

Abstract Submitted
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Theoretical explanation for the enhanced water-splitting catalytic activity in delithiated LiCoO_2 MICHAL BAJDICH, SUNCAT Center for Interface Science and Catalysis, Chemical Engineering, Stanford University and SLAC, ZHIYI LU, Department of Material Science and Engineering, Stanford University and SLAC, JENS K. NORSKOV, SUNCAT Center for Interface Science and Catalysis, Chemical Engineering, Stanford University and SLAC, YI CUI, Department of Material Science and Engineering, Stanford University and SLAC — Layered LiCoO_2 (LCO) is important battery material not well known for its electrochemical catalytic activity. On the other hand, layered 3d-metal-oxyhydroxides, including CoOOH , are very active water-splitting (oxygen-evolution reaction, OER) catalysts in alkaline media with structure very similar to LCO. In this work, we use DFT+U calculations to explain the enhancement effect in OER catalytic activity in the electrochemically delithiated LCO (De-LCO). We analyze the surface stability and OER activity of the 5 most stable surface facets of LCO and the De-LCO, with 50% Li removed. Using standard thermodynamic approach of the theoretical OER overpotential, we show that all surface facets have more active sites under Li removal. Particularly, the non-polar facets are identified to be highly active and are further activated by the delithiation process, while the dominant (0001) surface has negligible activity. These findings are in very good agreement with our experimental investigation of LCO and De-LCO nanosheets and nanoparticles with well defined surface morphology.

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