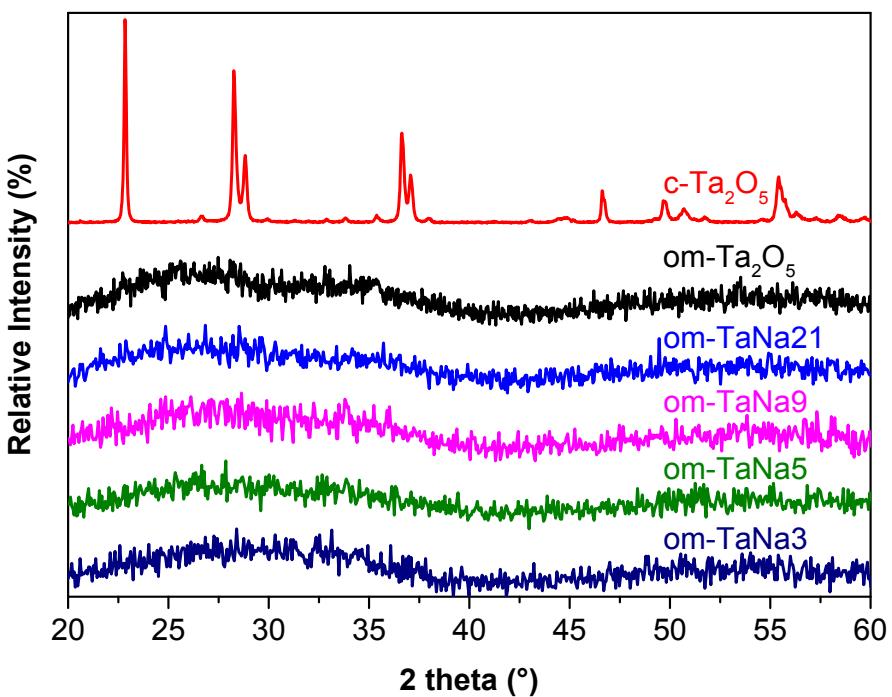


Supporting Information

Alkali metals incorporated ordered mesoporous tantalum oxide with enhanced photocatalytic activity for water splitting

Tobias Grawe, and Harun Tüysüz*

Max-Planck-Institut für Kohlenforschung, Kaiser-Wilhelm-Platz 1, 45470 Mülheim an der Ruhr, Germany

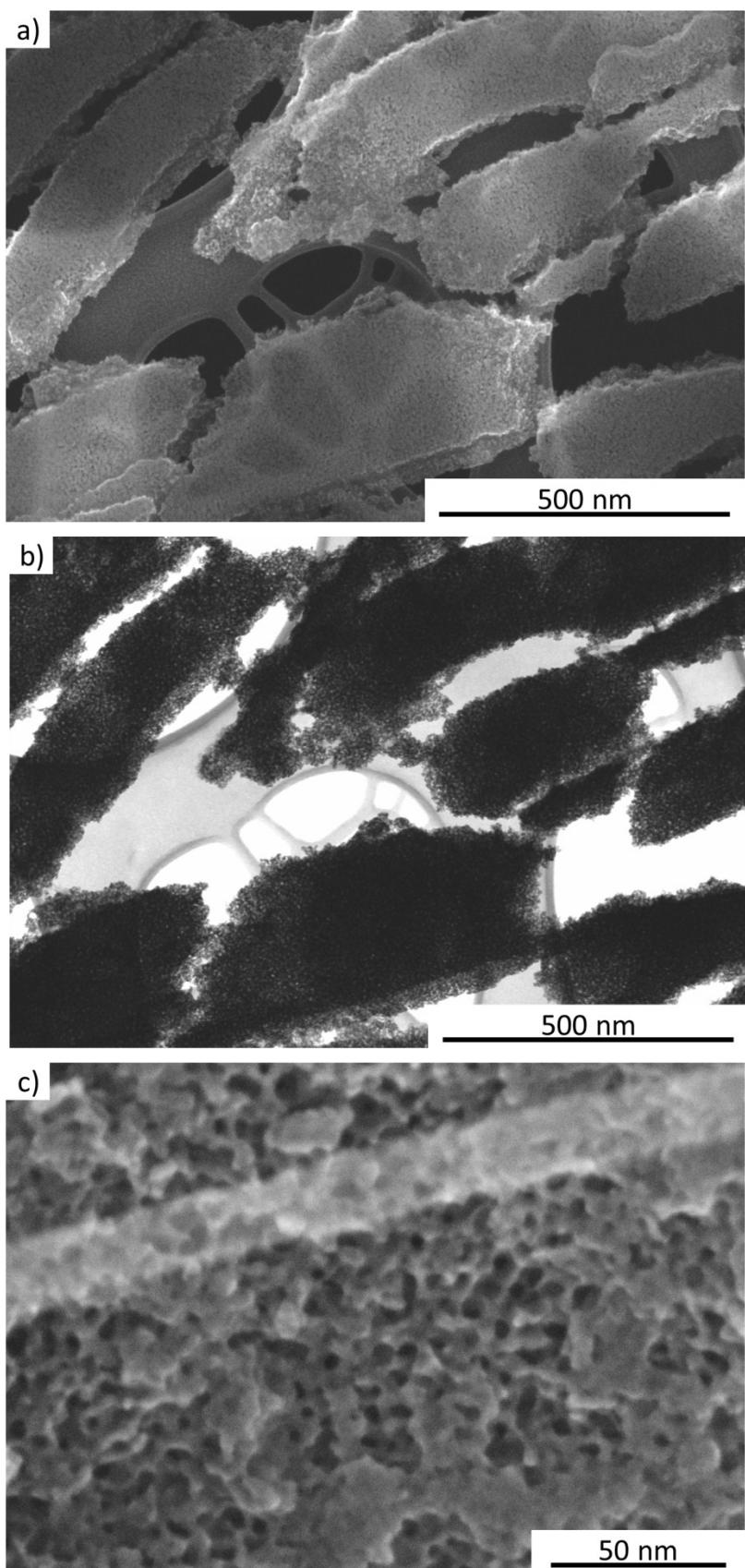


SI Figure 1. XRD patterns of om- Ta_2O_5 and sodium loaded samples om-TaN21, om-TaN9, om-TaN5 and om-TaN3. For comparison, the XRD pattern of the commercial reference sample c- Ta_2O_5 is shown as well. The abbreviation *om-* and *c-* represent *ordered mesoporous* and *commercial*, respectively.

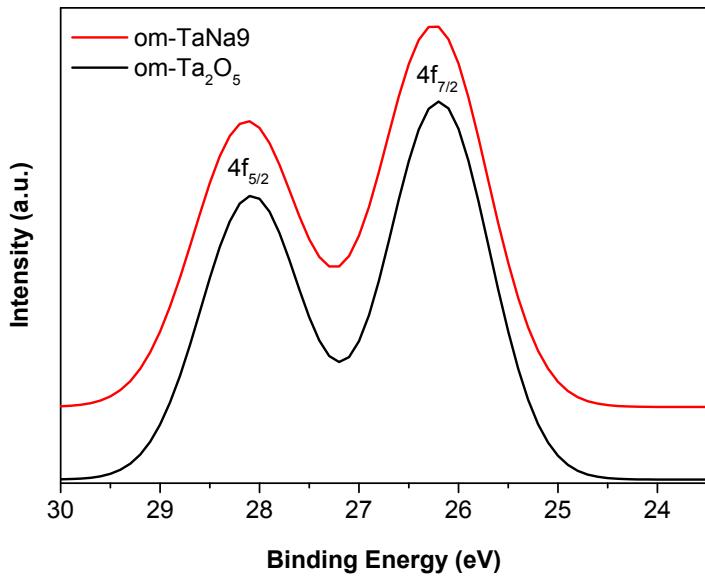
SI Table 1. EDX analysis data of the om-TaN sample series.

The abbreviation *om-* represents *ordered mesoporous*.

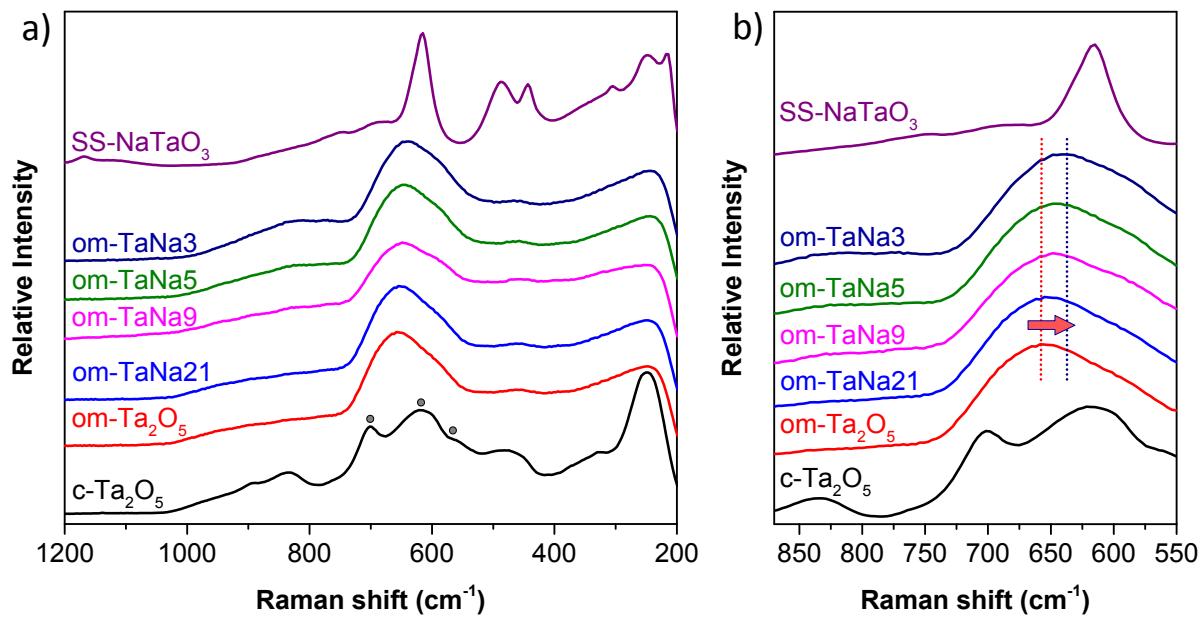
Sample	Atom-%		Ta/Na ratio
	Ta	Na	
om-TaN21	96.1	3.9	24.6
om-TaN9	90.4	9.6	9.4
om-TaN5	87.0	13.0	6.7
om-TaN3	77.8	22.2	3.5



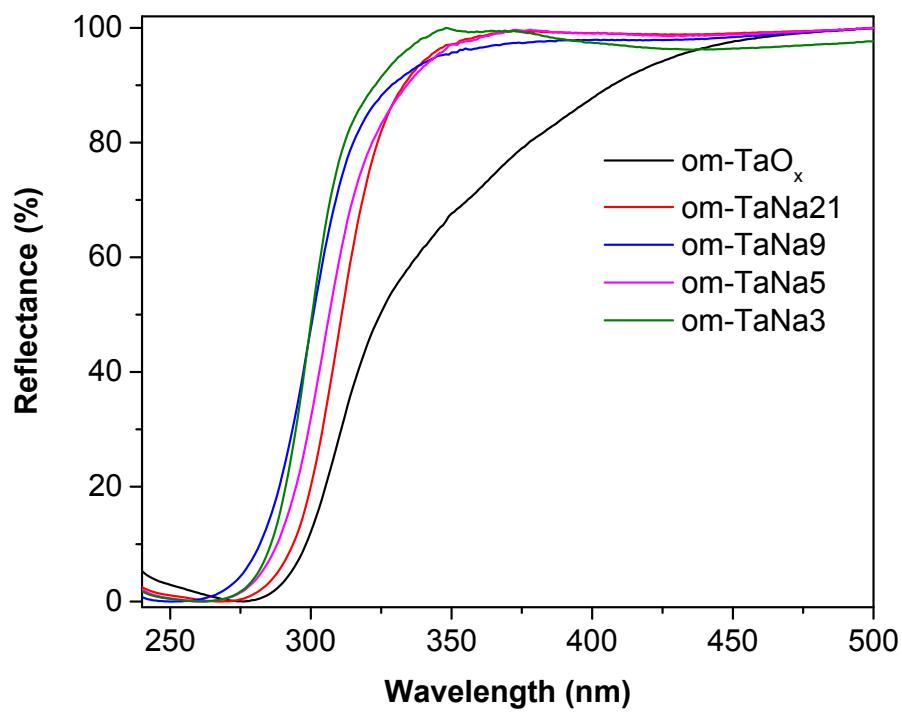
SI Figure 2. (a) Cross-sectional SEM image and (b) an image in bright field STEM mode of the same area of of om-TaNa9; (c) SEM image of the surface of om-Ta9.



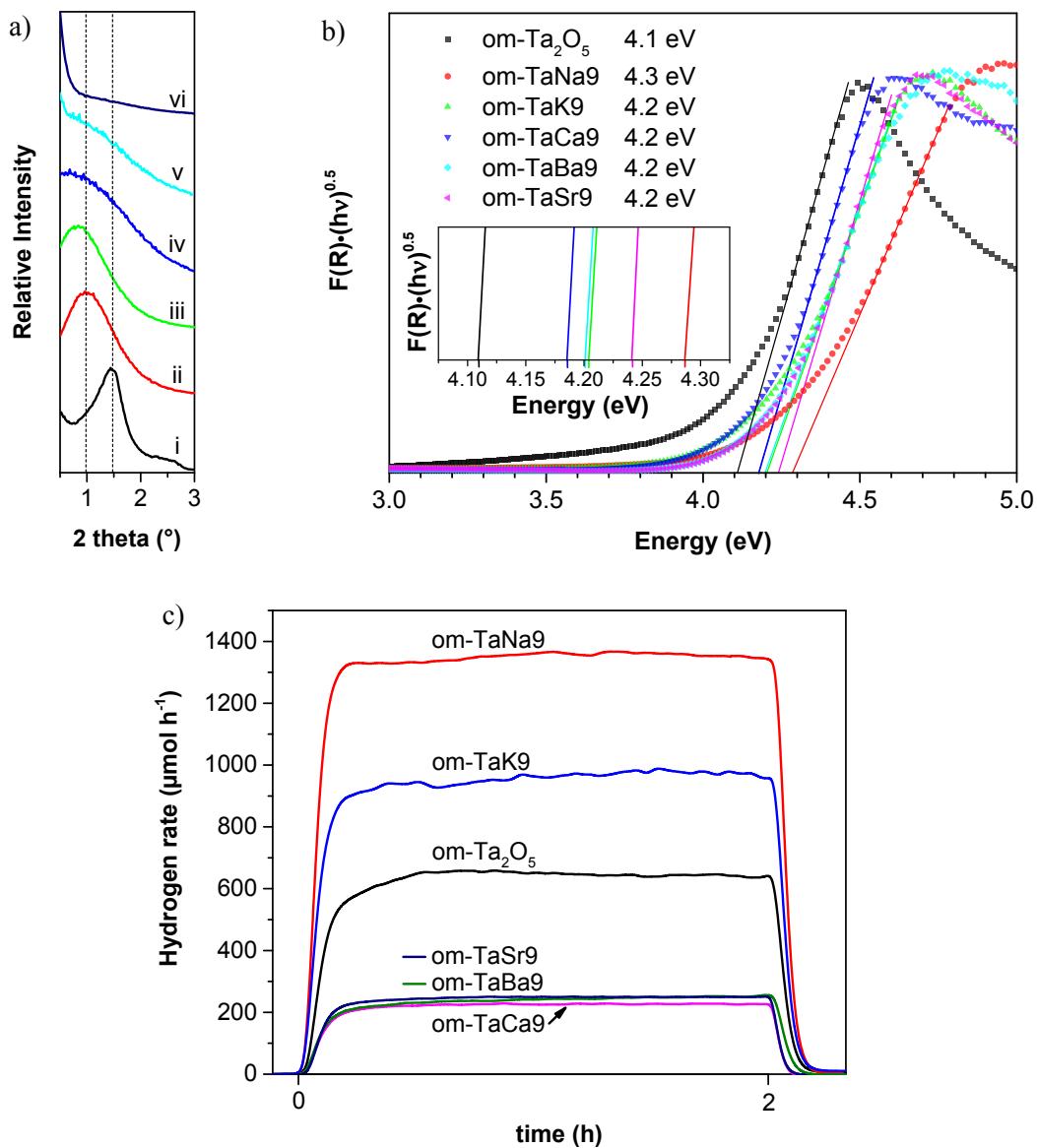
SI Figure 3. XPS spectra of Ta 4f binding energies of om-Ta₂O₅ and om-TaNa9. The abbreviation *om-* represents *ordered mesoporous*.



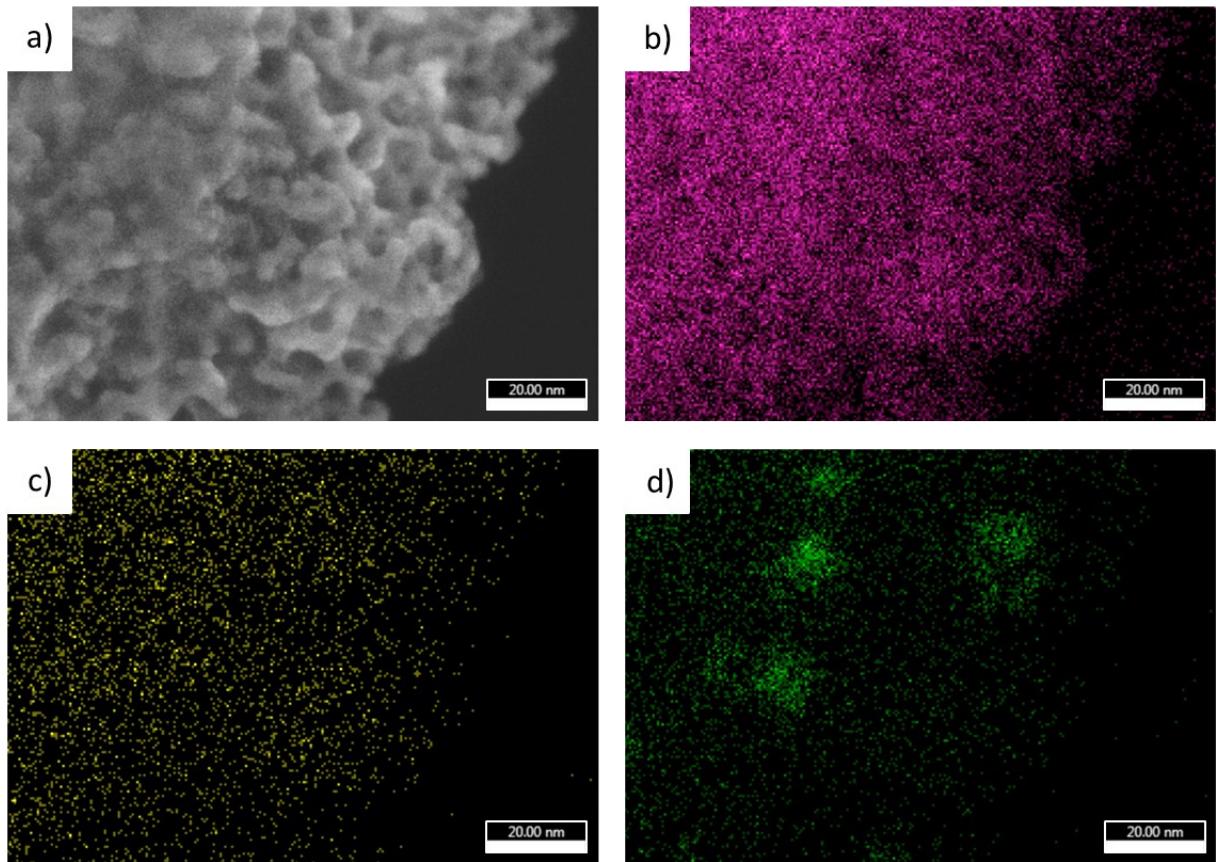
SI Figure 4. Raman spectroscopy data of the om-TaNa sample series and reference samples. (a) An overview of the measured spectra shows the position of the bands for all samples. The circles in the spectrum of c-Ta₂O₅ indicate the triply split peaks of the TaO₆ octahedron. (b) In a higher resolution, the shift of the main TaO₆ mode is depicted. The abbreviation *om-*, *c-* and *SS-* represent *ordered mesoporous*, *commercial* and *solid state* respectively.



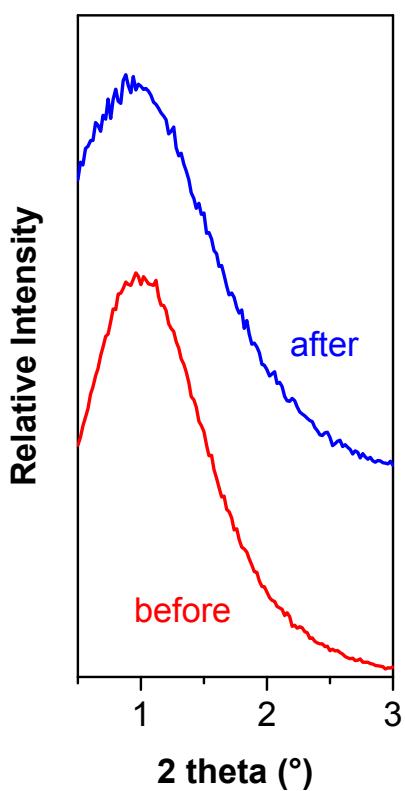
SI Figure 5. Diffuse reflectance UV-Vis spectra of om-Ta₂O₅ and sodium loaded samples. The abbreviation *om-* represents *ordered mesoporous*.



SI Figure 6. (a) Low angle XRD patterns of (i) om-Ta₂O₅, (ii) om-TaNa9, (iii) om-TaK9, (iv) om-TaCa9, (v) om-TaBa9 and (vi) om-TaSr9. (b) Tauc plots (inset: close-up of intersection with x-axis) and (c) hydrogen evolution rates of om-Ta₂O₅ and om-TaX9 with x = Na, K, Ca, Ba and Sr. Hydrogen evolution was tested in 10 vol-% methanol/water solution. The abbreviation *om-* represents *ordered mesoporous*.



SI Figure 7. STEM study of om-TaNa9 with 5 wt-% NiO_x loading, including elemental mapping; (a) SE image of the region of interest; elemental distribution of (b) Ta, (c) Na, and (d) Ni. The abbreviation *om-* represents *ordered mesoporous*. EDX analysis of this sample gave atomic ratios of $\text{Ta/Na} = 10.1$ (9.0) and $\text{Ta/Ni} = 6.6$ (7.4). The theoretical values are shown in brackets.



SI Figure 8. Low angle XRD patterns of sodium loaded ordered mesoporous tantalum oxide with Ta/Na ratio of 9 (om-TaNa9) and 2.5 wt-% NiO_x measured before and after overall water splitting. The sample was irradiated in the reactor for 30 h in total.