarize, the QNM computation and normalization (the prerequisite to using **QNMtoolbox_alpha**) are performed with **QNMEig**, using COMSOL software. The script extracts the normalized QNM fields inside the resonator domain, performs the overlap integral, and computes the modal excitation coefficients, the extinction and absorption cross sections in a Matlab environment. It shares many common features with the Matlab script **Script_cross_sections_FV.m** used in the QNMPole toolbox to compute the cross-sections, see the Userguide QNMPole.

2. SET-UP: COMPUTATION OF THE EXCITATION COEFFICIENTS

We recommend that the user starts with the bowtie example that is provided to become familiar with **QNMtoolbox_alpha** before calculating the excitation coefficients for its own nanoresonator. To calculate and normalize QNMs, follow the following steps:

1/ Build on a COMSOL model sheet for your problem (see details below), or first use the supplied bowtie model sheet **QNMEig_bowtie.mph**.

2/ Open the Matlab script **QNMtoolbox_alpha.m** and make sure that the COMSOL model in use is the folder.

3/ In **QNMtoolbox_alpha.m**, check the parameters in the ***Input file name and Computing setting, Material parameters, and Computational settings*** sections of the program. In particular, please check the following parameters

- COMSOL.file: the name of the COMSOL file where the QNMs were computed.
- COMSOL.dataset: The tag of the data set of the QNM solution.
- COMSOL.resonator: the index of the resonator domain.

Details on how to correctly set these 3 parameters are given in section 4 of this document.

4/ Run the script. For every real frequency ω, α_m will be computed for a plane wave excitation of amplitude $E_0 = 1\,\mathrm{V/m^2}$ polarized along the x-axis, propagating along the z-axis. The corresponding cross sections will then be calculated in SI units.

3. FREQUENTLY ASKED QUESTIONS

What does the QNM structure contain?

When N QNMs are computed by the COMSOL model, the QNM structure defined inside **QNMtoolbox_alpha.m** contains the following elements.

Name of variable	Description	Size
QNM.omega	QNM frequencies $\tilde{\omega}_m$	$N \times 1$
QNM.QN	QNM Normalization coefficients	$N \times 1$
QNM.eps	Material permittivity evaluated at QNM	$N \times 1$

	eigenfrequency	
QNM.cord	Gauss pattern sampled $x, y,$ and z coordinates inside the resonator volume. Column 1 is x, Column 2 is y, Column 3 is z	$3 \times X$ X depends on COMSOL mesh
QNM.Ex	QNM Electric field x component inside resonator	$N \times X$
QNM.Ey	QNM Electric field y component inside resonator	$N \times X$
QNM.Ez	QNM Electric field z component inside resonator	$N \times X$
QNM.mesh_volume	"Weight" of sampled points inside resonator volume (used for integration)	$1 \times X$

How are the overlap integrals performed?

The values of the QNM fields are extracted for the coordinates contained in QNM.coord. The incident Electric field that overlaps with the QNM fields is defined analytically using the x, y, z coordinates in QNM.cord.

```
k=omega/Phy.c*sqrt(Mat.eps_b);              % wavenumber in background
p=exp(1i*k*QNM.cord(1,:)*Comp.K(1)+...
    1i*k*QNM.cord(2,:)*Comp.K(2)+...
    1i*k*QNM.cord(3,:)*Comp.K(3));          % plane wave phase
E_inc_x=p*Comp.E(1); E_inc_y=p*Comp.E(2);  E_inc_z=p*Comp.E(3);        % incident electric fields
```

The values of the overlap integral between a QNM mode and the incident field are stored inside the variable E_int :

```
% Field overlap integration between incident field and QNM field
E_int=sym_factor.*sum( bsxfun(@times,QNM.Ex,E_inc_x.*QNM.mesh_vol)+...
        bsxfun(@times,QNM.Ey,E_inc_y.*QNM.mesh_vol)+...
        bsxfun(@times,QNM.Ez,E_inc_z.*QNM.mesh_vol),...
        2);
```

An overlap integral using this method entails the scalar product of the fields with QNM.mesh_volume.

If your model uses symmetries, you need to be aware of the value of the variable sym_factor, that is used when computing integrals. In the case of the bowtie model, since only an eighth of the 3D space is meshed, it is set to 8.

For example, the overlap integrals of the QNM fields with itself inside the resonator volume would be written:

```
int_E_self=sym_factor*(QNM.Ex.*QNM.Ex+QNM.Ey.*QNM.Ey+QNM.Ez.*QNM.Ez)*QNM.mesh_vol.';
```

How could one extract the magnetic field?

To extract a component of the QNM magnetic field from COMSOL model use the following lines:

temp=mpheval(model, 'emw.Hx', 'solnum', 'all','pattern','gauss','selection', COMSOL.resonator_domain,'Complexout','on');

QNM.Hx=temp.d1; % Magnetic field x component

The lines to extract the magnetic field components are included in the **QNMtoolbox_alpha.m** script, in the "Read data from COMSOL file" section, and these lines are simply commented.

How are the modal excitation coefficients computed inside the program?

The prefactors to the modal excitation coefficients at frequency ω are stored inside the variable "alpha_QNM" which is

alpha_QNM $= \left(\varepsilon_b - \varepsilon_\infty - \left(\Delta\varepsilon(\tilde{\omega}_m)\right)\frac{\tilde{\omega}_m}{\tilde{\omega}_m-\omega}\right)/N_{\mathrm{m}} = \frac{1}{\omega-\tilde{\omega}_m}\left(-\omega(\varepsilon_\infty-\varepsilon_b)-\tilde{\omega}_m(\varepsilon(\tilde{\omega}_m)-\varepsilon_\infty)\right)/N_m$, where N_m is the normalization coefficient of the m^{th} QNM.

The modal excitation coefficients for a single frequency are obtained by the performing following product:

alpha_QNM $*$ E_int % Modal Excitation coefficients

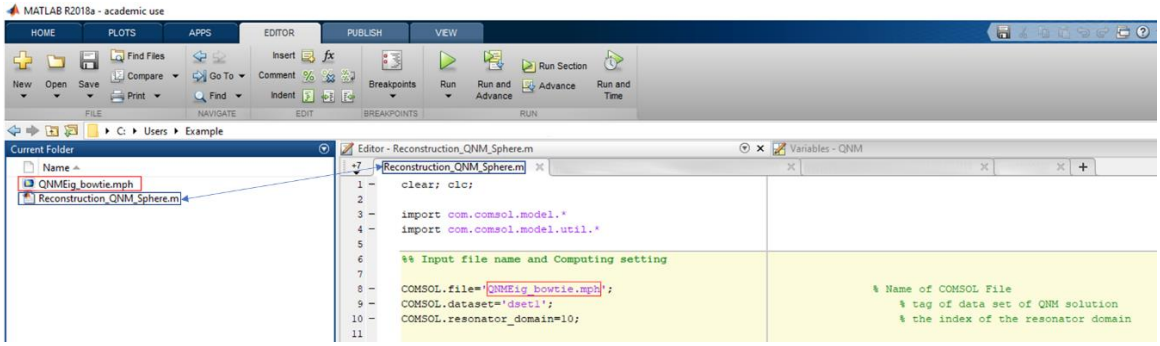
4. TROUBLESHOOTING

This sections constains a few ways to find some of the COMSOL model information that you need to modify the **QNMtoolbox_alpha.m** script to your liking.

The essential prerequisite step before using **QNMtoolbox_alpha** is to compute QNMs using a COMSOL model present in the QNMEig package or model modified from these. This operation is detailed in the **QNMEig** user guide included in the MAN Package versions greater than 6.

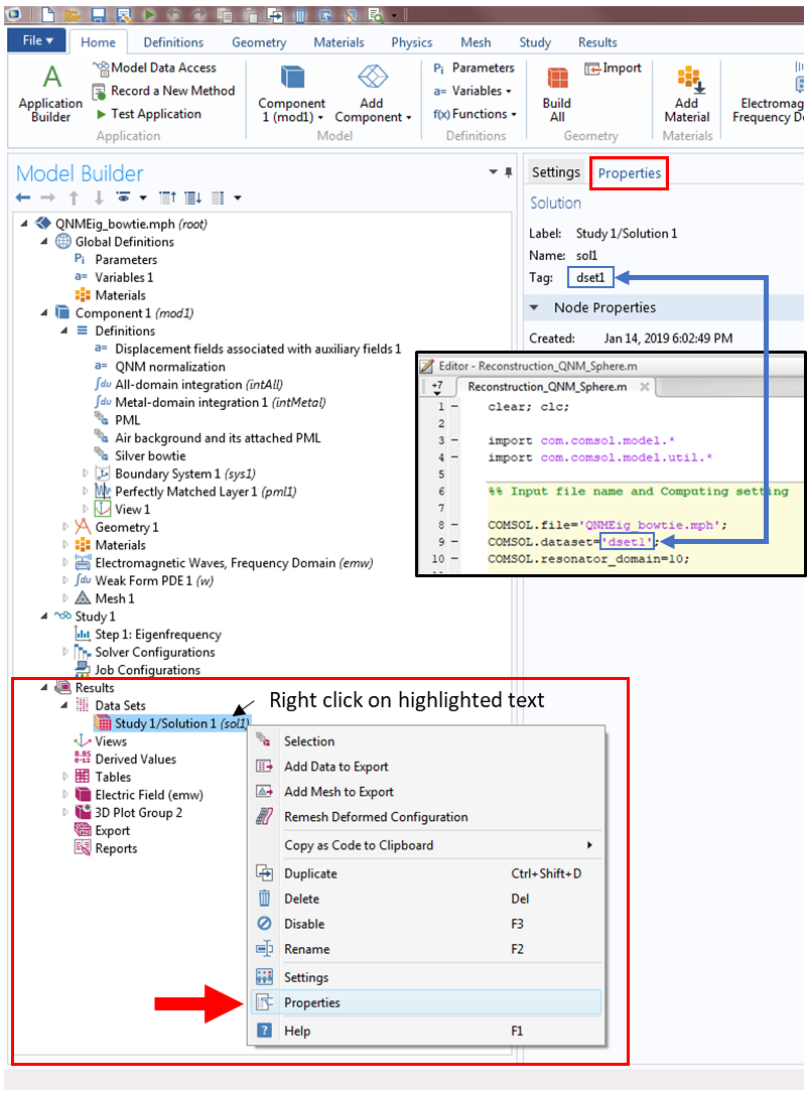
Once the QNM modes are computed inside the COMSOL model file, **QNMtoolbox_alpha.m** needs to be modified for use with the specific COMSOL model.

→The COMSOL model file should be placed in the same folder as the **QNMtoolbox_alpha.m** and the COMSOL.file variable should be defined as the complete name of the COMSOL file (file extension included).



The COMSOL model can be placed in another folder but you'll have to specify the location of the file in the COMSOL.file variable.

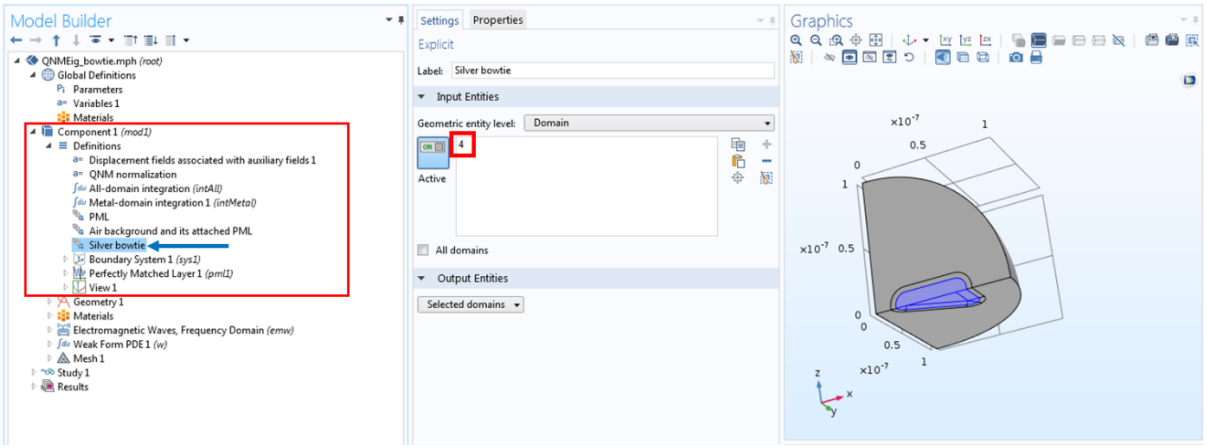
→The COMSOL.dataset variable must correspond to the name COMSOL dataset that contains the QNMs. This can be checked directly in COMSOL.



a. Open the COMSOL model file using COMSOL.
b. In the Model Builder window expand the "Results" section, by left clicking on the triangle on the left of "Results" line. This should make the "Data Sets" line appear. Click on the triangle on the left of the "Data sets" to expand the "Data Sets" section.
c. Right click on the StudyX/Solution Y (solZ) line that corresponds to the QNM calculation (X,Y,Z are the numbers that correspond to the QNM data set) and select "Properties". It should bring up the Properties tab for the QNM dataset.
d. The name of the dataset to be entered in the **QNMtoolbox_alpha.m script** is the **"Tag"**

→COMSOL.resonator_domain corresponds to the domain label (a positive integer) in the COMSOL model file that corresponds to the resonator domain. A way to check this would be to look inside the model in COMSOL. In the QNMEig model files, the different materials are split into different "explicit selections" to distinguish them.

→In the Model Builder window, expand the "Component 1 (mod1)" section, then the "Definitions" section to reveal the "explicit selections" denoted by the symbol. There should be one that corresponds to the QNMEig model's resonator domain (For example, the selection for the bowtie model is labeled "Silver Bowtie" and the corresponding domain is #4. This information can also be found inside the integration operators defined inside the COMSOL models, denoted by the $\int du$ symbols. Here, "Metal-domain integration 1" should also contain that information.



5. REFERENCES

[1] W. Yan, R. Faggiani, P. Lalanne, Phys. Rev. B **97**, 205422 (2018).
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