Supporting Information

Enhancement of Deep Ultraviolet Chiral Molecular Sensing Performance by Collective Lattice Resonances of Diamond Nanostructure Arrays

Shengsui Cai,^{#,a} Jing Wang,*,^{#,a} Wenxuan Liu,^a Zhaolong Cao,^a Huanjun Chen,^a Lei Shao,*,^a and Shaozhi Deng^a

^aState Key Laboratory of Optoelectronic Materials and Technologies, Guangdong Provincial Key Laboratory of Display Materials and Technologies, School of Electronics and Information Technology, Sun Yat-Sen University, Guangzhou, 510275 China

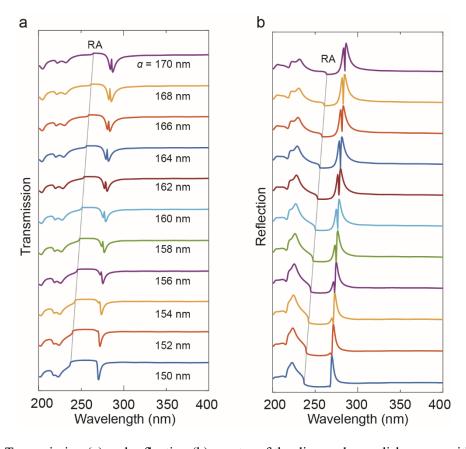


Fig. S1 Transmission (a) and reflection (b) spectra of the diamond nanodisk arrays with the period a varying from 150 to 170 nm. The diameter and height of the nanodisk unit were set at d = 121 nm and h = 51 nm, respectively.

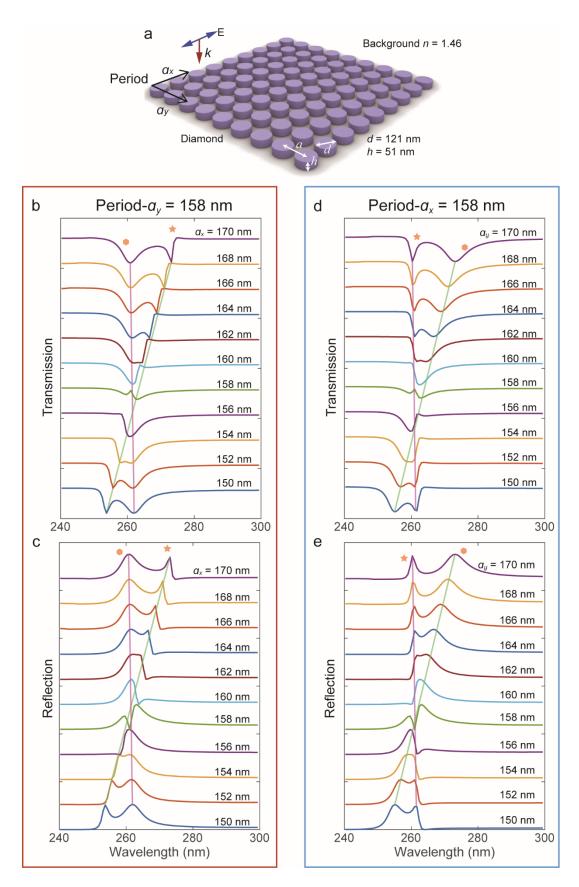


Fig. S2 Dependence of the collective resonance modes on the lattice constants of the diamond nanodisk array. (a,b) Transmission (a) and reflection (b) spectra of the nanodisk arrays with

the lattice constant along x axis a_x varying from 150 to 170 nm and the lattice constant along y axis a_y fixed at 158 nm. (c,d) Transmission (c) and reflection (d) spectra of the diamond nanodisk arrays with a_y varying from 150 to 170 nm and a_x fixed at 158 nm. The excitation light is always linearly polarized along the x-direction.

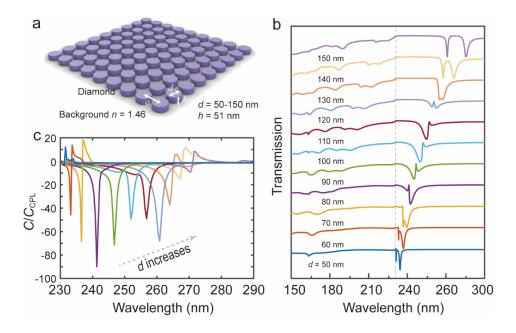


Fig. S3 Dependence of the collective resonance modes and the optical chirality on diameter of the diamond nanodisk unit in the array. (a) Schematics showing a square array of diamond nanodisks in a surrounding medium with n = 1.46. The diameter d of the nanodisk unit varies from 50 nm to 150 nm. The lattice constant of the array a and height h were fixed at 158 nm and 51 nm, respectively. (b) Transmission spectra of the diamond nanodisk array shown in (a) with varying d. (c) Averaged C enhancement spectra of the nanodisk arrays with different d. The averaged C enhancements were calculated by averaging the value of $C/|C_{CPL}|$ outside the nanodisk over an area of $a \times a$ in the horizontal central plane of the nanodisk unit as a function of wavelength, with the diamond nanodisk placed in the centre.

Methods

The simulation in this paper is accomplished by the Wave Optics Module of COMSOL Multiphysics. The refractive index of PMMA and molecules are derived by fitting the following equations:

$$\varepsilon = \varepsilon_b - \gamma \left(\frac{1}{\hbar \omega - \hbar \omega_0 + i \Gamma} - \frac{1}{\hbar \omega + \hbar \omega_0 + i \Gamma} \right)$$

$$\kappa = \beta \left(\frac{1}{\hbar \omega - \hbar \omega_0 + i\Gamma} - \frac{1}{\hbar \omega + \hbar \omega_0 + i\Gamma} \right)$$

 ε_b =2.14 is background permittivity, γ_1 = 0.007 eV, γ_2 = 0.3 eV, $\omega_{0,1}$ = 3.65 eV, $\omega_{0,2}$ = 4.65 eV, Γ_1 = 0.07 eV, Γ_2 = 0.22 eV, where the subscripts 1 and 2 represent PMMA and molecule respectively. The constant β = -1.5×10^{-5} eV for the chiral molecule. The built-in Electromagnetic Waves, Frequency Domain equations in COMSOL Multiphysics were reformulated by substituting κ into Maxwell's equations. This modified formulation included the introduction of chiral variables, allowing for chiral correlation calculations to be performed. In Fig. 4c, the ratio of molecule: PMMA = 1.17×10^{-5} . To calculate the optical chirality enhancement, we first extracted electromagnetic field data from a 153×153 nm² region using MATLAB and computed the $C/|C_{CPL}|$ values. A zero matrix was then applied to exclude the nanostructure region, focusing exclusively on enhancement in the non-structural region. The average enhancement was obtained by taking the mean of all non-zero values in the unmasked area.