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Water adsorption on $Sr_3Ru_2O_7$ and $Ca_3Ru_2O_7$ WERNFRIED MAYR-SCHMOELZER, ULRIKE DIEBOLD, DANIEL HALWIDL, FLORIAN MITTENDORFER, GARETH PARKINSON, JIRI PAVELEC, JOSEF REDINGER, MICHAEL SCHMID, BERNHARD STOEGER, Inst. of Applied Physics, TU Wien, Vienna, DAVID FOBES, ZHIQIANG MAO, JIN PENG, Dept. of Physics, Tulane University, New Orleans — Perovskite oxides are promising materials for a wide range of applications as diverse as sensors, fuel cells and catalysts. Surprisingly an atomic scale knowledge of their surface chemistry is still rather poor. Here we present a combined DFT, low-temperature STM and XPS study of the first monolayer H_2O formation on the (001) surfaces of two Ruddelsden-Popper type compounds, $Sr_3Ru_2O_7$ and $Ca_3Ru_2O_7$. Both cleave nicely, yielding flat surfaces of rocksalt-like SrO and CaO type. Adsorbed H_2O monomers dissociate on both surfaces by transferring a proton to an apical O while the remaining OH resides at a nearby Sr-Sr or Ca-Ca bridge, respectively. The different tilting and rotations of the RuO_6 octahedra in the Sr and Ca perovskites cause different behaviour of the dissociated fragments: for $Sr_3Ru_2O_7$ a lone Sr-Sr bridge OH circles the apical OH with an activation energy of ≈187meV. At higher coverages dimers, followed by chains and cages are formed[1]. In contrast, the dissociated monomer fragments are immobile on $Ca_3Ru_2O_7$(001) and only chains along the [010] direction occur. [1]D. Halwidl et. al., Nature Materials, 15(4), 450-455.

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