Supplemental Information

Title: **A comprehensive design framework for all-dielectric metasurfaces by harnessing the interplay of controlled multiple multipoles excitation, Rayleigh anomaly, Mie and lattice resonances**

Tummaluru Khadar Basha,[1] Faraz A. Inam,[2] and Junaid Masud Laskar[1*],
Nanophotonics and Quantum Meta-Optics Group, Center for Nanophotonics, Department of Physics and Nanotechnology, Kattankulathur, Chennai, Tamil Nadu, PIN- 603203, India
Department of Physics, Aligarh Muslim University, Aligarh, Uttar Pradesh, PIN-202002, India
(*Electronic mail: junaidmb@srmist.edu.in)

Theoretical background

Electromagnetic wave scattering cross-section (C_{sca}^{total}) of a meta-atom

Multipole moments of different nature and orders, electric dipole (p_α), magnetic dipole (m_α), electric quadrupole $(Q_{\alpha\beta}^{e})$ and magnetic quadrupole $(Q_{\alpha\beta}^{m})$, can be excited in a meta-atom on excitation by an electromagnetic wave, as shown in Fig. 1[1]. The resonant excitation of multipoles take place on satisfying the following conditions. First, meta-atom physical dimensions should be of the order of excitation wavelength $(\lambda_{excitation})$. Secondly, the meta-atom refractive index should have high real values, while having lower value for the imaginary component. On excitation of a dielectric meta-atom (TiO_2, $n_{TiO_2} = 2.49 \text{ @ } \lambda_{excitation} = 488\, nm$) by an electromagnetic wave $(\lambda_{excitation} = 488\, nm)$ [Fig. 1], the total electromagnetic wave scattering cross-section (C_{sca}^{total}) can be expressed using multipolar decomposition, considering the contributions from different individual multipole moments- electric dipole (p_α), magnetic dipole (m_α), electric quadrupole $(Q_{\alpha\beta}^{e})$ and magnetic quadrupole $(Q_{\alpha\beta}^{m})$, as given below

$$C_{sca}^{total} = C_{sca}^{p} + C_{sca}^{m} + C_{sca}^{Q^e} + C_{sca}^{Q^m} \tag{1}$$

$$C_{sca}^{total} = \frac{k^4}{6\pi\varepsilon_0^2|E_{Inc}|^2}\left[\sum_{\alpha}\left(|p_\alpha|^2\right) + \sum_{\alpha}\left(|m_\alpha|^2\right) + \frac{1}{120}\left[\sum_{\alpha\beta}\left(|kQ_{\alpha\beta}^{e}|^2\right) + \sum_{\alpha\beta}\left(\left|\frac{kQ_{\alpha\beta}^{m}}{c}\right|^2\right)\right]\right] \tag{2}$$

Here, C_{sca}^{p}, C_{sca}^{m}, $C_{sca}^{Q^e}$, and $C_{sca}^{Q^m}$ are the cross sections corresponding to electric dipole (ED), magnetic dipole (MD), electric quadrupole (EQ), and magnetic quadrupole (MQ), as shown in Fig. 1c. The notations $|E_{inc}|^2$, k and c are the amplitude of the incident electric field, wave vector, and speed of light, respectively. The electromagnetic multipole moments are deduced from the distribution of induced electric current density (J_ω) of a meta-atom, on considering the surrounding

medium as air $\left[n_{air} = \sqrt{\epsilon_0} = 1\right]$. The induced current density (J_ω) in the meta-atom is expressed as

$$J_\omega(r) = -i\omega\epsilon_0\left[\epsilon_r(r) - 1\right]E\,(r) \tag{3}$$

Here, ϵ_0 and $\epsilon_r(r)$ are the permittivity in vacuum and relative permittivity at the position coordinates r with respect to the surrounding medium air, respectively. The electric field $E\,(r)$ contains both the incident field and the scattered radiation by the meta-atom. The electromagnetic multipole moments can be expressed as an integral function of induced current density (J_ω), as given below.

Electric dipole moment-**ED**:

$$p^\alpha = -\frac{1}{i\omega}\left\{\int d^3r J_\alpha^\omega\, j_0(kr) + \frac{k^2}{2}\int d^3r\left[3\,(r\cdot J_\omega)r_\alpha - r^2 J_\alpha^\omega\right]\frac{j_2\,(kr)}{(kr)^2}\right\} \tag{4}$$

Magnetic dipole moment-**MD**:

$$m^\alpha = \frac{3}{2}\left\{\int d^3r(r\times J_\omega)_\alpha\frac{j_1\,(kr)}{kr}\right\} \tag{5}$$

Electric quadrupole moment-**EQ**:

$$Q_{\alpha\beta}^{e} = -\frac{3}{i\omega}\left\{\int d^3r\left[3\left(r_\beta J_\alpha^\omega + r_\alpha J_\beta^\omega\right) - 2(r\cdot J_\omega)\delta_{\alpha\beta}\right]\frac{j_1\,(kr)}{kr} + 2k^2\int d^3r\left[5r_\alpha r_\beta\,(r\cdot J_\omega) - (\right.\right. \tag{6}$$

Magnetic quadrupole moment-**MQ**:

$$Q_{\alpha\beta}^{m} = 15\int d^3r\left\{r_\alpha(r\times J_\omega)_\beta + r_\beta(r\times J_\omega)_\alpha\right\}\frac{j_2\,(kr)}{(kr)^2} \tag{7}$$

Here, α, β are the symbolic representations of x, y, z position co-ordinates.

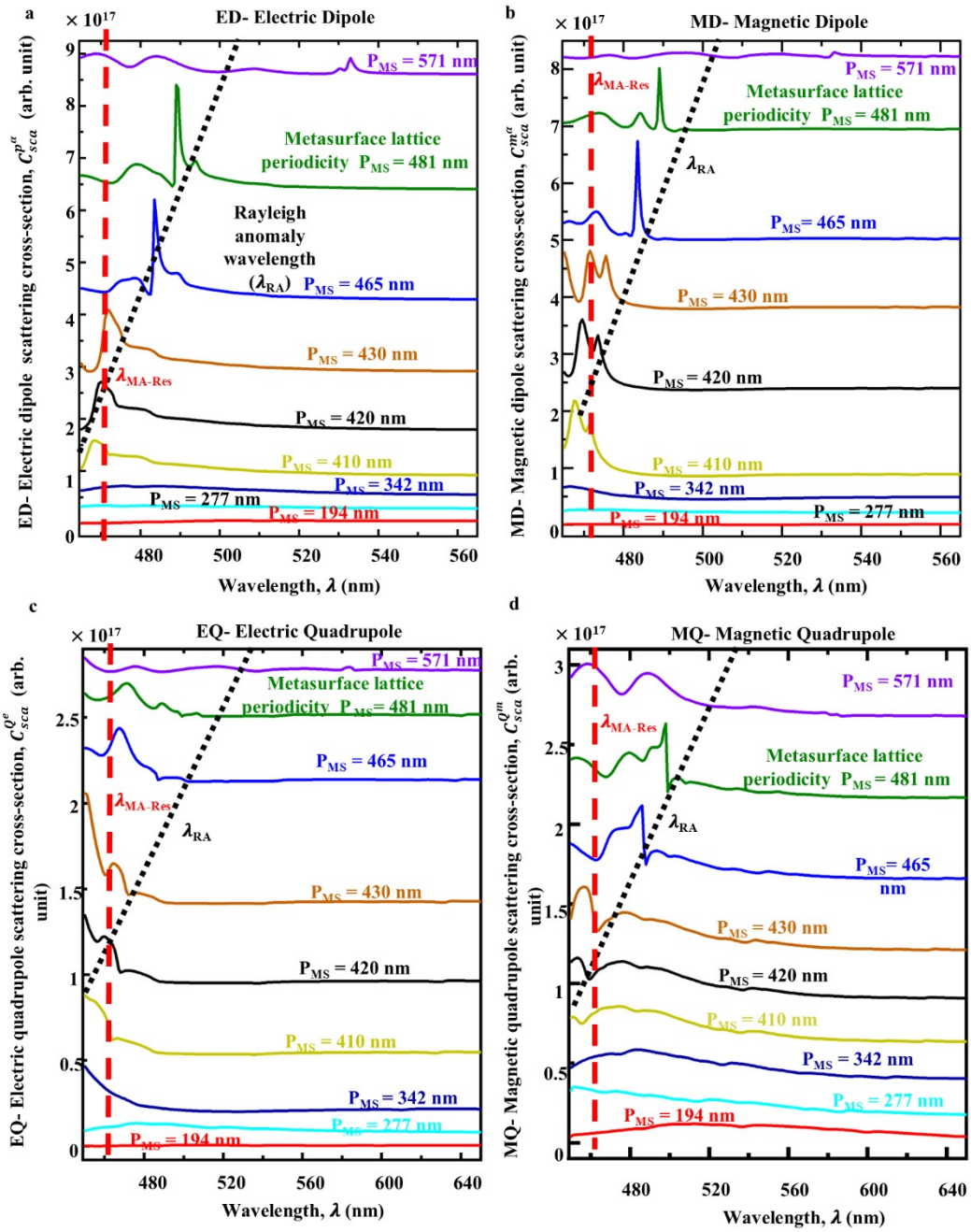
Effective refractive index (n_{eff}) of a metasurface on an opaque substrate

The effective refractive index (n_{eff}) of a metasurface on an opaque substrate, as a function of the diameter (D_{MA}) of each meta-atom as well as the metasurface array lattice periodicity (P_{MS}), is given by the following expression[2]

$$n_{eff} = n_{TiO_2}\left(\frac{\pi\cdot D_{MA}^2}{3\cdot\sqrt{3}\cdot P_{MS}^2}\right) + n_{air}\left(1 - \frac{\pi\cdot D_{MA}^2}{3\cdot\sqrt{3}\cdot P_{MS}^2}\right) \tag{8}$$

Here, n_{TiO_2} and n_{air} are the refractive indices of the TiO_2 meta-atom and surrounding medium air, respectively.

Results



Lattice periodicity (P_{MS}) dictates coupling among Mie-resonance and lattice resonances

Figure S1: Multipole scattering cross-section (C_{sca}) EM spectra of metasurface for different lattice periodicities (P_{MS})

Number of meta-atoms in finite metasurface dictates spatial hybridization of EM multipoles

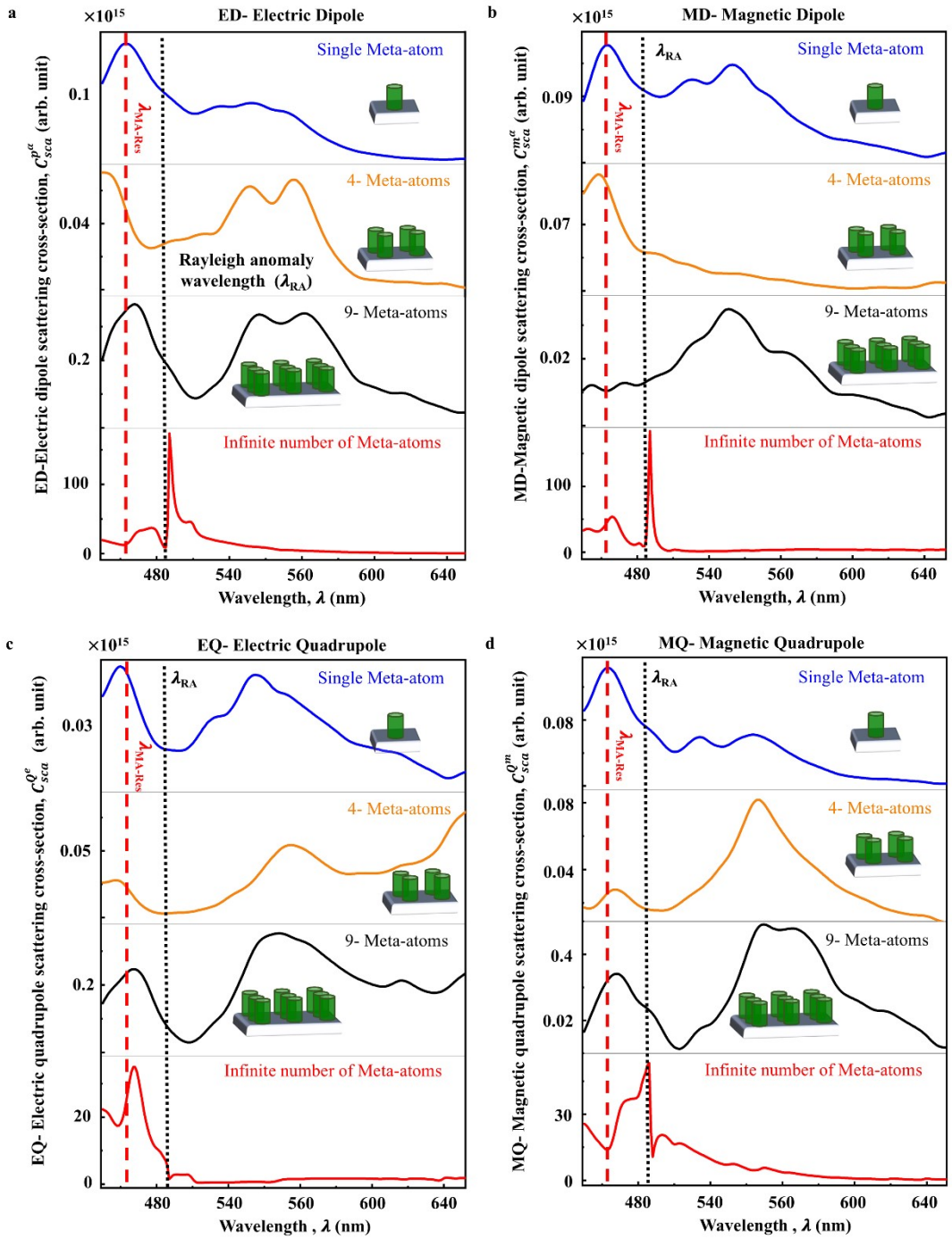


Figure. S2: Multipole scattering cross-section (C_{sca}) EM spectra of metasurface for different number of meta-atoms.

References

1 R. Alaee, C. Rockstuhl and I. Fernandez-Corbaton, *Optics Communications*, 2018, **407**, 17–21.

2 D. Visser, D. Y. Chen, Y. Désières, A. P. Ravishankar and S. Anand, *Scientific Reports*, 2020, **10**, 1-11.