Water adsorption on Sr$_3$Ru$_2$O$_7$ and Ca$_3$Ru$_2$O$_7$

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$_2$O formation on the (001) surfaces of two Ruddelsden-Popper type compounds, Sr$_3$Ru$_2$O$_7$ and Ca$_3$Ru$_2$O$_7$. Both cleave nicely, yielding flat surfaces of rocksalt-like SrO and CaO type. Adsorbed H$_2$O 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$_3$Ru$_2$O$_7$ a lone Sr-Sr bridge OH circles the apical OH with an activation energy of \(\approx 187\) meV. At higher coverages dimers, followed by chains and cages are formed\[1\]. In contrast, the dissociated monomer fragments are immobile on Ca$_3$Ru$_2$O$_7$(001) and only chains along the [010] direction occur. [1]D. Halwidl et. al., Nature Materials, 15(4), 450-455.

Wernfried Mayr-Schmlzzer
Vienna Univ of Technology

Date submitted: 11 Nov 2016

Electronic form version 1.4