Supplementary Information
for
Photonic Band Structure Calculation of 3D-Finite Nanostructured Supercrystals

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Table S1: High symmetry (critical) points and symmetry lines in the first Brillouin zone of a simple cubic lattice.

Symmetry points (u,v,w)	$[k_x,k_y,k_z]$
Γ: (0,0,0)	[0,0,0]
X: (½, 0 ,0)	[π/a,0,0]
M: (½,½,0)	[$\pi/a,\pi/a$,0]
R: (½,½,½)	[$\pi/a,\pi/a,\pi/a$]

Symmetry lines	**Length**
Δ: (0,v,0), $0 < v < ½$	$\overline{\Gamma X} = \pi/a$
T: (½,½,w), $0 < w < ½$	$\overline{MR} = \pi/a$
Λ: (w,w,w), $0 < w < ½$	$\overline{\Gamma R} = \sqrt{3}\pi/a$
Σ: (u,u,0), $0 < u < ½$	$\overline{\Gamma M} = \sqrt{2}\pi/a$
S: (u,½,u), $0 < u < ½$	$\overline{XR} = \sqrt{2}\pi/a$
Z: (u,½,0), $0 < u < ½$	$\overline{XM} = \pi/a$

Table S2: Key physical parameters for each system: supercrystal overall size (L), unit cell volume (V_{cell}), nanoparticle volume (V_{NP}), and filling fraction ($F=V_{NP}/V_{cell}$).

Supercrystals	L [μm]	V_{cell} [nm^3]	V_{NP} [nm^3]	F
Spherical NPs, a=100 nm	2.0	10^6	2.68×10^5	0.268
Spherical NPs, a=130 nm	3.5	2.20×10^6	2.68×10^5	0.122
Nanorods, a=100 nm	2.0	10^6	8.38×10^4	0.084

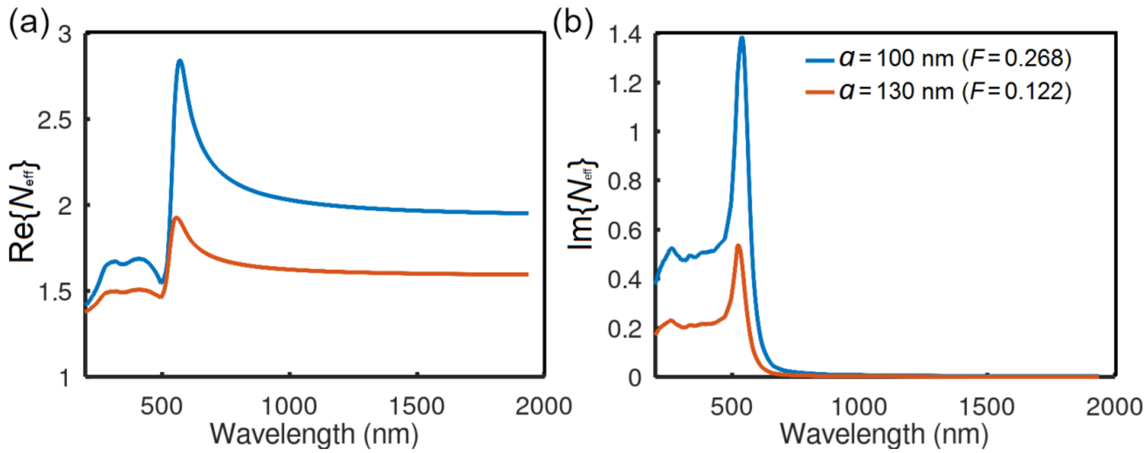

Figure S1: (a) Real and **(b)** imaginary parts of the effective refractive index of superlattices composed by Au NPs of 80 nm in diameter arranged in a simple cubic lattice and with lattice parameters of a=100 nm (blue) and a=130 nm (red). The refractive index of the Au NPs is taken from Johnson and Christy's experimentally tabulated data and the refractive index of the medium is n_m=1.33 (water). F is the filling factor.

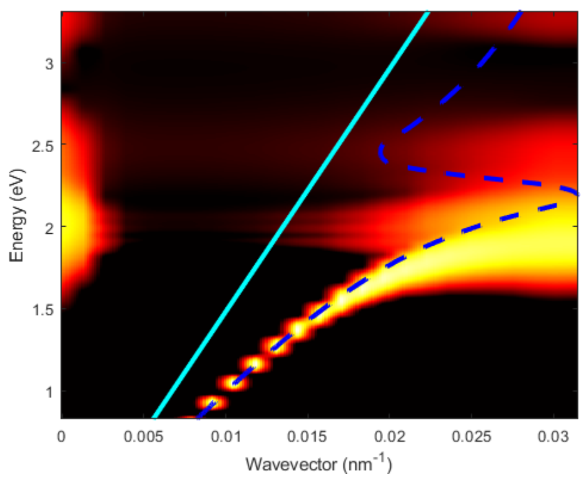

Figure S2: Dispersion relation of an infinite Au-NPs supercrystal with a lattice parameter of 100 nm, light dispersion in water (cyan solid line), and dispersion relation of the light in the effective medium (blue dashed line).

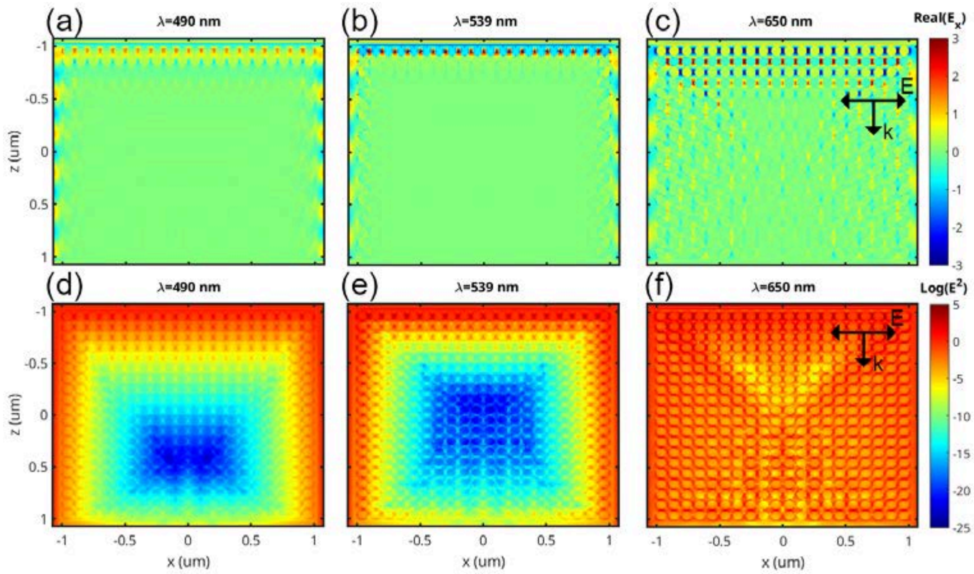

Figure S3: Real part of the *x*-component of the electric field (upper panels) and electric field intensity enhancement in log-scale (lower panels) of a cubic supercrystal composed of 80-nm Au NPs in a cubic array of lattice parameter *a*=100 nm. The cubic supercrystal is excited with a plane wave of $\mathbf{k} = \mathbf{k}_X$ (**X** point of the Brillouin zone) and at wavelengths corresponding to (**a**, **d**) the upper branch, (**b**, **e**) the polaritonic band gap, and (**c**, **f**) the lower branch of the photonic band structure (**Figure 4a**).

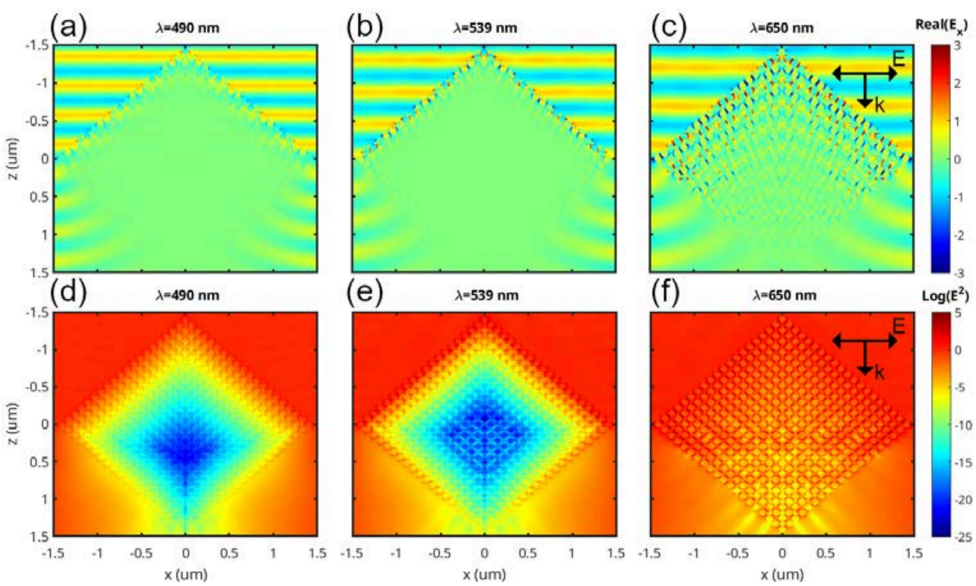

Figure S4: Real part of the *x*-component of the electric field (upper panels) and the electric field intensity enhancement in log-scale (lower panels) of a rhombic dodecahedral supercrystal composed of 80-nm Au NPs in a cubic array of lattice parameter *a*=100 nm. The cubic supercrystal is excited with a plane wave of $\mathbf{k} = \mathbf{k}_M$ (**M** point of the Brillouin zone) and at wavelengths corresponding to (**a**, **d**) the upper branch, (**b**, **e**) the polaritonic band gap, and (**c**, **f**) the lower branch of the photonic band structure (**Figure 4c**).

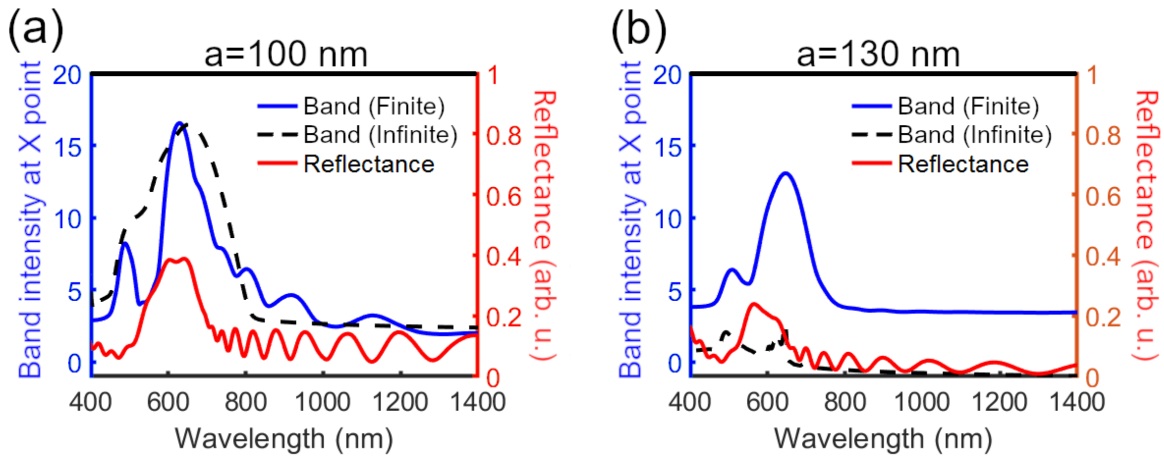

Figure S5: Band structure at **X** point (**k** = $\mathbf{k}_X$), blue line, and reflectance, red line, of a cubic Au NPs supercrystal with a lattice parameter of **(a)** 100 nm and **(b)** 130 nm. The band structure for the infinite case is also plotted, dashed black line.

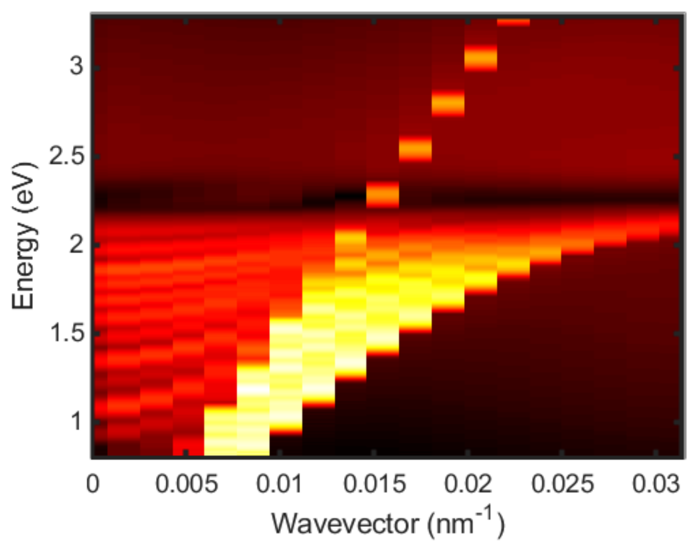

Figure S6: Dispersion relation of slab with effective refractive index (N_{eff}) representing a Au-NPs supercrystal with a lattice parameter of 100 nm in water.

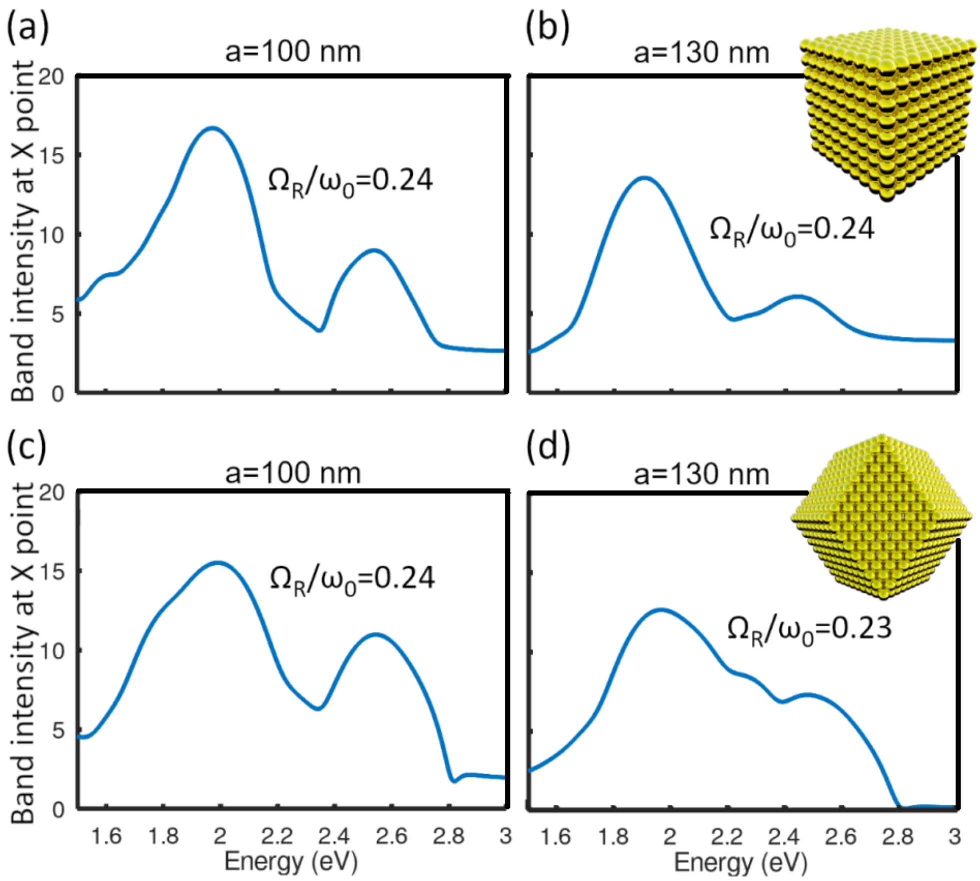

Figure S7: Photonic bands and mode splitting to plasmonic mode energy ratios (Ω_R/ω_0) at the **X** point for the finite supercrystals with cubic (**a**, **b**) and rhombic dodecahedral (**c**, **d**) habits. The LSPR energy is $\hbar\omega_0 \sim 2.3$ eV.