Synthesis of hydrated KTaWO₆ nanoparticles and Sn(II) incorporation for visible light absorption

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Results and Discussion



Fig. S1: TEM image with indexed lattice planes of $KTaWO_6$ nanoparticle, prepared at 20 °C for 12h in 25% ammonia solution.



Fig. S2: XRD patterns of KTaWO₆ samples (left) and crystallite sizes and BET surface areas (right) prepared at 150 °C for 12 h in different concentrated ammonia solutions.







Fig. S4: Raman spectra of $KTaWO_6$ samples prepared for different times at 120 °C in 25% ammonia solution (left) and of samples prepared at for 12 h 150 °C with different ammonia concentrations. Bands marked with an asterisk can be attributed to the glass plate supporting the sample.



Fig. S5: UVVIS spectra and bandgaps of $KTaWO_6$ samples prepared for different times at 120 °C in 25% ammonia solution (left) and of samples prepared at for 12 h 150 °C with different ammonia concentrations.



Fig. S6: Particle size distributions according to DLS of $KTaWO_6$ samples prepared for different times at 120 °C in 25% ammonia solution (left) and of samples prepared at for 12 h 150 °C with different ammonia concentrations.



Fig. S7: Zeta-potential for all samples.



Fig. S8: In situ XRD patterns of KTaWO₆ measured at different temperatures.



Fig. S9: Calculated relative XRD intensities for anhydrous $KTaWO_6$ for three different Wyckoff positions of the potassium ion, assuming a lattice constant of 10,424 Å.



Fig. S10: Crystal structures of anhydrous $KTaWO_6$ for 8b (left), 16d (middle) and 32e (right) positions of the potassium ions, based on the data published by Kuznetsova et al.^[1]



Fig. S11: Raman spectra of dry and hydrated KTaWO₆. Bands marked with an asterisk can be attributed to the glass plates supporting and covering the sample.



Fig. S12: Water physisorption isotherms of KTaWO₆.



Fig. S13: TGA-MS (right) data of KTaWO₆. It should be noted, that these temperatures cannot be compared directly with those from *in situ* XRD, due to the long equilibration and measuring times of the XRD.



Fig. S14: DRIFT spectra of dried $KTaWO_6$. The time denotes the time the sample spent in ambient air before starting the measurement.



Fig. S15: Tauc-plots and bandgaps of $Sn_xK_{1-2x}TaWO_6$, in which the base material has been prepared at different temperatures.



Fig. S16: Tauc-plots and band gaps of $Sn_xK_{1-2x}TaWO_6$, in which the base material has been prepared for different times.



Fig. S17: Tauc-plots and band gaps of $Sn_xK_{1-2x}TaWO_6$, in which the base material has been prepared with different 25 % ammonia amounts.



Fig. S18: Elemental composition of all samples as determined by EDX (circles) and by titrating the not exchanged tin in solution (crosses).



Fig. S19: Calculated relative XRD intensities for anhydrous $KTaWO_6$ and $Sn_xK_{1-2x}TaWO_6$, under the assumption that K and Sn both occupy 32e sites and a lattice constant of 10.424 Å.



Fig. S20: XRD patterns (left) and Raman spectra (right) of $Sn_xK_{1-2x}TaWO_6$, in which the base material has been prepared at different temperatures.



Fig. S21: XRD patterns (left) and Raman spectra (right) of $Sn_xK_{1-2x}TaWO_6$, in which the base material has been prepared for different times. Raman bands marked with an asterisk belong to the glass plate supporting the sample.



Fig. S22: XRD patterns (left) and Raman spectra (right) of $Sn_xK_{1-2x}TaWO_6$, in which the base material has been with different ammonia amounts. Raman bands marked with an asterisk belong to the glass plate supporting the sample.

[1] A. V. Knyazev, M. Maczka, N. Y. Kuznetsova, *Thermochim. Acta* **2010**, *506*, 20–27.