Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

An alternative structure of TiO2 with higher energy valence band edge SINISA COH, UC Riverside, PETER Y. YU, UC Berkeley and LBL, YUTA AOKI, SUSUMU SAITO, Tokyo Institute of Technology, STEVEN G. LOUIE, MARVIN L. COHEN, UC Berkeley and LBL — We propose an alternative structure of TiO2 anatase that has a higher energy oxygen p-like valence band maximum than the pristine TiO2 anatase and thus has a much better alignment with the water splitting levels. This alternative structure is unique when considering a large subspace of possible structural distortions of TiO2 anatase. We propose two ways to access this state experimentally and argue that one of them might have been realized in the recently discovered so-called black TiO2. This work was supported by NSF Grant No. DMR-1508412 and the theory of Materials Program at the Lawrence Berkeley National Lab funded by the Director, Office of Science, Office of Basic Energy Sciences, Materials Sciences and Engineering Division, U.S. Department of Energy under Contract No. DE-AC02-05CH11231. Computational resources have been provided by the DOE at Lawrence Berkeley National Laboratory's NERSC facility. We acknowledge support from the MEXT Japan Elements Strategy Initiative to Form Core Research Center, MEXT Japan KAKENHI Grant No.25107005, and JSPS Grant No.14J11856.

Sinisa Coh
UC Riverside

Date submitted: 11 Nov 2016 Electronic form version 1.4