

Files included in dataset “Singlet Oxygen Generation by Laser Irradiation of Gold Nanoparticles”

NP characterisation.opj

Origin file with UVvis spectra and DCS size distributions for nanoparticles used in this study

DPBF 532.xls

Excel file with UVvis spectra of 1,3-Diphenylisobenzofuran (DPBF) samples (all freshly prepared, some after bubbling with nitrogen) during irradiation with cw laser light at 532 nm at different powers, taken at intervals of 10 minutes up to a maximum irradiation time of 60 minutes. All experiments from 14 April 2015 were undertaken with beam diameter 8mm, all before 14 April 2015 with beam diameter 1.85mm.

DPBF 532 0.03W old vs new.xls

Excel file with UVvis spectra of DPBF samples (one prepared several days before the experiment, one freshly prepared) during irradiation with cw laser light at 532 nm, 0.03 W, taken at intervals of 10 minutes up to a maximum irradiation time of 60 minutes.

15nm NPs 532.xls

Excel file with UVvis spectra of DPBF+ 15nm citrate-NP samples (some after bubbling with nitrogen) during irradiation with cw laser light at 532 nm, 1 W (+ one set at 0.1W), taken at intervals of 10 minutes up to a maximum irradiation time of 60 minutes.

15nm PEG-NPs 532.xls

Excel file with UVvis spectra of DPBF+ 15nm PEG-NP samples during irradiation with cw laser light at 532 nm, 1 W, taken at intervals of 10 minutes up to a maximum irradiation time of 60 minutes.

15nm PEG-NPs 532 80%EtOH.xls

Excel file with UVvis spectra of DPBF-only and DPBF+ 15nm PEG-NP samples in 80/20 EtOH/H₂O (all other irradiation experiments in this data collection were taken in 50/50 EtOH/H₂O) during irradiation with cw laser light at 532 nm, 1 W, taken at intervals of 10 minutes up to a maximum irradiation time of 60 minutes.

46nm NPs 532.xls

Excel file with UVvis spectra of DPBF+ 46nm citrate-NP samples during irradiation with cw laser light at 532 nm, 0.5 or 1 W, taken at intervals of 10 minutes up to a maximum irradiation time of 60 minutes.

NRs 532.xls

Excel file with UVvis spectra of DPBF+PEG-Nanorod samples during irradiation with cw laser light at 532 nm, 1 W, taken at intervals of 10 minutes up to a maximum irradiation time of 60 minutes.

NRs 800.xls

Excel file with UVvis spectra of DPBF-only and DPBF+PEG-Nanorod samples during irradiation with cw laser light at 800 nm, 1 W, taken at intervals of 10 minutes up to a maximum irradiation time of 60 minutes.

Pulsed Laser.xls

Excel file with UVvis spectra of DPBF-only and DPBF+15nm NP samples during irradiation with 5 ns laser pulses at 532 nm, 0.15 W, 10 Hz repetition rate, taken at intervals of 5 minutes up to a maximum irradiation time of 30 minutes, or at intervals of 10 minutes up to a maximum irradiation time of 60 minutes.

two-T-simulations.OPJ

Origin file showing Time-dependent temperatures of the conduction band electrons, T_{el} , lattice, T_{ph} , and first solvent layer, T_s , calculated for 15 nm spherical NPs in 50/50 EtOH/water, 5 ns laser pulses with 0.15 J cm^{-2} intensity, and for 40 nm spherical NPs in 80/20 EtOH/water, 7 ns laser pulses with 0.03 J cm^{-2} intensity, using the “two-temperature model” for the electron and phonon heat baths, coupled to finite-element heat transfer and diffusion simulations in the surrounding solvent. Also included are simulations for ps-pulses for verification (by direct comparison with experimental data) and tests that sufficiently small time steps were used. Also included are the time-dependent densities (normalized to the number of gold atoms) of the occupied NP electronic states at the energy of the oxygen $^1\Delta$ state, calculated from the time-dependent electron temperatures for the two experimental conditions.