

Abstract Submitted  
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**Unexpected carboxylate like CO adsorption at the  $\text{Sr}_3\text{Ru}_2\text{O}_7$  (001) surface** MARCEL HIECKEL, FLORIAN MITTENDORFER, JOSEF REDINGER, BERNHARD STOEGER, ZHIMING WANG, MICHAEL SCHMID, ULRIKE DIEBOLD, Vienna University of Technology — Oxide perovskite materials have attracted enormous attention because of a variety of intriguing physical properties ranging from catalysis to multiferroicity. We present a combined experimental and ab-initio (DFT) study with the Vienna Ab initio Simulation Package (VASP) on the adsorption of CO at the  $\text{Sr}_3\text{Ru}_2\text{O}_7$  (001) surface. We identify both a physisorbed and a chemisorbed CO configuration. Unexpectedly, in the latter case adsorption occurs in a carboxylate (COO) like state. Both configurations have been confirmed by detailed STM experiments and simulations. In addition we find only a small barrier for the carboxylate formation on the surface. Work supported by the Austrian FWF, SFB F45 (FOXSI).

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