

## Supporting Information

# Computational modelling of nanoparticle-based tunable photonic crystal sensors

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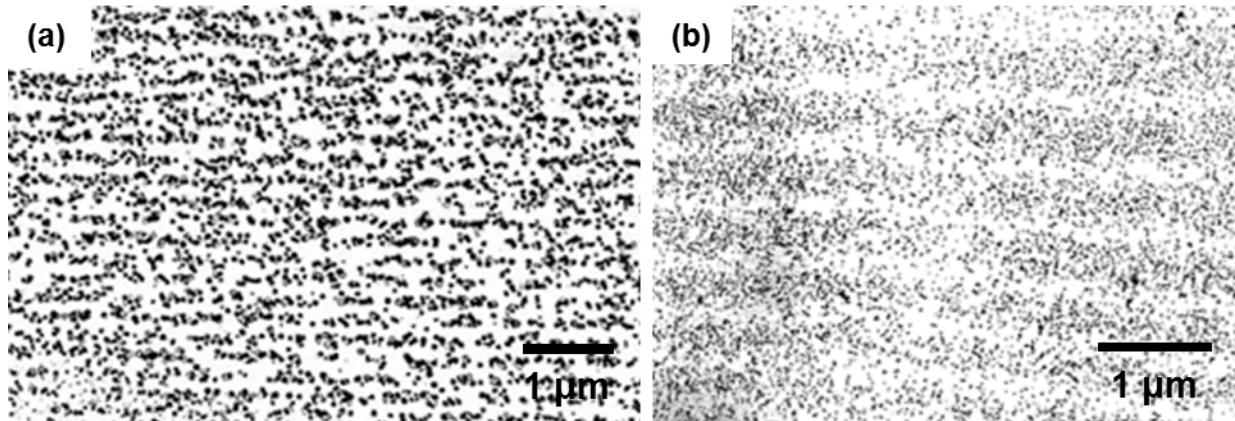
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This file contains information about the materials and equipment used in the fabrication of  
photonic crystal devices and provides a protocol for its fabrication.

## Diffraction gratings of photonic crystals

Figure S1 shows diffraction gratings produced through laser writing.



**Figure S1.** The electron micrographs of hydrogel-based photonic crystal cross sections recorded using a HeNe laser operated at 632.8 nm. (a) A Lippmann phase photonic crystal. Reprinted with permission from ref [1]. Copyright 1988 The Optical Society of America. (b) A phase diffraction grating. Reprinted with permission from ref [2]. Copyright 1999 The Royal Photographic Society.

## MATERIALS AND METHODS

**Materials.** 3-(Trimethoxysilyl)propyl methacrylate (98%), acetone (99.9%), 2-hydroxyethyl methacrylate (HEMA) (ultrapure 99+%), ethylene dimethacrylate (EDMA), methacrylic acid (MAA) (99%), 2-dimethoxy-2-phenylacetophenone (DMPA) (99%), silver perchlorate ( $\text{AgClO}_4$ ) (99%), lithium bromide (99%), 1,1'-diethyl-2,2'-cyanine iodide (photosensitizing dye) sodium phosphate dibasic ( $\text{Na}_2\text{HPO}_4$ ) (99.0%), L-ascorbic acid (99%), sodium carbonate (99.9%) and sodium hydroxide (98.0%) were purchased from Sigma-Aldrich. All chemicals were of analytical grade and used without further purification. Methanol, propan-2-ol, and ethanol were purchased from Fisher Scientific, U.K. 4-methylaminophenol sulfate was purchased from Acros

Organics. sodium thiosulphate (10% w:v) (hypo/x-ray fixer) was purchased from Champion Photochemistry (Essex, U.K.).

**Equipment.** Microscope slides (1.2 mm thick) were purchased from Fisher Scientific. Single-side aluminised polyester film was purchased from HiFi Industrial Film Ltd. (Stevenage, U.K.). Stratalinker 2400 UV Crosslinker ( $\sim 350\text{ nm}$ ,  $4000\text{ }\mu\text{watts/cm}^2$ ) was purchased from RS Components (Corby, U.K.). Nd-Yttrium-Aluminum-Garnet pulsed laser (high power compact Q-switched Nd:YAG oscillator with super gaussian resonator,  $700\text{ mJ @ 1064 nm, 10 Hz}$ ) with a second harmonic generator,  $350\text{ mJ @ 532 nm 10 Hz}$ , thermally stabilized with wavelength separation) was purchased from Lambda Photometrics (Harpden, U.K.). AvaSpec 2028 spectrophotometer, 2048-pixel InstaSpec IV CCD detector and a bifurcated cable (FC UV 600-2,  $600\text{ }\mu\text{m}$  fibre, 2 m length, SMA terminations) were purchased from Avantes (Apeldoorn, The Netherlands). FE20 FiveEasy pH meter was purchased from Mettler Toledo (Leicester, U.K.). Abbé refractometer (Atago 4t) with an LED was purchased from Atago USA (Bellevue, WA). AvaSoft (v8.0) software and COMSOL Multiphysics (v4.3b) were used for data processing and simulations. Lumix DMC-FZ20 camera was used for imaging.

**Silane Coupling.** 3-(Trimethoxysilyl)propyl methacrylate and acetone 1:50 (v/v) was poured onto glass microscope slides in an aluminum tray. After thorough coating, the excessive acetone/silane mix was poured off whilst slides remaining *in situ* due to surface tension. The slides stored in the tray overnight in the dark, before removal and dark storage at room temperature.

**Synthesis of poly(HEMA) Films (pH 4.5-7).** Prepolymer solution consisted of EDMA (2.5 mol%), MAA (6 mol%) and HEMA (91.5 mol%). The solution was mixed by 1:1 (v:v) with 2% (w:v) DMPA in propan-2-ol. 200  $\mu\text{l}$  of the solution was pipetted as a lateral blob on an

aluminum coated polyester sheet, aluminum side facing up. Silanised side facing down, the slide was placed on the lateral blob. Bubbles can be prevented by lowering one side of the slide over the blob, then laying the rest of the slide on the lateral blob. The system was exposed to UV light for 1 hour. The slide was lifted off from the aluminum coated sheet, and finally rinsed with deionized water and ethanol, respectively.

**Photosensitisation of poly(HEMA) Films with Silver Halide Chemistry.** Under red safe lighting, 200  $\mu$ l of 0.3 M  $\text{AgClO}_4$  dissolved in propan-2-ol and DI water (1:1 v/v) was pipetted as an elongated blob onto a glass sheet. Polymer film side down, the slide was placed on the elongated blob. The slide was remained *in situ* for three minutes to allow diffusion of  $\text{AgClO}_4$  into the polymer film. The slide was lifted off and excess  $\text{AgClO}_4$  solution was wiped with a squeegee. The film was dried under a tepid air current for five seconds. A solution consisting of 1,1'-diethyl-2,2'-cyanine iodide (1 ml) (1:500, w/v, 1 ml) in methanol and lithium bromide (0.3 M, 40 ml) in 3:2 (v/v) methanol: $\text{H}_2\text{O}$  was dispensed into a Petri dish. Polymer film side facing up, the slide was immersed in the Petri dish for 30 s (Figure 3f). The slide was washed thoroughly with deionized water.

## References

- [1] T. Kubota, "Cross-Sectional View of Lippman Hologram Gratings," *Applied Optics*, vol. 27, pp. 4358-4360, Nov 1 1988.
- [2] J. Blyth, R. B. Millington, A. G. Mayes, and C. R. Lowe, "A diffusion method for making silver bromide based holographic recording material," *Imaging Science Journal*, vol. 47, pp. 87-91, 1999.