Electronic Supporting Information for

Interactions of iodoperfluorobenzene compounds with gold nanoparticles

Idriss Blakey,*[a] Zul Merican,[a] Llewellyn Rintoul,[c] Ya-Mi Chuang,[a] Kevin S. Jack [b] and Aaron S. Micallef[a]

[a] *The University of Queensland, Australian Institute for Bioengineering and Nanotechnology, Centre for Advanced Imaging,* [b]*Centre for Microscopy and Microanalysis, Brisbane, Queensland 4072, Australia.*

[c]*Queensland University of Technology, Brisbane Australia.*

***Corresponding author i.blakey@uq.edu.au**

Supplementary Results

UV-Vis spectra

The UV-Vis spectra for 1,2-DITFB dispersed in water at concentrations ranging from 0.85-11.1 μM are shown in Fig S1. The UV spectrum of 1,2-DITFB dispersed in water exhibits peaks at 270 nm (4.6 eV), 235 nm (5.28 eV) and 215 nm (5.77 eV).

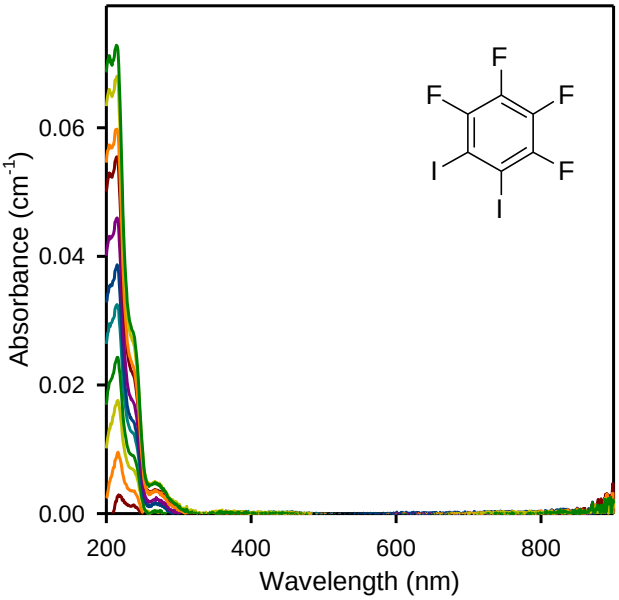

Figure S1 1,2-DITFB dispersed in water, 0.85 – 11.1 μM, for zoomed in view of UV region see Figure S4 left.

The UV-Vis spectra for different amounts of 1,2-DITFB added to a solution of AuNPs is shown in Fig S2. A dampening at the maximum of the SPR and enhancement of the shoulder at about 600 nm can be observed. An isobestic point can

also be observed. To enhance these changes, difference spectra (with respect to the unmodified AuNP SPR) are shown in the main text.

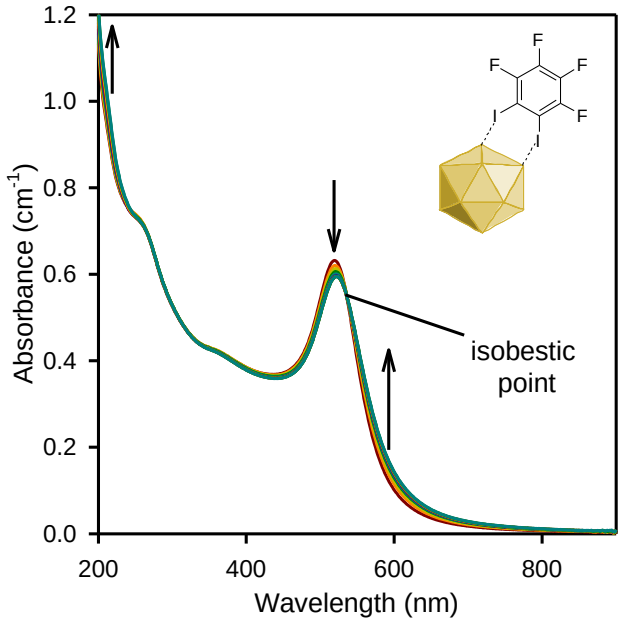

Figure S2 UV-Vis spectra of mixtures of AuNP and 12DIFTB (AuNP concentration: 1.05 nM, 1,2-DITFB concentration: 0 – 11.1 µM)

Fig S3 shows a calculated bathochromic red shift for the SPR of gold nanoparticles (left) and the calculated difference spectra (right). This is the sort of shift that is expected by changing the refractive index of the surrounding medium. No isobestic point is observed for a bathochromic shift.

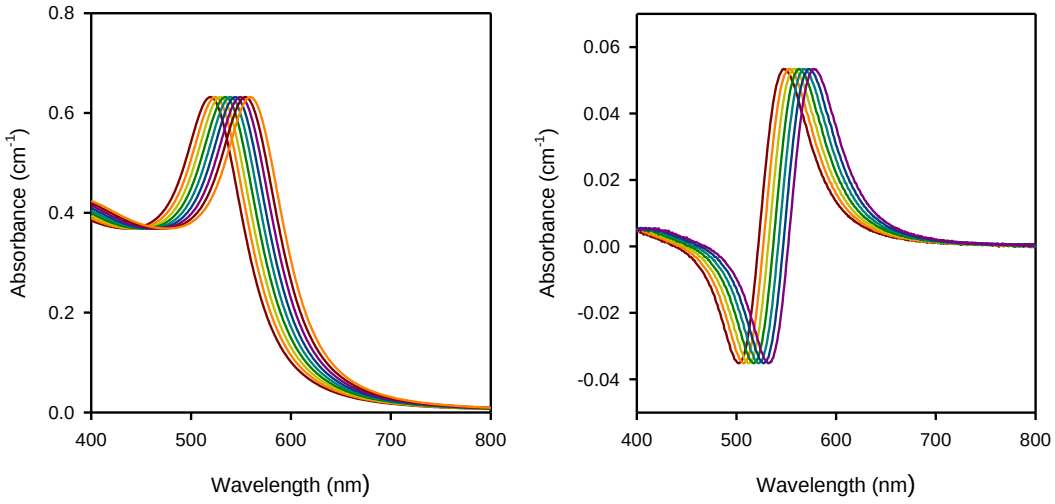

Figure S3 (left) Simulation of a bathochromic shift for the SPR of a solution of the AuNPs (right) and the same calculations plotted as a difference spectra, as described in the text..

Fig S4 shows the zoomed in region of the UV region for 1,2-DITFB dispersed in water (left) and the UV region for different amounts of 1,2-DITFB (0.85 - 11.1

μM). The UV spectra of the 1,2-DITFB when bound to the gold nanoparticles becomes distorted.

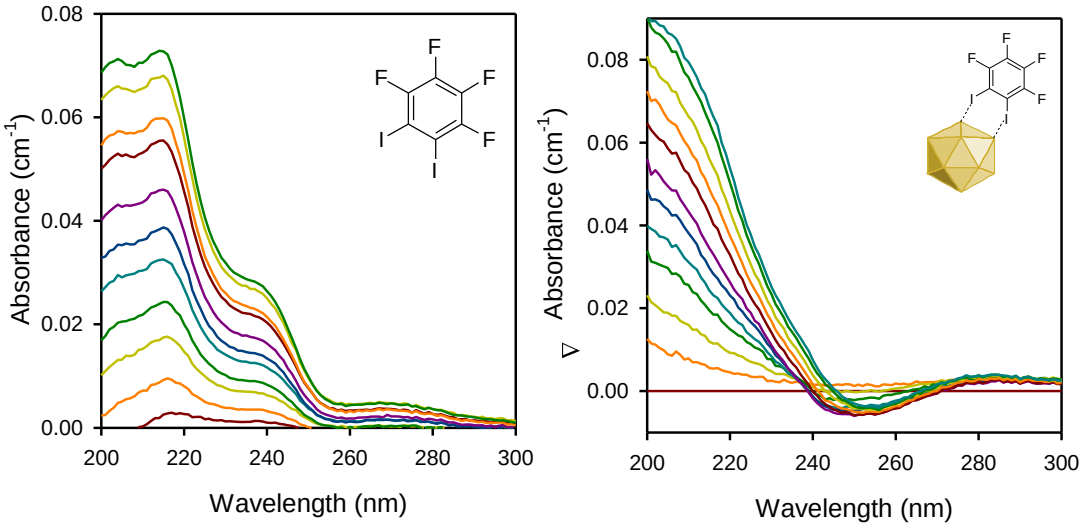

Figure S4 left UV spectrum of 1,2-DIFTB in water 0.85-11.1 μM, right UV difference spectrum of AuNP/1,2-DIFTB mixture

Raman

The normal Raman of 1,2-DITFB is shown in Fig S7. As expected the spectrum is virtually identical to 633 nm excitation (shown in main text). This demonstrates that the differences observed in the SERS spectra are not due to changes in the detector sensitivity for the different excitation wavelengths.

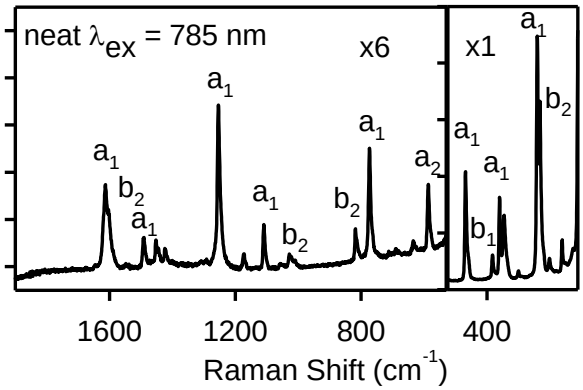

Figure S5 Raman spectrum of neat 1,2-DITFB using a laser excitation wavelength of 785 nm. Major bands are labelled with their symmetry modes.

Synchrotron XPS

AuNPs that were treated with TFB did not exhibit a peak in the F 1s region (Fig S6 (a)), which indicates that binding did not occur. This demonstrates that binding of 1,2-DITFB does not occur through the fluorine atoms. AuNPs treated with 1,2-DIB exhibited peaks in the I 3d region, which are assigned to the I $3d^{5/2}$ and I $3d^{3/2}$ peaks. This shows that 1,2-DIB binds to AuNPs and as described in the text this provides

further evidence of binding through the iodine atoms. The 1,2-DITFB on AuNPs exhibits a smaller shift of the F1s compared to the I 3d peaks when compared to neat 1,2-DITFB on silicon.

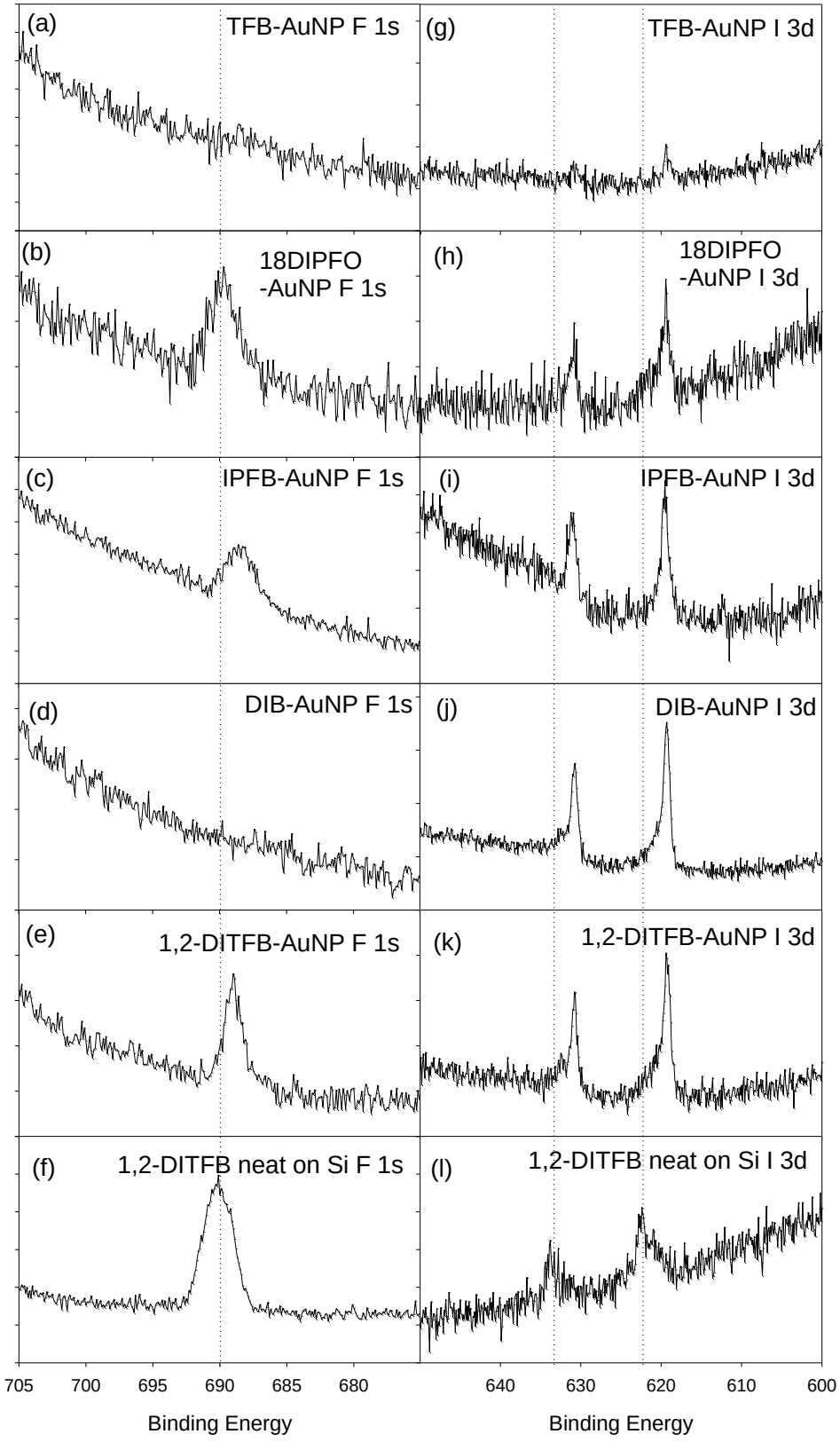

Figure S6 High resolution XPS in the F1s region for dried solutions of AuNPs treated with (a) tetrafluorobenzene (TFB), (b) 1,2-diiodobenzene (c) 1,2-DITFB and washed with water and IPA as well as (d) neat 1,2-DITFB on a silicon wafer. High resolution XPS in the I 3d region for dried solutions of AuNPs treated with (a) tetrafluorobenzene (TFB), (b) 1,2-diiodobenzene (c) 1,2-DITFB and washed with water and IPA as well as (d) neat 1,2-DITFB on a silicon wafer.

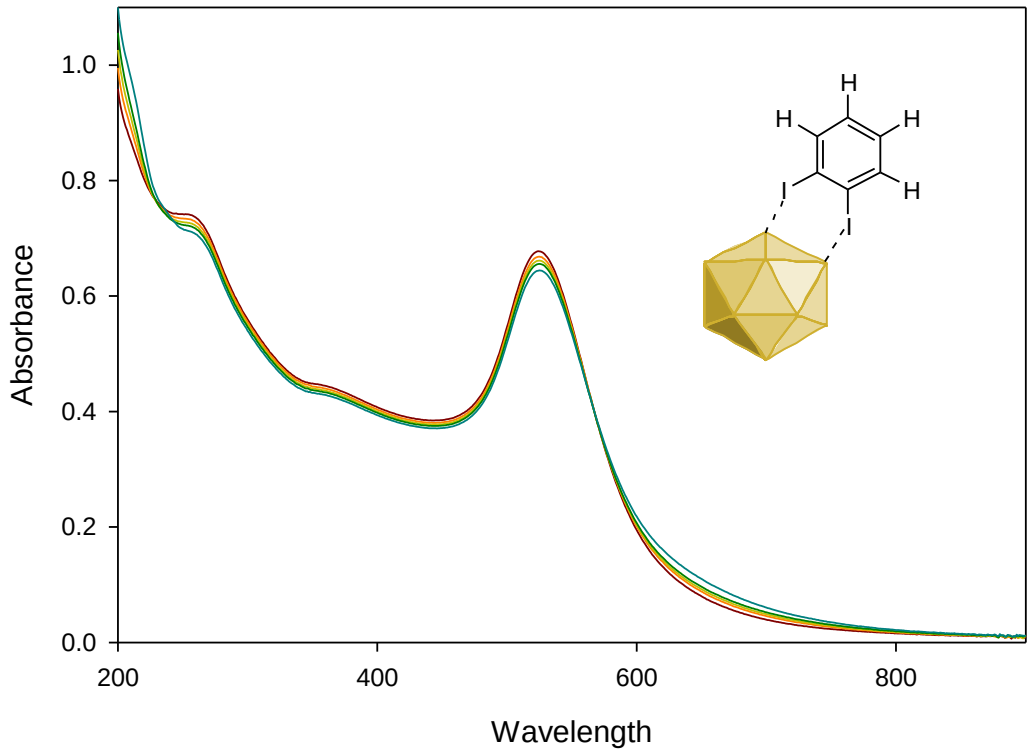

Figure S7 UV-Vis spectra of mixtures of AuNP and 12DIB (AuNP concentration: 1.05 nM, 1,2-DIB concentration: 0, 0.44, 0.89, 1.4 and 3.6 µM)

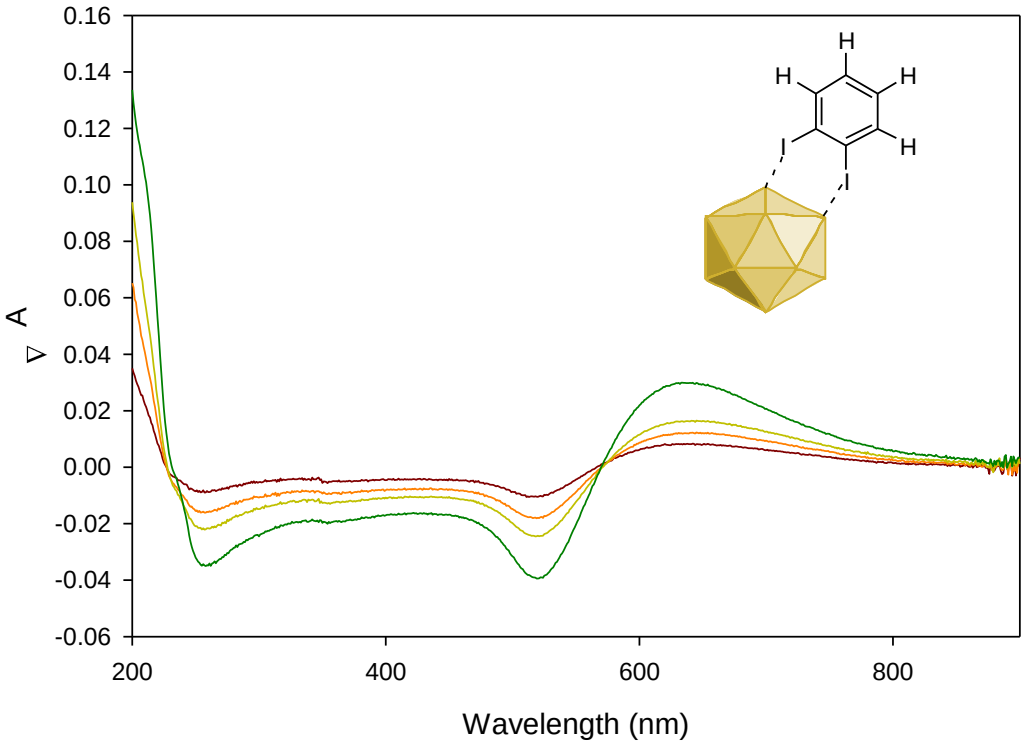

Figure S8 UV-Vis difference spectra of mixtures of AuNP (1.05 nM) and 1,2-DIB (1,2-DIB concentrations: 0.44, 0.89, 1.4 and 3.6 µM.