

Abstract Submitted  
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**Ab initio study of the charge storage mechanism of ruthenium dioxide as an electrochemical ultracapacitor** YONGDUO LIU, FEI ZHOU, VIDVUDS OZOLINS, University of California, Los Angeles — The charge storage mechanisms of ruthenium dioxide were investigated by first principles calculations. Both H-injected bulk and H-adsorbed RuO<sub>2</sub>(110) surface have been studied in order to obtain a whole picture of the discharging process of ruthenium dioxide as a supercapacitor. We have predicted the crystal structure of ruthenium-oxy-hydroxide (ROOH). By ab-initio voltage calculations, we also found that the RuO<sub>2</sub>(110) surface is completely hydrated before the usual voltammogram measurements, which suggests that the redox reactions happen in deep layers and should be diffusion dominated processes.

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