Theory-guided design of cobalt-incorporated birnessite as an improved water oxidation catalyst.

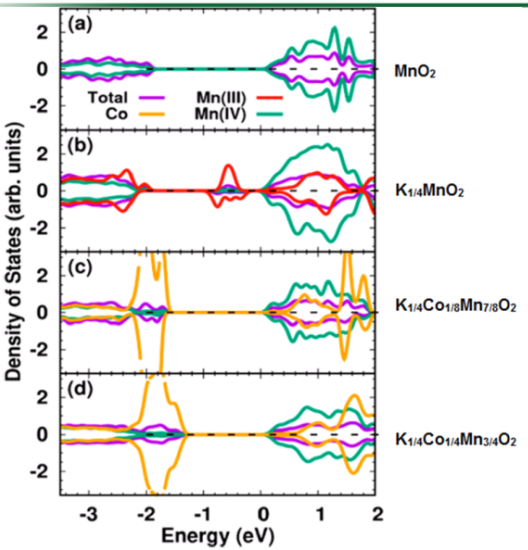

Figure 1. Calculated Density of States from DFT (optB86b).

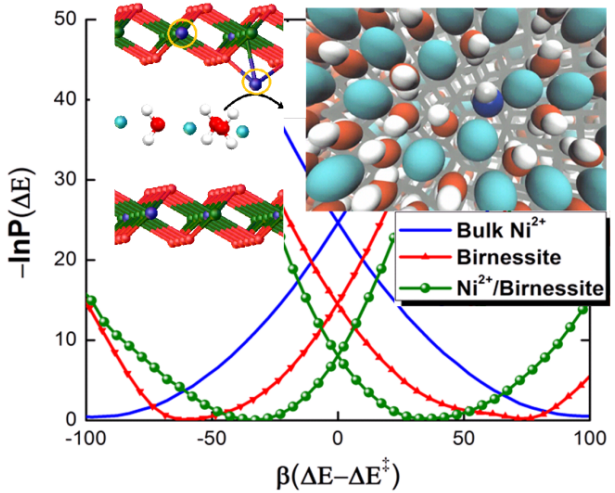

Figure 2. MD prediction of decreased reorganization energy and activation barrier to electron transfer from enhanced water dynamics. (Thenuwara et. al., *Angew. Chem. Int. Ed.* **2016**, *55*, 1 – 6

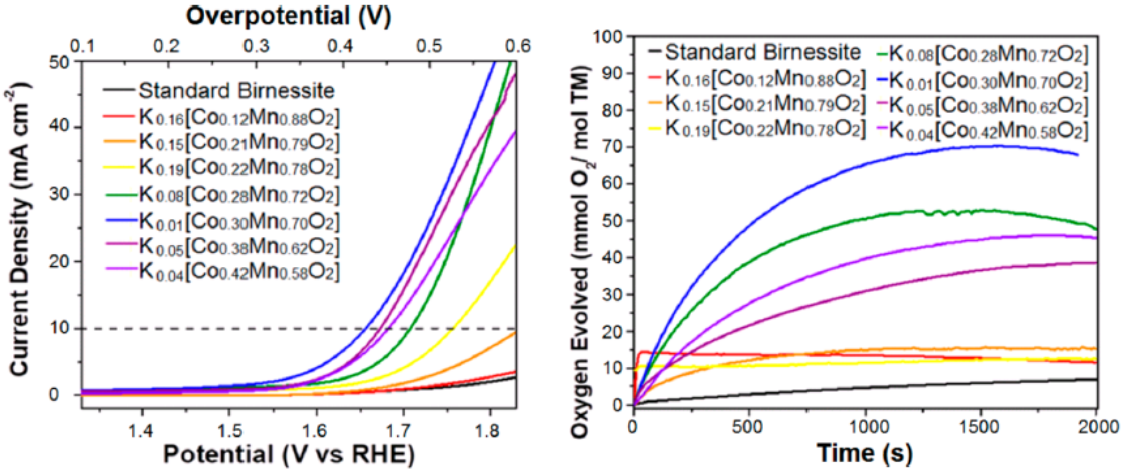

Figure 3. Examination of catalytic activity by linear sweep voltammetry at pH = 14 (left), and by chemical oxidation by Ce^{4+} at pH = 2 (right).

McKendry, I. G. et al. *Inorg. Chem.* DOI: 10.1021/acs.inorgchem.7b01592
Work performed at Temple University

Scientific Achievement

Features theoretically advantageous to water oxidation, are incorporated into a new layered catalyst.

Significance and Impact

Use of theory and modelling in the successful design of catalysts, and generation of a new water oxidation catalyst with good performance.

Research Details

- Predictions on physical properties of layered MnO_2 from DFT & MD encourage
  - In-layer cobalt and inter-layer transition metals for hole mobility.
  - Increased charge for enhanced water dynamics, speeding electron transfer.
- These elements are incorporated by systematic inclusion of Co as 1/3 of transition metal content. Overpotential (η) = 420 mV, Tafel slope (*b*) = 81 mV/dec.

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