

Electronic and surface properties of PbS nanoparticles exhibiting efficient multiple exciton generation

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Supplementary Material

1. The Effect Stirring Rates on Absorption Transients

Figure 1 compares a typical pump-induced transmittance transient observed when the sample was unstirred with ones obtained when the sample was stirred at 500 rpm and 1000 rpm. The ratio of the initial amplitude of the unstirred transient (at $t=0$ ps) to its amplitude at 600 ps is considerably greater than the corresponding ratio for either of the stirred transients, indicating that significant photocharging occurs if the sample is not stirred. In contrast, this ratio is approximately constant for stirring at 500 rpm or 1000 rpm. If significant photocharging were still occurring for samples stirred at 500 rpm then a further reduction of the ratio would be expected on increasing the stirring rate to 1000 rpm. The absence of such a reduction indicates that stirring at 500 rpm is sufficient to suppress the effects of photocharging on our data.

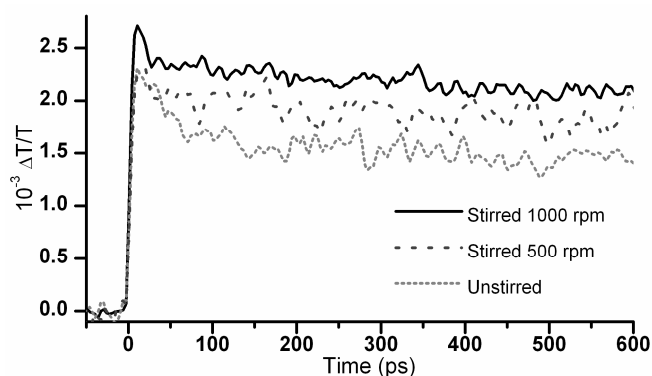


FIG. 1. Pump-induced transmittance transients for the nanoparticle sample with a band gap of 1.1 eV, excited with a pump energy 3.6 times E_g , stirred at 0, 500 and 1000 rpm.

2. Valence Band Spectra of PbS Nanoparticles

Figure 2 shows valence band spectra of PbS nanoparticles deposited on a gold substrate. The VBM was found to be 0.75 ± 0.1 eV, indistinguishable from the VBM position of the 4.6 nm diameter nanoparticles deposited on ITO-coated glass (0.75 ± 0.1 eV, Figure 4, main text).

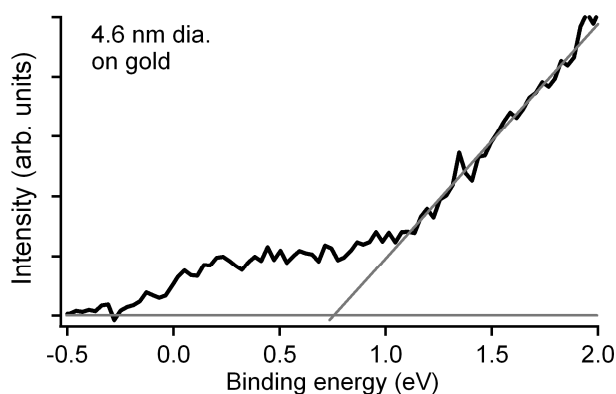


FIG. 2. Photoemission spectra of the valence band edge region of butylamine-capped PbS nanoparticles deposited on gold. A linear fit to the valence band edge is shown as a grey line.

3. Valence Band Spectra of 'Aged' and 'Fresh' PbS Nanoparticles

Figure 3 shows valence band spectra of 'fresh' and 'aged' samples of 2.7 nm diameter PbS nanoparticles deposited on an ITO-coated glass substrate. The VBM was found to be shifted from 0.75 ± 0.1 eV to a higher binding energy (0.89 ± 0.1 eV) in the 'aged' sample. The samples shown here gave the XPS spectra shown in figures 5 (g) & (h) ('fresh') and 5 (i) & (j) ('aged') of the main text.

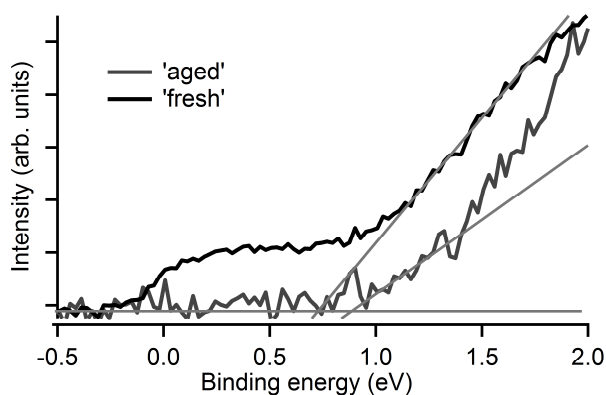


FIG. 3. Photoemission spectra of the valence band edge region of 'aged' (dark grey line) and 'fresh' (black line) butylamine-capped 2.7 nm diameter PbS nanoparticles deposited on ITO-coated glass. Linear fits to the valence band edges are shown as grey lines.

4. Absorption Spectra of Olive-Oil-Capped PbS Nanoparticles

Figure 4 shows absorption spectra of olive-oil-capped PbS nanoparticles (of approximately 3.6 nm diameter) in hexane. Shortly after synthesis the 1S absorption peak position was 1.29 eV. After 18 months of storage in the dark at $\sim 4^{\circ}\text{C}$ the peak was found to be shifted to 1.31 eV.

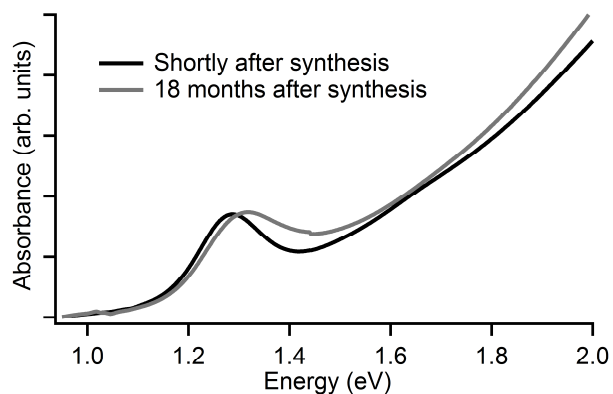


FIG. 4. Absorption spectra of olive-oil-capped PbS nanoparticles shortly after synthesis (black line), and after 18 months (grey line).