Electronic Supplementary Information

The shift of optical absorption band edge of ZnO/ZnS core/shell nanotube arrays beyond quantum effects

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† Electronic Supplementary Information (ESI) available: [details of any supplementary information available should be included here]. See DOI: 10.1039/x0xx00000x

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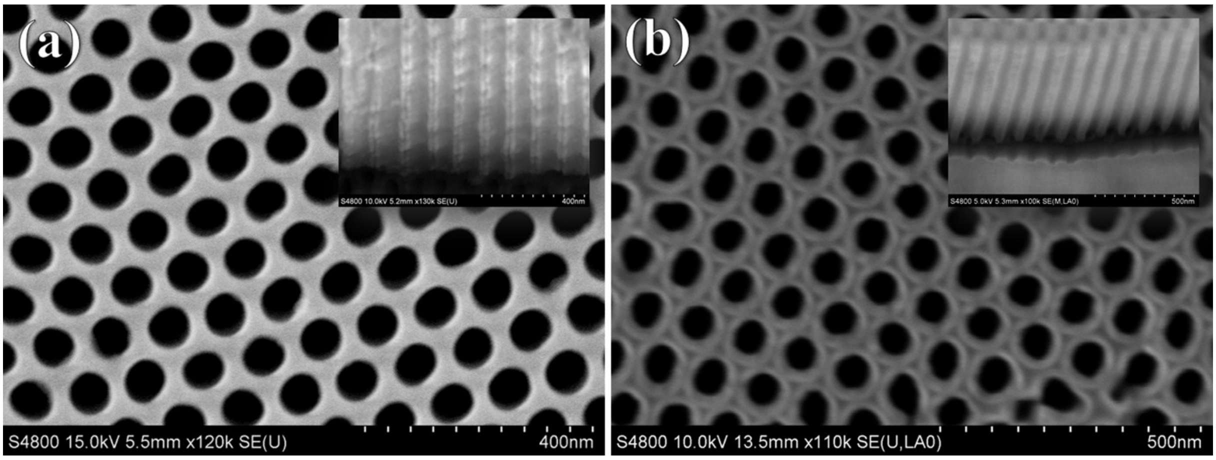

Figure S1. SEM images of (a) Top view of the prepared AAO template with pore diameter around 70 nm after 35 min of pore widening process; the inset is the cross-sectional view of AAO template after 30 min anodizing at 2 °C. (b) Uniform ZnO layer deposited by 300 cycles ALD after an ion milling process with 5 kV for 10 min; the inset is the cross-sectional view, showing that the ZnO is covering the entire surface of AAO template pores.

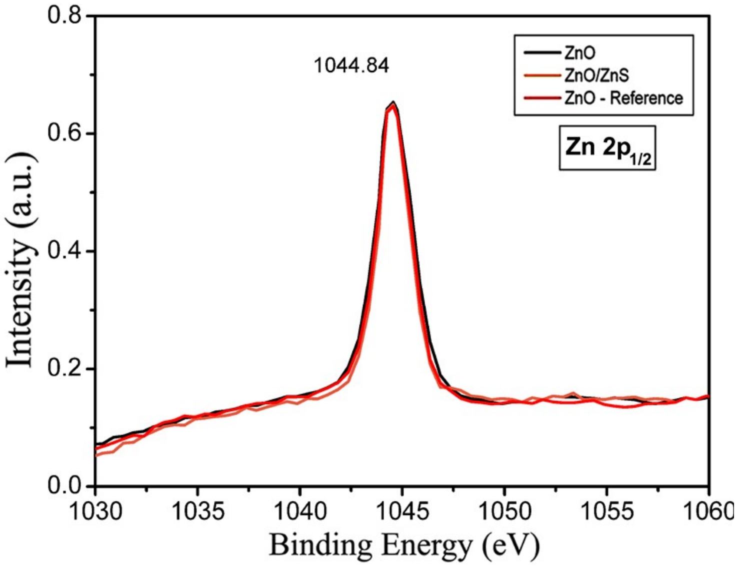

Figure S2. Resolved Zn $2p_{1/2}$ peaks for the three samples.

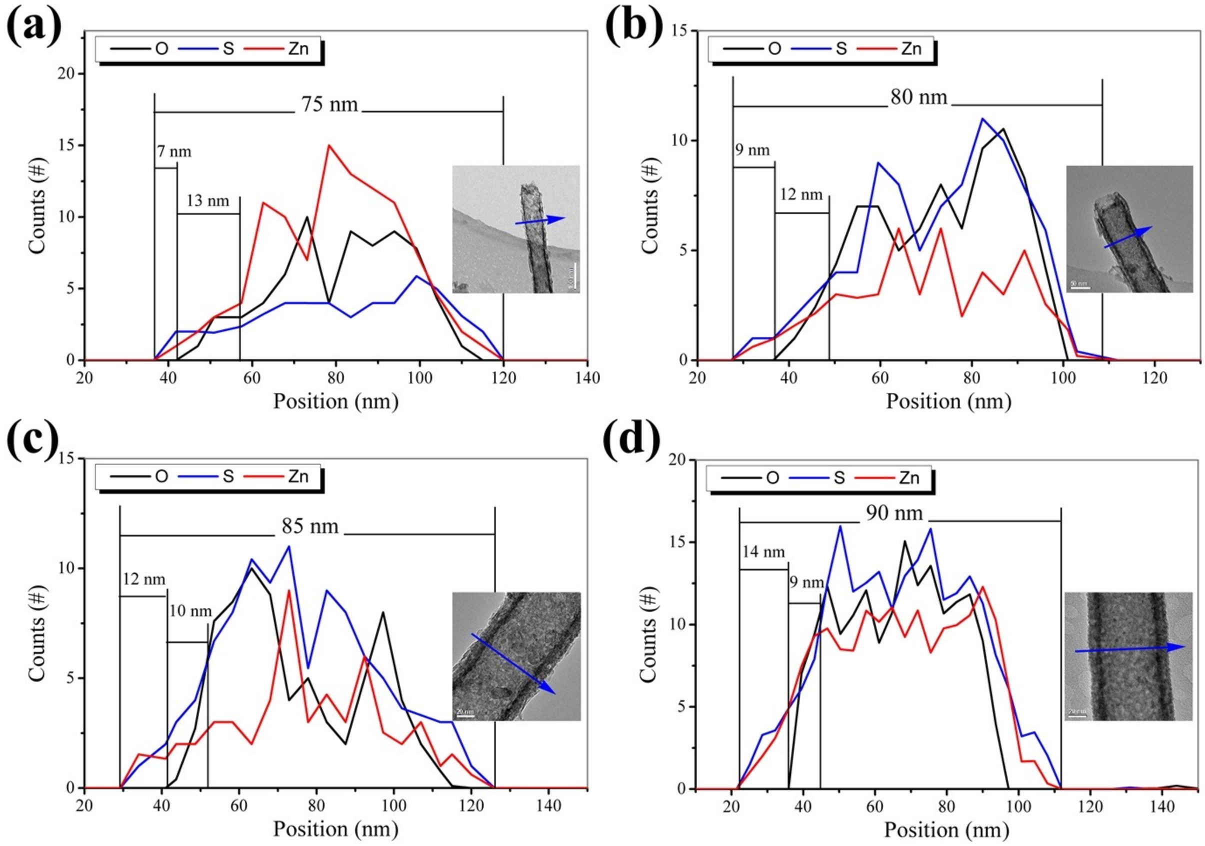

Figure S3. TEM-EDX line scan for four sets of nanotube arrays with different geometric features.

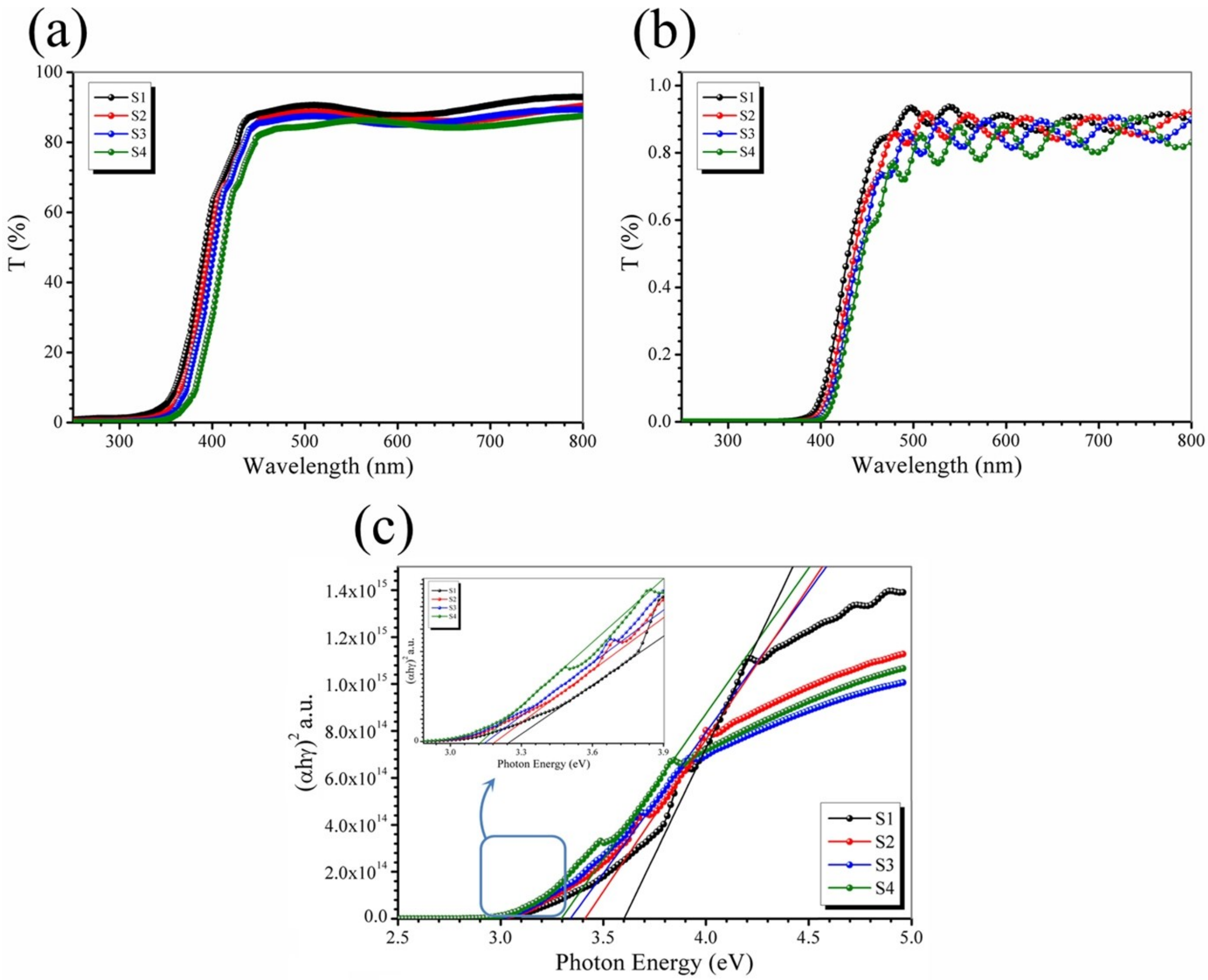

Figure S4. (a, b) Experimental and FDTD simulated transmittance spectra of the prepared ZnO/ZnS nanotube arrays. (c) Tauc plots of direct optical band gap calculations from FDTD results.

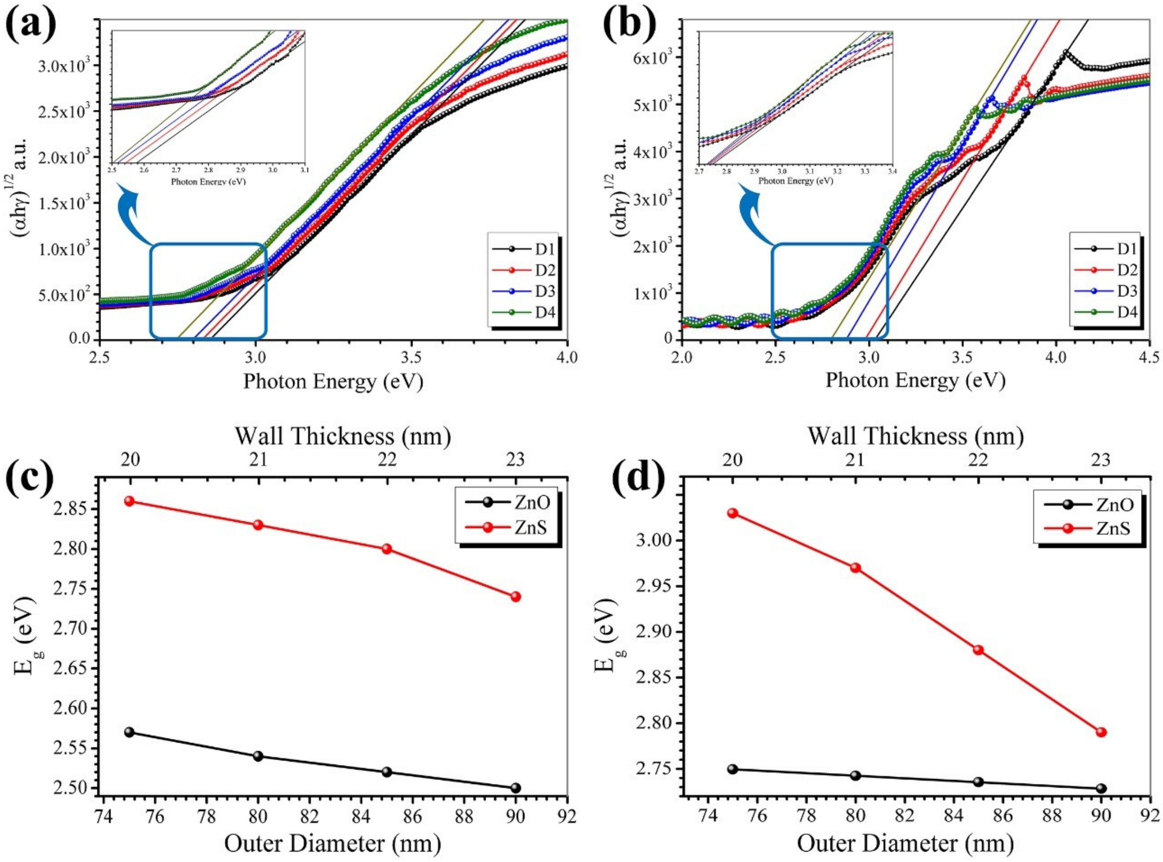

Figure S5. (a, b) Band gap calculations based on indirect band gap transition model for the experimental and simulated absorbance spectra of ZnO/ZnS nanotube arrays, respectively. (c, d) Dependence of the resulting band gap values of ZnO and ZnS (from experimental and simulated spectra, respectively) on geometric parameters of the composite nanostructure arrays.

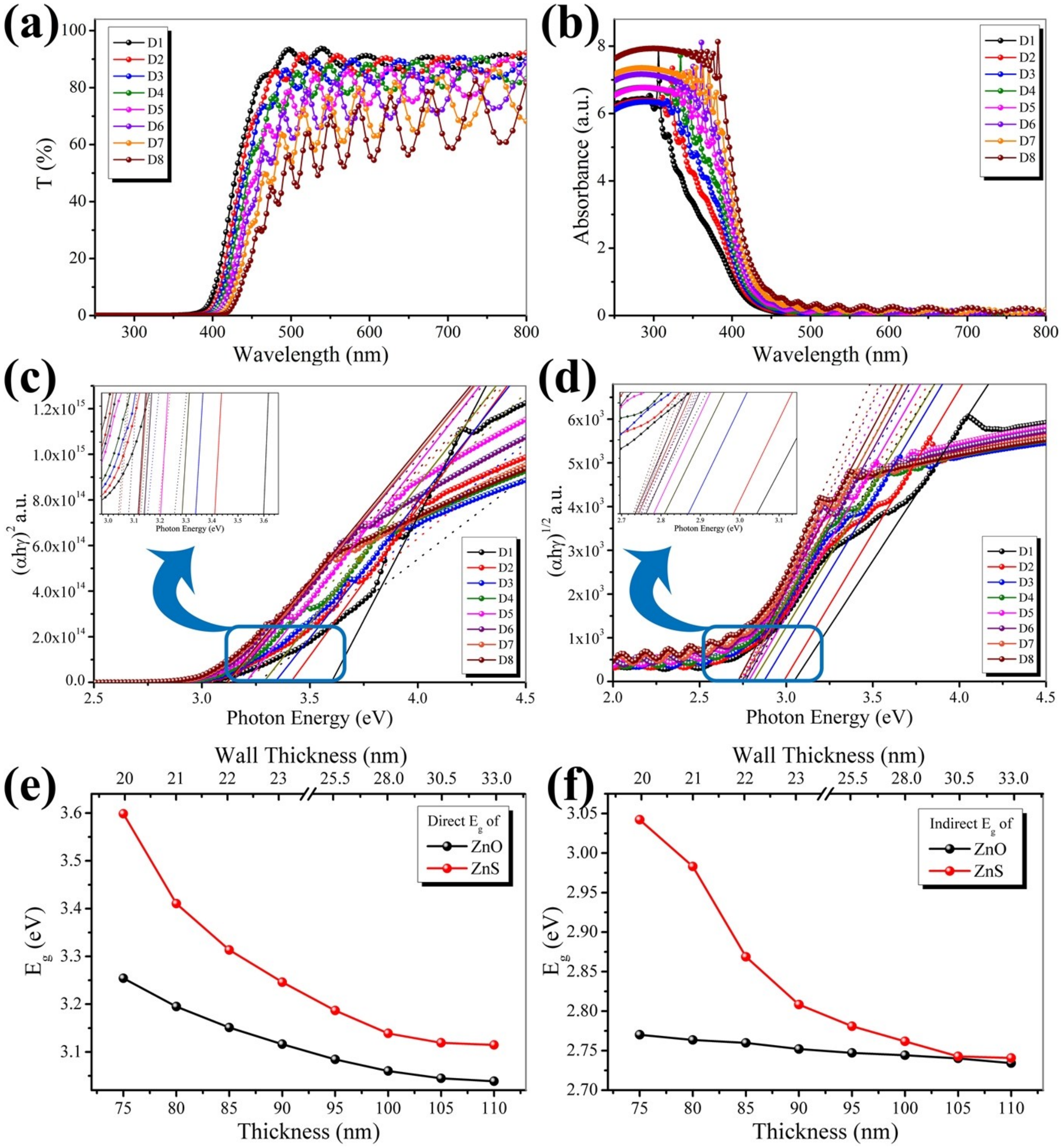

Figure S6. (a, b) FDTD simulated transmittance and absorbance spectra of ZnO/ZnS nanotube arrays with the increase of the diameter and tube thickness until the gaps of between the tubes are filled. (c, d) Direct and indirect band gap calculations for the two materials. (e, f) Dependence of the calculated direct and indirect band gaps on the geometrical features of the composite nanotube arrays.

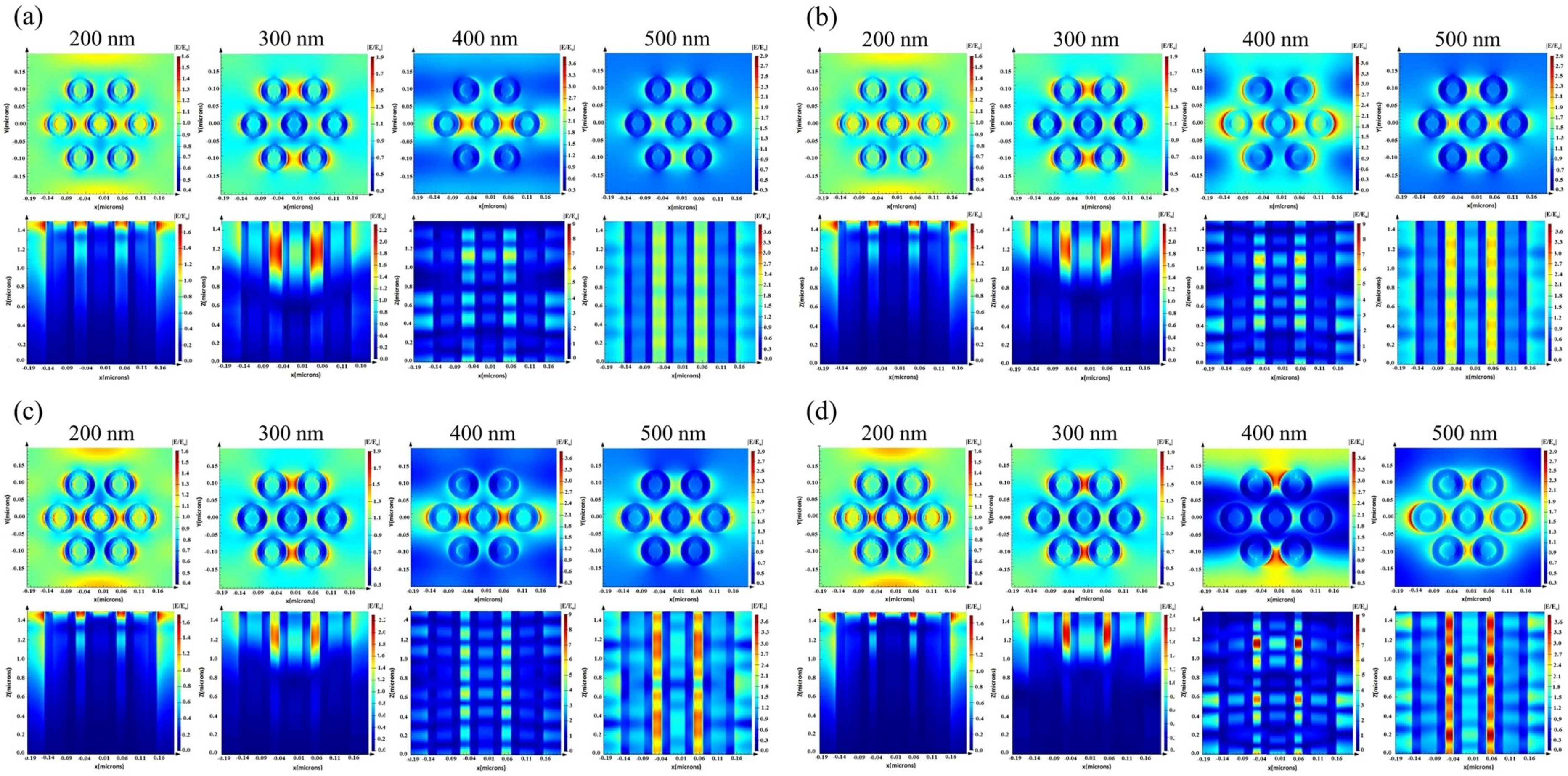

Figure S7. FDTD simulations of E-field amplitude distributions under illuminations of the wavelength at 200 nm, 300 nm, 400 and 500 nm, respectively.(a) D1, (b) D2, (c) D3, (d) D4.