

Supporting Information

Deposition of an Oxomanganese Water Oxidation Catalyst on TiO₂ Nanoparticles: Computational Modeling, Assembly and Characterization

Gonghu Li, Eduardo M. Sproviero, Robert C. Snoeberger III, Nobuhito Iguchi, James D. Blakemore, Robert H. Crabtree*, Gary W. Brudvig* and Victor S. Batista*

Department of Chemistry, Yale University, P. O. Box 208107, New Haven, CT 06520-8107

*Email Addresses: robert.crabtree@yale.edu; gary.brudvig@yale.edu; victor.batista@yale.edu

Supporting Figures

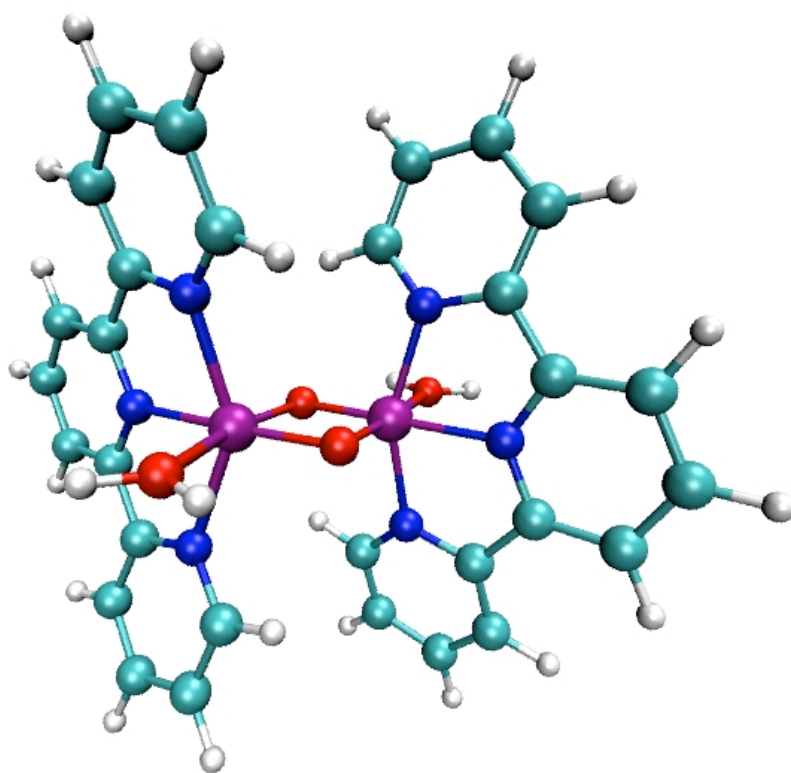


Figure S1. Optimized structure of complex **1** in vacuum. Color scheme: C(light-blue), H(white), Mn(purple), N(blue), O(red).

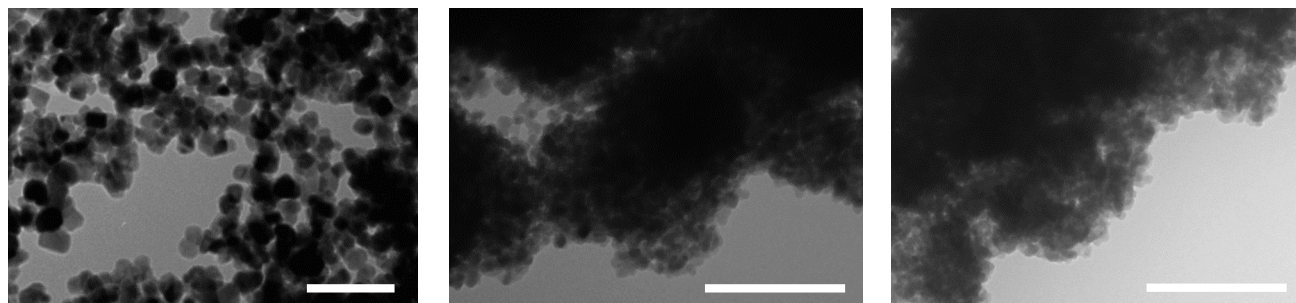


Figure S2. TEM images of Degussa P25 (left), D450 (middle), and D70 (right). Scale bars 100 nm.

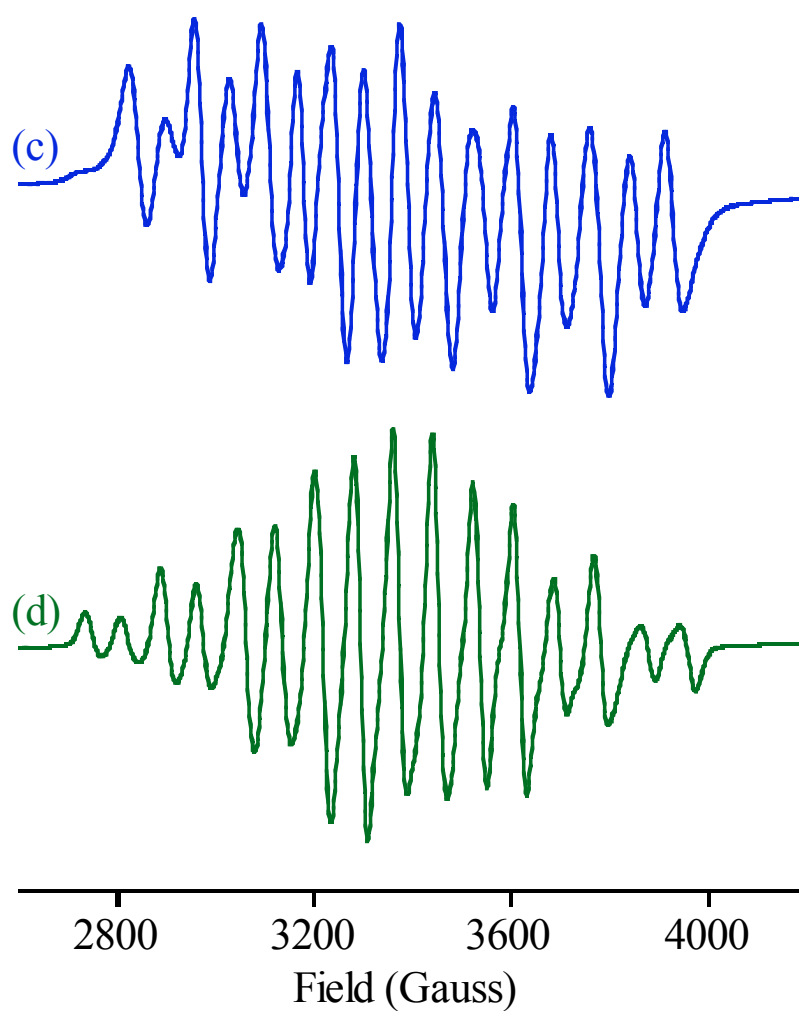


Figure S3. EPR spectra of (c) **1**-D70 dispersed in water and (d) isolated **1** in a HOAc/NaOAc buffer (pH 4.5) solution. These are expanded from Figure 3 in the text.

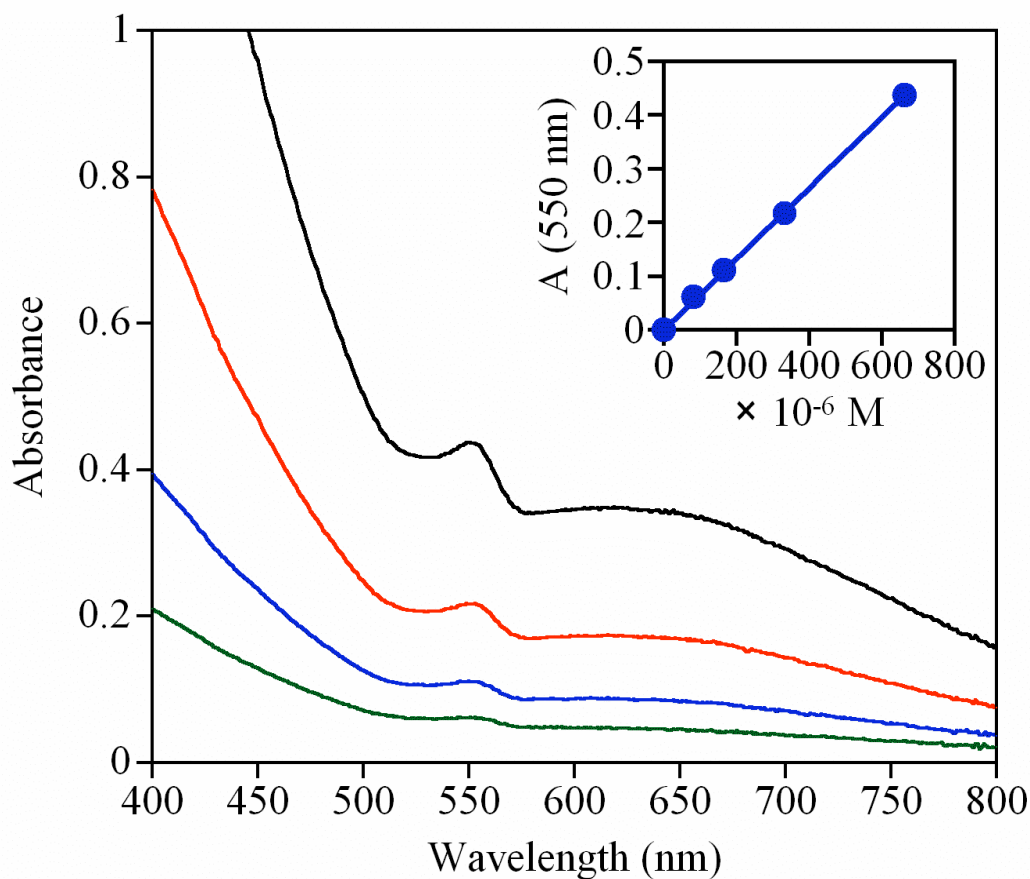


Figure S4. UV-visible spectra of complex **1** in H_2O at different concentrations (from top to bottom): 663, 332, 166, 83 μM . Inset: a calibration curve showing the absorbance of complex **1** at 550 nm as a function of concentration. These data give an extinction coefficient for complex **1** at 550 nm of $660 \text{ M}^{-1} \text{ cm}^{-1}$.

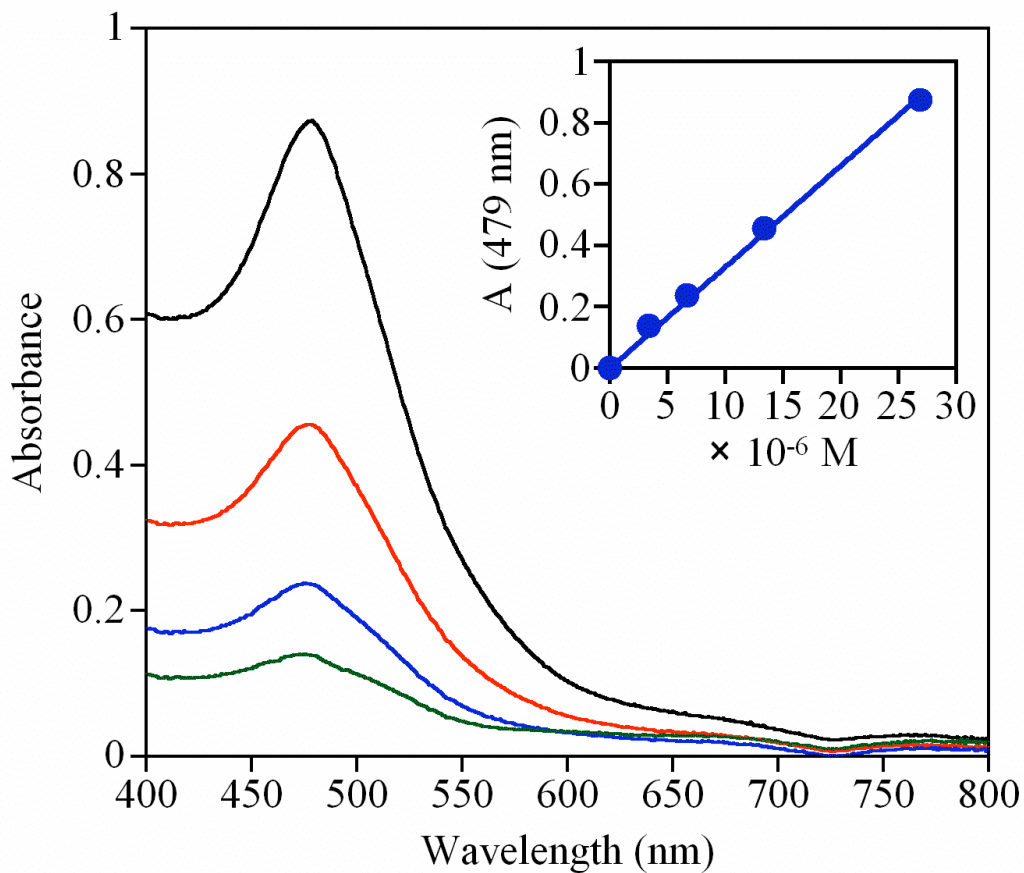


Figure S5. UV-visible spectra of complex 2 in 0.3 M HNO_3 at different concentrations (from top to bottom): 26.9, 13.4, 6.7, 3.4 μM . Inset: a calibration curve showing the absorbance of complex 2 at 479 nm as a function of concentration. These data give an extinction coefficient for complex 2 at 479 nm of $33000 \text{ M}^{-1} \text{ cm}^{-1}$.