

## Synthesis and Photocatalytic Activity of the Oxysulfide Perovskite $\text{KTaO}_{3-x}\text{S}_x$

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### INTRODUCTION & AIM

Oxide perovskite  $\text{KTaO}_3$  is a promising photocatalytic material due to its high chemical and structural stability, however, its use in the visible range is limited by a wide band gap ( $E_g \approx 3.6$  eV) due to the formation of a valence band by O 2p-states and a conduction band by d states of  $\text{Ta}^{5+}$ .

One of the ways to modify the structure is the partial anionic substitution of oxygen with sulfur to form oxysulfide phases  $\text{KTaO}_{3-x}\text{S}_x$ , which leads to an increase in the valence band due to S 3p-states and contributes to a narrowing of the band gap and an expansion of absorption into the visible region of the spectrum.

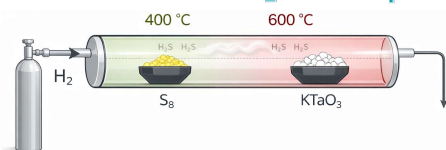


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### METHOD

#### PREPARATION OF $\text{KTaO}_{3-x}\text{S}_x$

$\text{KTaO}_{3-x}\text{S}_x$  powders were obtained in two steps:  $\text{KTaO}_3$  was first synthesised by a solid-state reaction between  $\text{K}_2\text{CO}_3$  and  $\text{Ta}_2\text{O}_5$  at 800 °C for 8 h, and then  $\text{KTaO}_3$  was treated at 600 °C in an  $\text{H}_2\text{S}$  atmosphere.



#### CHARACTERIZATION OF $\text{KTaO}_{3-x}\text{S}_x$

**Composition** were studied using scanning electron microscopy (SEM) on a JSM-7600F (JEOL, Japan) equipped with an EDS detector (Oxford Instruments, UK).

**Crystal structure changes** were monitored using XRD on a DRON-3 X-ray diffractometer (NPO Burevestnik, Russia) using  $\text{CoK}\alpha$  radiation at 40 kV.

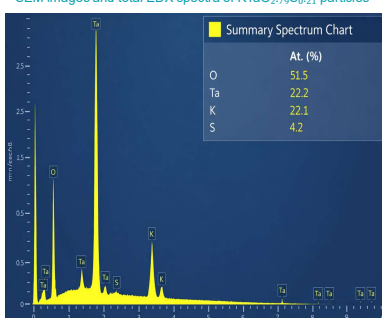
#### PHOTOCATALYTIC TESTS OF $\text{KTaO}_{3-x}\text{S}_x$

The **photocatalytic activity** of  $\text{KTaO}_{3-x}\text{S}_x$  particles was assessed by the degree of RhB decomposition under sunlight exposure, and the **contribution of various catalytically active particles** to the process was assessed using scavenger experiments (IPA, BQ, DMSO, EDTA).

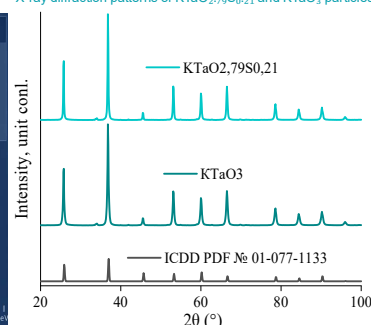
### RESULTS & DISCUSSION

✓ Oxysulfide perovskites  $\text{KTaO}_{3-x}\text{S}_x$  with sulfur contents of 1.8, 4.2 and 7.4 at.% were obtained.

SEM images and total EDX spectra of  $\text{KTaO}_{2.79}\text{S}_{0.21}$  particles

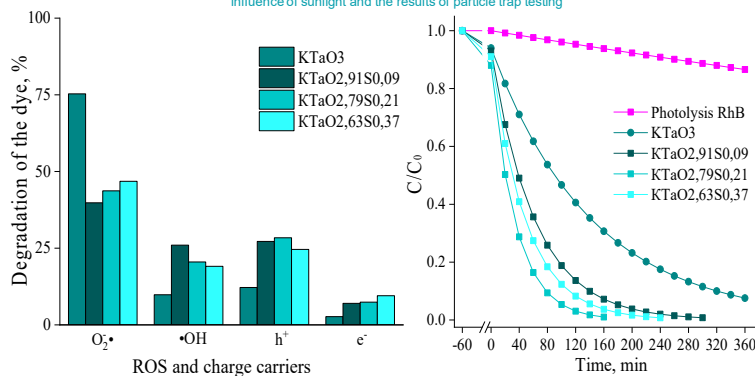


X-ray diffraction patterns of  $\text{KTaO}_{2.79}\text{S}_{0.21}$  and  $\text{KTaO}_3$  particles



The samples are single-phase, and the  $\text{KTaO}_3$  structure is preserved over the entire sulfur-doping range studied.

Photodegradation of 50 mL of RhB solutions (10 mg/L) containing 40 mg of  $\text{KTaO}_{3-x}\text{S}_x$  particles under the influence of sunlight and the results of particle trap testing



The  $\text{KTaO}_{2.79}\text{S}_{0.21}$  sample (4.2 at.% S) exhibits the highest photocatalytic activity under solar-light irradiation: in RhB degradation its activity is **2.25** times higher than that of pristine  $\text{KTaO}_3$ , with superoxide anion  $\text{O}_2^{\bullet-}$  being the main active species.

### CONCLUSION

It is shown that sulfurization of  $\text{KTaO}_3$  in  $\text{H}_2\text{S}$  vapour enables controlled formation of the oxysulfide perovskite  $\text{KTaO}_{3-x}\text{S}_x$ . Sulfur doping increases the photocatalytic activity by more than a factor of two: the composition containing 4.2 at.% S exhibits an **activity of  $12.5 \text{ mg}\cdot\text{g}^{-1}\cdot\text{h}^{-1}$**  in RhB degradation under solar-light irradiation.

### ACKNOWLEDGEMENTS

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