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(Invited) Unequal {110} Facets: The Critical Role of Surface Termination in Determining Photoelectrochemical Activity of Single BiVO₄ Particles

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BiVO₄ particles are attractive visible light-absorbing semiconductors to drive the water oxidation half reaction in a photoelectrochemical cell or for the overall water splitting reaction in a photocatalytic reactor. Ensemble-level and single particle-level measurements previously showed that photogenerated electrons and holes tend to accumulate and react at top {010} and lateral {110} facets, respectively. However, multiple possible surface terminations exist for these low-index facets, and it is unclear to what extent different surface facet terminations influence the overall current or reaction rate of a single BiVO₄ particle. Here we use correlative scanning photoelectrochemical microscopy (SPCM), facet-dependent electrical measurements, electron beam induced current (EBIC) mapping, and mid-IR scattering scanning near-field optical microscopy (s-SNOM) measurements to quantify the water and sulfite oxidation photocurrent among different lateral and top facets of 62 BiVO₄ particles. SPCM measurements confirmed that illuminating lateral {110} facets generates higher photocurrents for water and sulfite oxidation than top {010} facets. However, they also unexpectedly revealed that different lateral facets within the same particle produce varying photocurrents, despite electron microscopy images showing no clear structural differences between them. Facet-dependent electrical and EBIC measurements further indicated that no significant space charge regions form at inter-facet junctions or metal-BiVO₄

contacts under vacuum. This result is significant because it is highly unlikely that photogenerated holes generated in the particle interior beneath the top {010} facet transport to the lateral {110} facets and contribute to the water/sulfite oxidation reaction. Additionally, nano-FTIR spectroscopy revealed that materials chemistry heterogeneity exists not only between particles but also within individual facets of a single particle. These findings suggest the presence of distinct surface termination chemistries across different facets, consistent with theoretical predictions, and emphasize the need to control atomic-level surface termination during sample growth to enhance photocatalytic performance.