VI. Supporting information available

Here we show the calculated energies and voltages for various hydrogen-adsorbed surface configurations on RuO_2(110). This information is available free of charge via the Internet at http://pubs.acs.org.

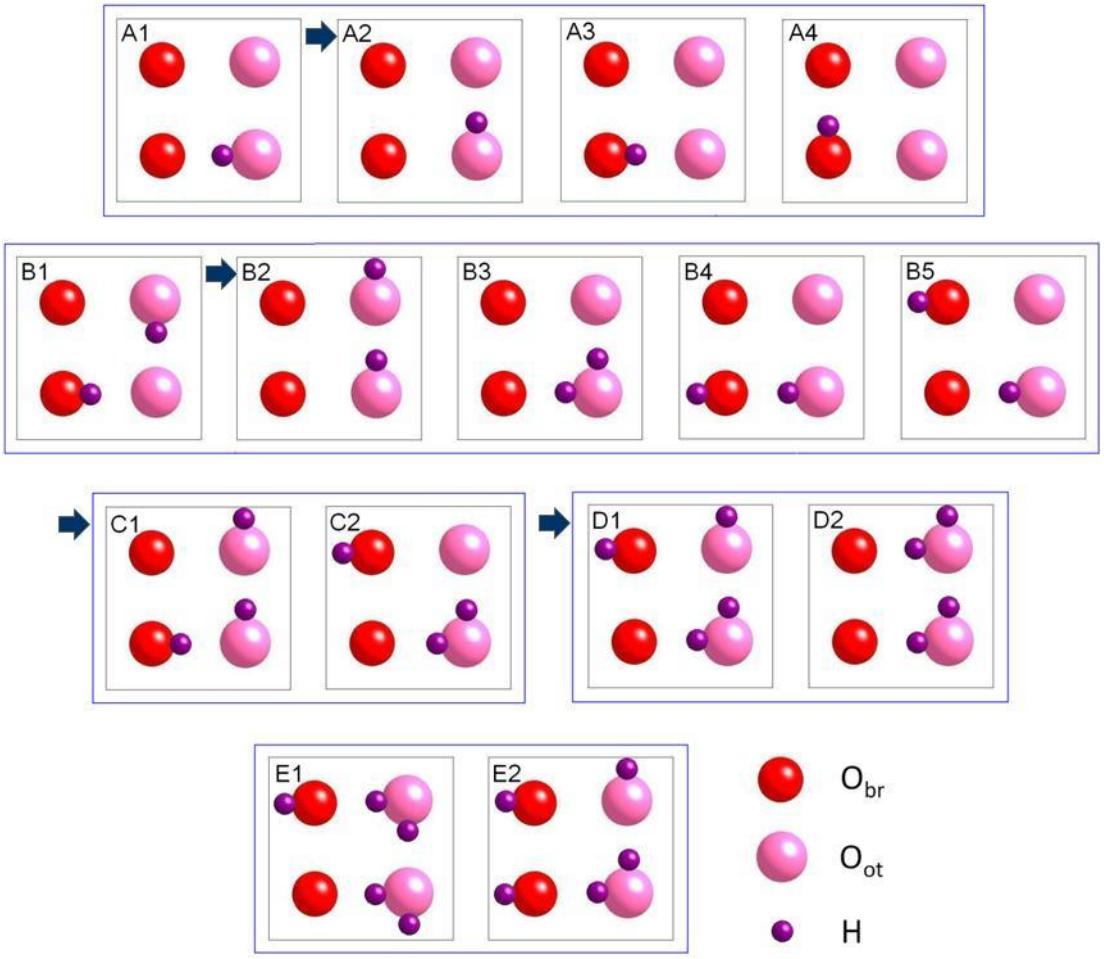

Figure 9. Top view of the 2×1 surface unit cell of the selected surface adsorption configurations categorized by the coverage of protons. The red sphere illustrates the bridge-oxygen, the big pink sphere is the on-top oxygen, and the little purple sphere is the proton. The arrow indicates the ground state structure of each coverage category.

Table 3. Adsorption energies calculated through static energies [$E_{adsorption}$(eV/H_2)] or free energies [$G_{adsorption}$(eV/H_2)], as well as voltages of H-complexes on oxygen covered RuO_2(110) as determined by DFT calculations.

Structure	Number of protons	$G_{adsorption}$ (eV/H_2)	Voltage (vs.RHE)	$E_{adsorption}$ (eV/H_2)	$E_{adsorption}$ (literature)
A1	1	2.33		2.93	
A2	1	2.49	1.25	3.09	
A3	1	2.27		2.87	
A4	1	1.95		2.55	
B1	2	2.34		2.94	2.94[24]
B2	2	2.57	1.33	3.17	3.21[24]
B3	2	2.54		3.14	
B4	2	2.5		3.1	
B5	2	2.26		2.86	2.91[24]
C1	3	2.55	1.27	3.15	
C2	3	2.36		2.96	
D1	4	2.49	1.22	3.09	
D2	4	2.38		2.98	
E1	5	1.9		2.5	
E2	5	1.98		2.58	
E3 (subsurface)	5	2.46	1.21	3.06	