

## Investigation of Ta-based materials for the oxygen evolution reaction in acid medium

by Ebrahim Ghasemy, Kulbir K. Ghuman, Daniel Guay and Ana C. Tavares in the frame of the NSERC Alliance (ALLRP 576728-22) and PRIMA (R24-13-001-PME) collaborative project

### Summary

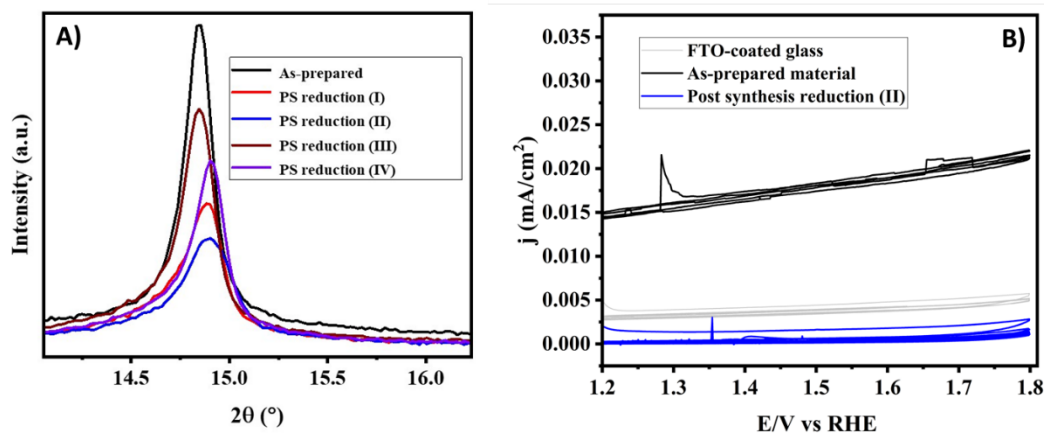
Proton exchange membrane water electrolyzers (PEMWEs) operate in an acidic environment and require the use of Ru and Ir -based electrocatalyst on the anode, which introduces risks associated with high-cost and scarcity. Development of catalysts exempt from platinum group metals is being pursued to mitigate these risks and to diversify catalyst materials supply.

Tantalum-based oxides are known for their good stability under acidic media. However, they are insulators in their pristine form and their use in oxygen evolution reaction (OER) - the reaction occurring at the anode of the PEMWE - has been less explored.

In this work, we attempted to unlock the electrocatalytic activity of Tantalum-based oxides for OER. To this end, we first employed density functional theory (DFT) calculations, as a primary computational tool to: i) understand the structure dependence of electronic properties of polycrystalline materials and how they can be modified by doping, creating defects, forming heterostructures; and ii) predict the electrocatalytic performance of materials prior to experimental tests:

- 1) DFT calculations on three different Ta<sub>2</sub>O<sub>5</sub> facets, pristine and with O or Ta defects, revealed that the OER activity of the oxide is facet-dependent according to the following trend (200) > (120) > (001). The trend inversely correlated with the Ta density on the topmost atomic layer. The lowest overpotentials were observed at a Ta–O site (0.61 V) and at a Ta site (0.63 V) of the pristine and of Ta-defect (200) facets, respectively. As a conductive phase is often added to insulating materials in experiments, the (200) Ta<sub>2</sub>O<sub>5</sub>/graphene heterostructure was also studied. An overpotential as low as 0.39 V was found for the Ta–O sites of the heterostructure. Detailed analysis of the electronic properties of the facets (density of states and partial density of states) and their impact on OER activity can be found in [1].
- 2) Sodium tantalates, including NaTaO<sub>3</sub> and NaTa<sub>3</sub>O<sub>8</sub>, were also investigated by DFT as alternative Ta-based materials for OER electrocatalysis. The calculations indicated that Na sites on the (202) NaTa<sub>3</sub>O<sub>8</sub> facet are active centers and exhibited an onset potential of 0.59 V. Analysis of the PDOS revealed that the presence of Ta *d* orbitals at the Fermi level could play a key role in determining the OER activity of the material [2].
- 3) In parallel with the DFT-based theoretical investigations, experimental work was undertaken to synthesize NaTa<sub>3</sub>O<sub>8</sub>. According to the existing literature, this oxide had not previously been synthesized by hydrothermal synthesis, in contrast to other sodium tantalates. In this study, we demonstrated the first successful synthesis of the target phase via this method. The electrochemical characterization of samples with NaTa<sub>3</sub>O<sub>8</sub> as the major phase showed that the material was electrically resistive with no OER activity. Post-synthesis reduction treatments lead to defective materials with higher conductivity and stable electrochemical response to potential cycling, Figure 1. These results introduce reduced NaTa<sub>3</sub>O<sub>8</sub> as a stable electrocatalyst support for OER, but further

studies are necessary to study its long-term stability in acidic media under anodic polarization conditions. Additionally, the material synthesized in this work is polycrystalline and new synthesis strategies are needed to obtain  $\text{NaTa}_3\text{O}_8$  nanoparticles with high density of (202) facets [3].



**Figure 1.** (A) X-ray diffraction pattern of the pristine and reduced samples (PS) in the 14.5 to 15.5°  $2\theta$  range. The shift of the diffraction peak to higher  $2\theta$  values indicates a contraction of the lattice, consistent with the creation of oxygen defects. (B) Cyclic voltammograms in 1.2 to 1.8 V vs RHE potential window in 0.5 M  $\text{H}_2\text{SO}_4$  at 50 mV/s. The positive inclination of the cyclic voltammogram recorded with the pristine sample is indicative of a resistive electrode.

## References

- [1] Ebrahim Ghasemy, Ana C Tavares, Kulbir K Ghuman, *Facet-and graphene-support-dependent activity of  $\text{Ta}_2\text{O}_5$  for oxygen evolution reaction*, RCS Applied Interfaces, 2 (2025) 1631.
- [2] Ebrahim Ghasemy, *Developing Nb-and Ta-based Electrocatalysts for Oxygen Evolution Reaction*, in *PhD thesis in Sciences de l'Énergie et Matériaux*, June 2025, Université du Québec, Institut National de la Recherche Scientifique – Centre Énergie Matériaux Télécommunications.
- [3] Ebrahim Ghasemy, Kulbir K. Ghuman, Daniel Guay and Ana C. Tavares, *Optimizing the synthesis of Ta-based materials and their electrochemical characterization for the oxygen evolution reaction in acid medium*, report submitted to Niobay in the context of NSERC Alliance (ALLRP 576728-22) and PRIMA (R24-13-001-PME) collaborative project , April 2026, 27 pages (confidential).

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