

Supplementary Data:

Preparation of new sulfur-doped and sulfur/nitrogen co-doped CsTaWO₆ photocatalysts for hydrogen production from water under visible light

Roland Marschall^a, Aniruddh Mukherji^a, Akshat Tanksale^a, Chenghua Sun^b, Sean C. Smith^b, Gao Qing (Max) Lu^{a,*} and Lianzhou Wang^{a,*},

^a ARC Centre of Excellence for Functional Nanomaterials, School of Chemical Engineering and Australian Institute for Bioengineering and Nanotechnology, The University of Queensland, St Lucia, Brisbane, QLD 4072 Australia

^b Centre for Computational Molecular Science, Australian Institute for Bioengineering and Nanotechnology, The University of Queensland, St Lucia, Brisbane, QLD 4072 Australia

Experimental Details:

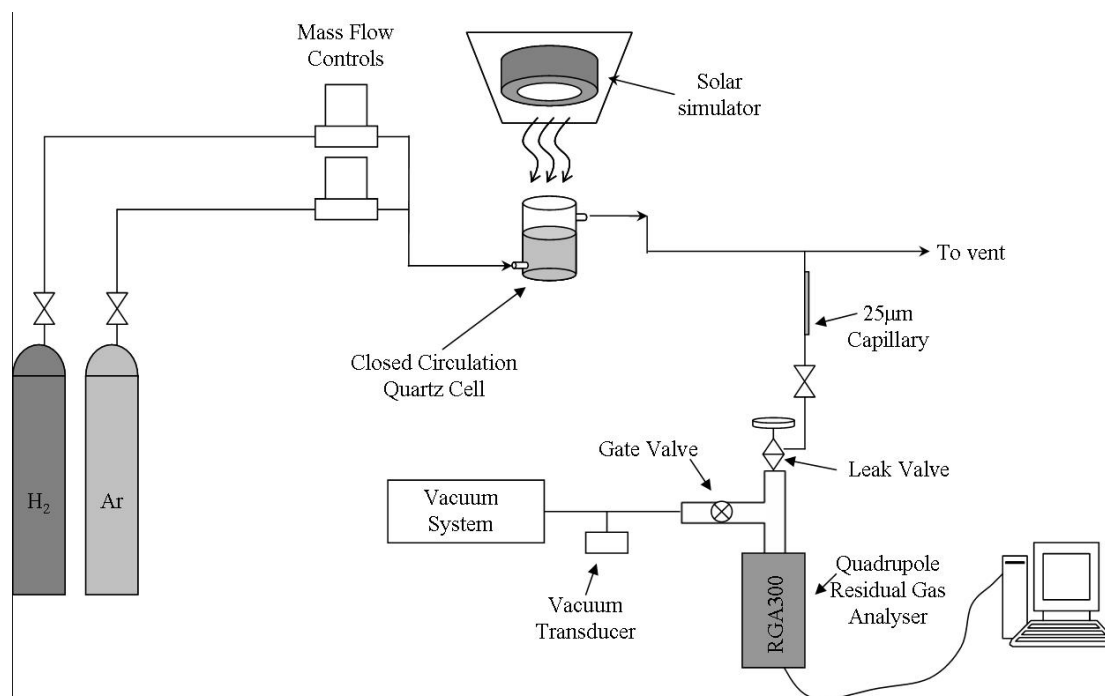
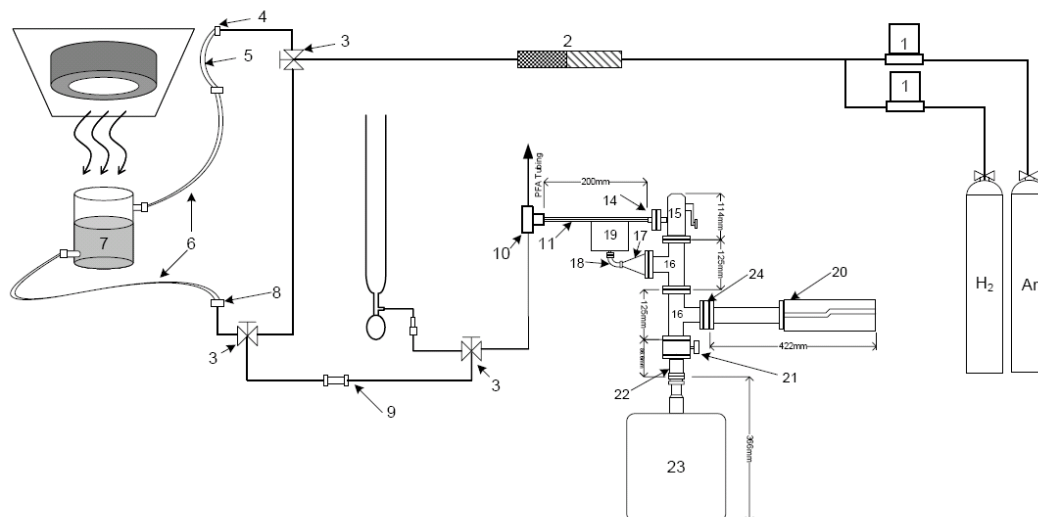


Figure SD01. Scheme of the water splitting reaction setup, including the gas detection system via mass spectrometer.



- | | | |
|-----------------------------------|--|----------------------------------|
| 1. Brooks MFC | 11. SGE 25 μ m Capillary | 23. MiniTASK KF40 Pumping System |
| 2. Molecular Sieve Moisture Trap | 14. Flange CF 1-1/3" to 1/4" Swagelok | 24. Double Sided CF275 Flange |
| 3. 3-Way Valve | 15. Variable Leak Valve | |
| 4. 1/8" to 1/4" Tube Fitting | 16. CF275 Tee Fitting | |
| 5. Metal Flexible Hose Assembly | 17. Conical Adapter Nipple NW-16-CF275 | |
| 6. 1/4" PTFE Hoses + Fittings | 18. Elbow, Radius NW 90 Degree | |
| 7. Closed circulation Quartz Cell | 19. EyeSys Mini-BA Vacuum Transducer | |
| 8. 1/4" to 1/8" Tube Fitting | 20. SRS Residual Gas Analyser 300AMU | |
| 9. 2 Micron Particulate Filter | 21. Butterfly Gate Valve | |
| 10. PFA Tube Fitting Union Tee | 22. Adapter CF275 to NW40, 2.0" Long | |

Figure SD02. Detailed diagram of the water splitting reaction setup, including the gas detection system and part/connector details.

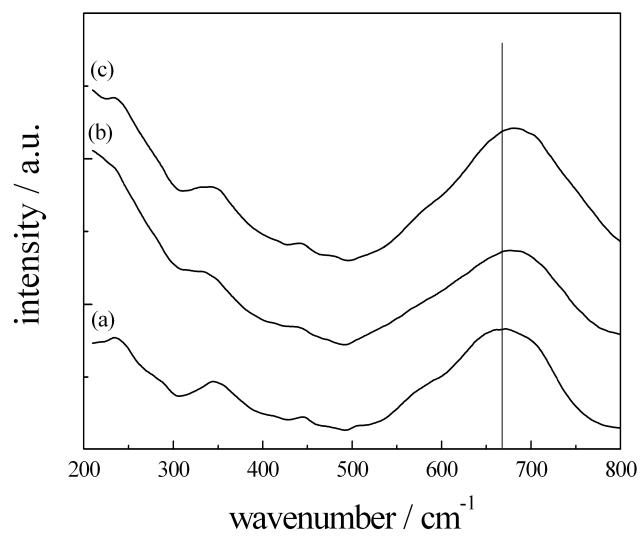


Figure SD03. Raman spectra of $\text{CsTaWO}_{6-x-y}\text{S}_x\text{N}_y$ (c) and $\text{CsTaWO}_{6-x}\text{S}_x$ (b), compared to CsTaWO_6 (a).