Abstract Submitted
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Atomic-scale roughness of Li metal surface evident in soft X-ray absorption spectroscopy[1] DAVID PRENDERGAST, LIWEN WAN, YUFENG LIANG, YI-DE CHUANG, Lawrence Berkeley National Laboratory (LBNL), RUIMIN QIAO, LBNL and Shandong University, China, SHISHEN YAN, Shandong University, WANLI YANG, LBNL — Realizing Li metal electrodes depends on fundamental understanding and efficient control of surface properties, which requires reliable characterization of the Li metal surface. Controlled experiments of Li K-edge soft X-ray absorption spectroscopy (XAS) reveal evidence of steady oxidation of the Li metal surface even under ultrahigh vacuum (UHV) conditions. The XAS of the short-lived Li metal surface, prepared by *in-situ* scratching, exhibits a prominent peak at 55.6 eV, more intense and at a slightly higher energy than the first peak expected for bulk Li metal at 55 eV. First-principles XAS calculations explain the origin of both the increased intensity and energy shift. This required the use of surface structural models with under-coordinated Li atoms and an estimated 4 Å inelastic mean-free-path for Auger electrons, implying extreme surface sensitivity of the measurements to the first 2-3 atomic layers. This work provides a benchmark on both experiment and theory for further studies of Li and other reactive metal surfaces, which are currently under scrutiny for next-generation energy storage devices.

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