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Electronic Supplementary Information

Early-stage formation of (hydr)oxo bridges in transition-metal catalysts for photosynthetic processes

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Table S1. Calculated effective potentials for each oxidation step [$U(S_{i+1}-S_i)$ (V)] for isolated and two-metal systems of Co, Mn, and Ni at *pH* 7.0, 6.0, and 13.0, respectively.

	Effective potential *U* (V)							
	Co (*pH* 7.0)		Mn (*pH* 6.0)		Ni (*pH* 13.0)			
Transition	Isolated	Two-metal	Isolated	Two-metal	Isolated	Two-metal	Isolated (less one H+)	Two-metal (less one H^+)
$S_0 \rightarrow S_1$	1.60	1.29	1.12	0.80	1.79	1.83	1.03	1.27
$S_1 \rightarrow S_2$	1.63	1.39	1.85	0.85	1.45	1.41		1.38
$S_2 \rightarrow S_3$				1.52		1.97		1.64
$S_3 \rightarrow S_4$				1.62		1.46		