

## **Supporting Information**

### **Heterobinuclear Light Absorber Coupled to Molecular Wire for Charge Transport across Ultrathin Silica Membrane for Artificial Photosynthesis**

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### Calculation of Surface Coverage of TMSA Anchor Molecules

The estimated surface area for 1.0 g SiO<sub>2</sub> nanoparticles is 200 m<sup>2</sup> g<sup>-1</sup>, which corresponds to 1.56 • 10<sup>21</sup> Si surface atoms, assuming a surface Si density of 7.8 nm<sup>-2</sup>.<sup>1</sup> TMSA occupies 3 surface Si atoms, which yields a maximum monolayer density of 2.6 TMSA nm<sup>-2</sup>. The amount of TMSA anchored onto 1.0 g SiO<sub>2</sub> nanoparticles was obtained from UV-vis measurements and is 0.105 mmol (24 % of the initial amount). 0.105 mmol are 6.33 • 10<sup>19</sup> molecules, which corresponds to 0.3 TMSA nm<sup>-2</sup>. This corresponds to 12 % surface coverage (0.3 / 2.6).

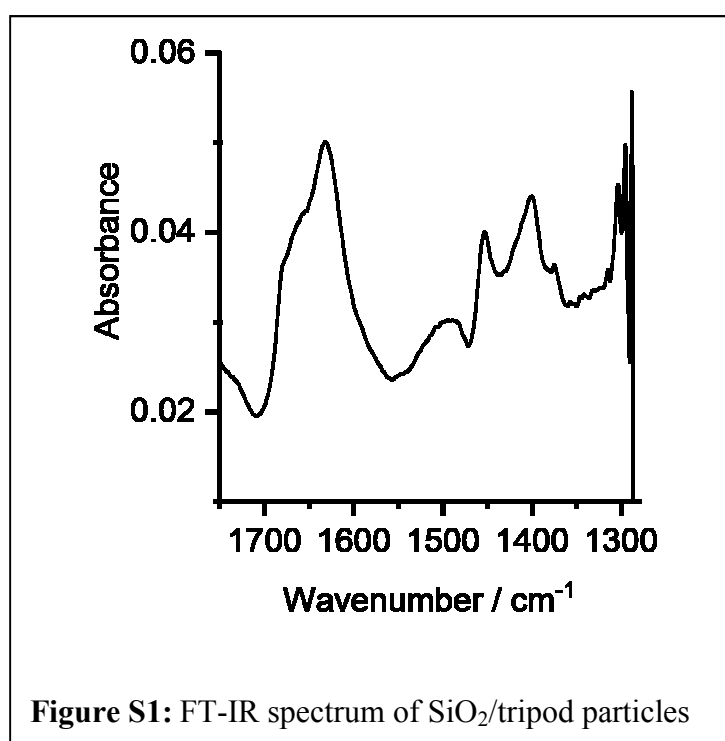
### Calculation of Surface Coverage of PV3 Molecules

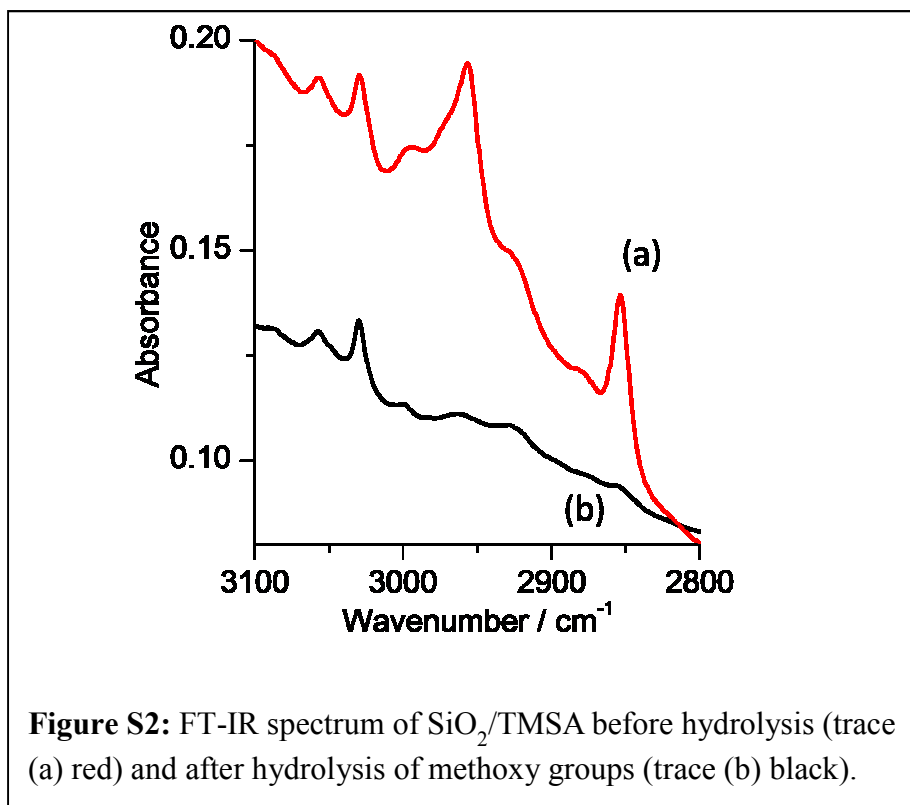
The estimated surface area for 0.1 g SiO<sub>2</sub> nanoparticles used is 20 m<sup>2</sup>/g, which corresponds to 1.56 • 10<sup>20</sup> Si surface atoms, assuming a surface Si density of 7.8 nm<sup>-2</sup>.<sup>1</sup> The SiO<sub>2</sub>/TMSA reactant has a TMSA density of 0.3 nm<sup>-2</sup> (see above). The amount of PV3 grafted onto 0.1 g SiO<sub>2</sub>/TMSA nanoparticles was obtained from UV-vis measurements and is 0.6 μmol, or 3.61 • 10<sup>17</sup> molecules, which corresponds to 0.02 PV3 nm<sup>-2</sup>. This corresponds to 0.8 % surface coverage (0.02 / 2.6).

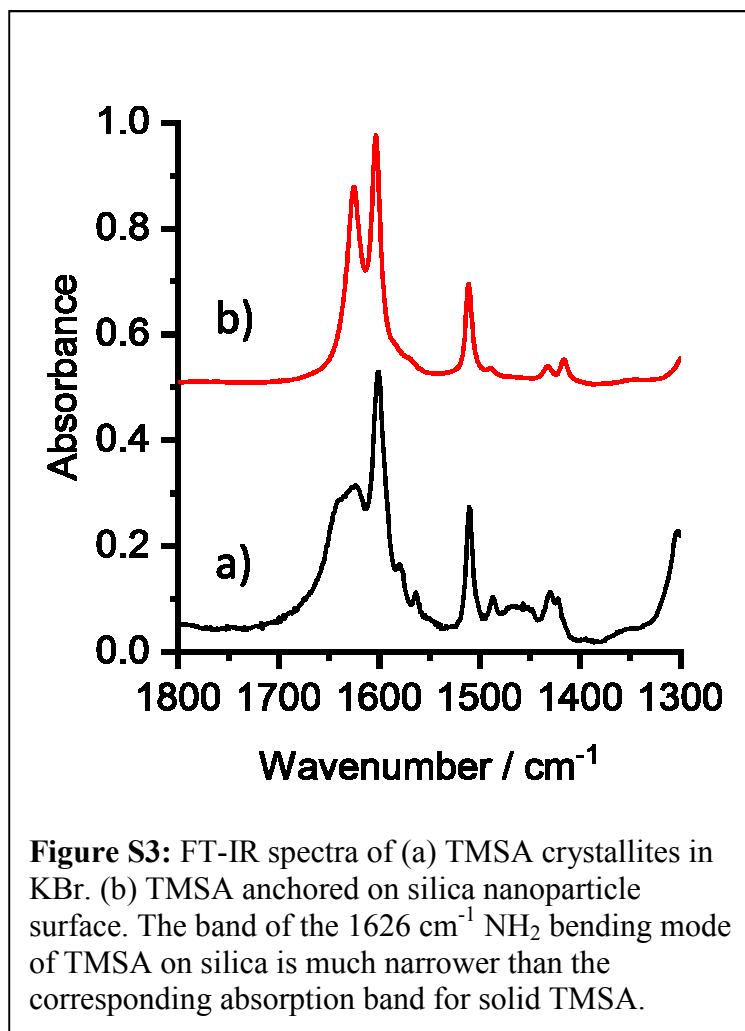
### Calculation of Surface Coverage of tripod anchor molecules

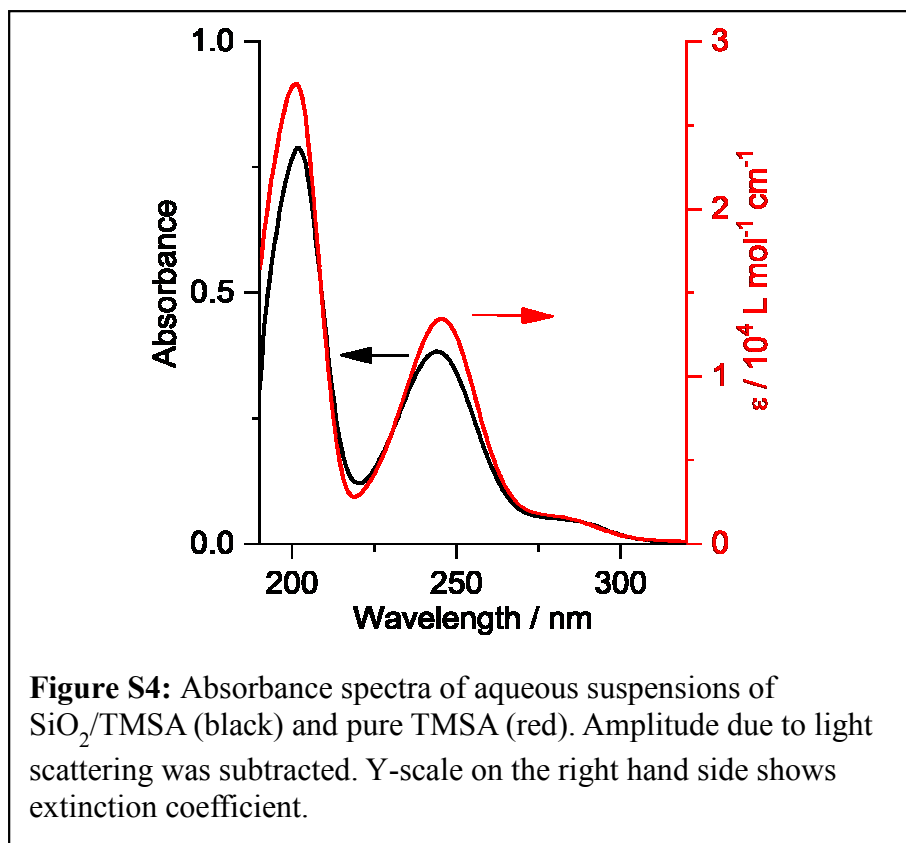
To roughly estimate the surface coverage of tripod molecules the NH<sub>2</sub> scissor deformation mode intensity at 1630 cm<sup>-1</sup> of an 18 mg pellet of SiO<sub>2</sub>/tripod in Figure S1 (absorbance 0.03) was compared to the NH<sub>2</sub> scissor deformation mode intensity at 1623 cm<sup>-1</sup> of a same-sized SiO<sub>2</sub>/TMSA (Figure 1Aa) (absorbance 0.36). From this comparison, the relative intensity of SiO<sub>2</sub>/tripod is 8%, which results in a surface coverage of 0.08 • 0.3 nm<sup>-2</sup> = 0.02 nm<sup>-2</sup> (assuming

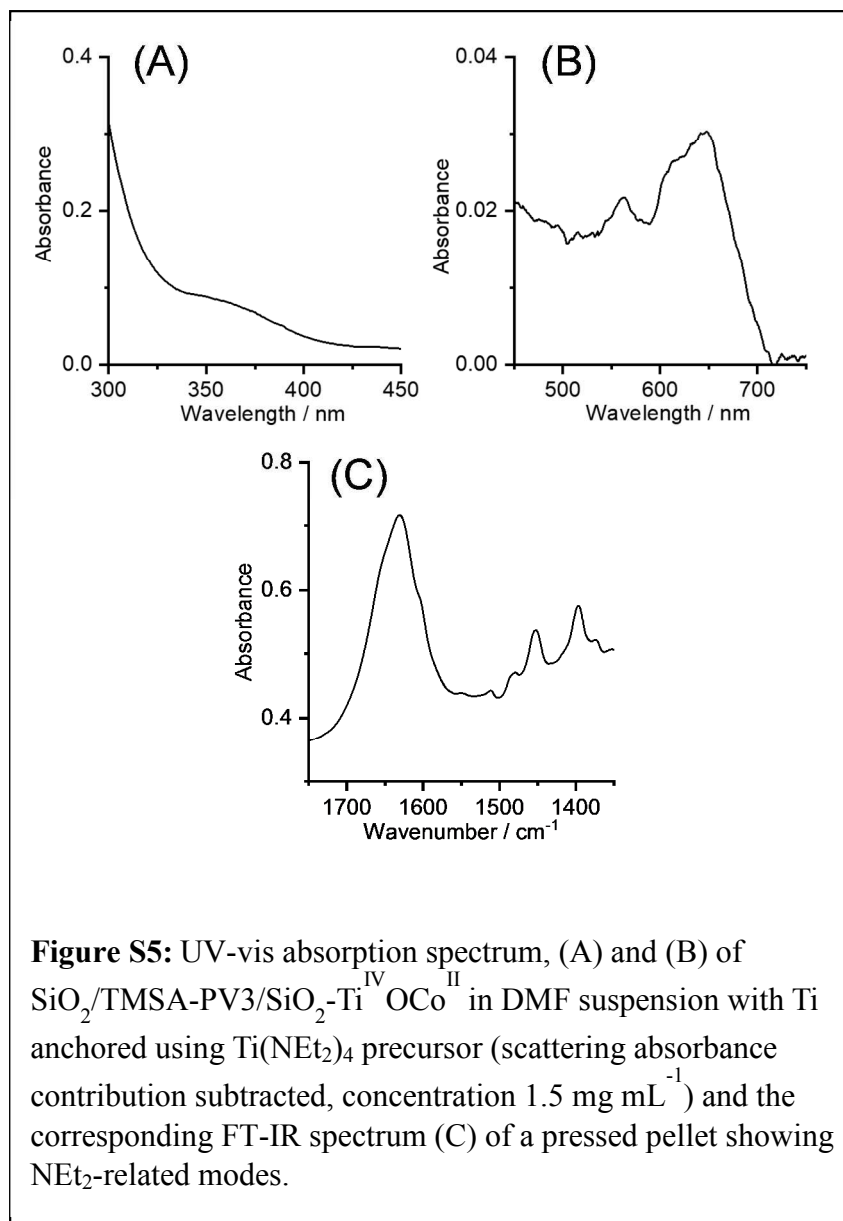
that the  $\text{NH}_2$  extinction coefficient of the two amines is the same). This corresponds to 0.8 % surface coverage.

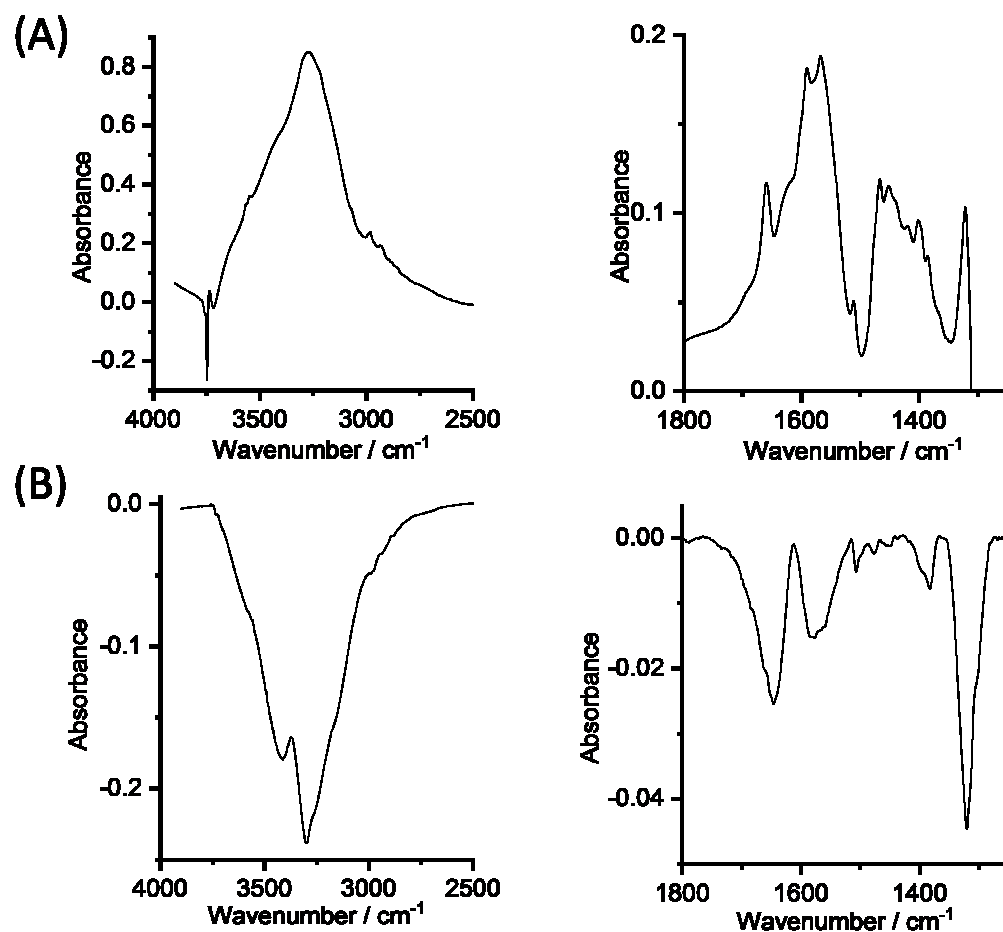












**Figure S6:** (A) FT-IR spectrum of SiO<sub>2</sub>-TiOCo particles with physisorbed PV3 (0.1 nm<sup>-2</sup>) and [Co(NH<sub>3</sub>)<sub>5</sub>Cl]Cl<sub>2</sub> (0.1 nm<sup>-2</sup>) acceptor. SiO<sub>2</sub> background subtracted. (B) FT-IR difference spectrum after 15 min irradiation with 476 nm continuous laser emission showing depletion of [Co(NH<sub>3</sub>)<sub>5</sub>Cl]<sup>2+</sup> under growth of adsorbed ammonia.

## References

- [1] Zhuravlev, L. T. The Surface Chemistry of Amorphous Silica. Zhuravlev model. *Colloids Surf. A: Physicochem. Eng. Aspects* **2000**, 173, 1-38.