Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Water Dissociation on MnO(1x1)/Ag(100)

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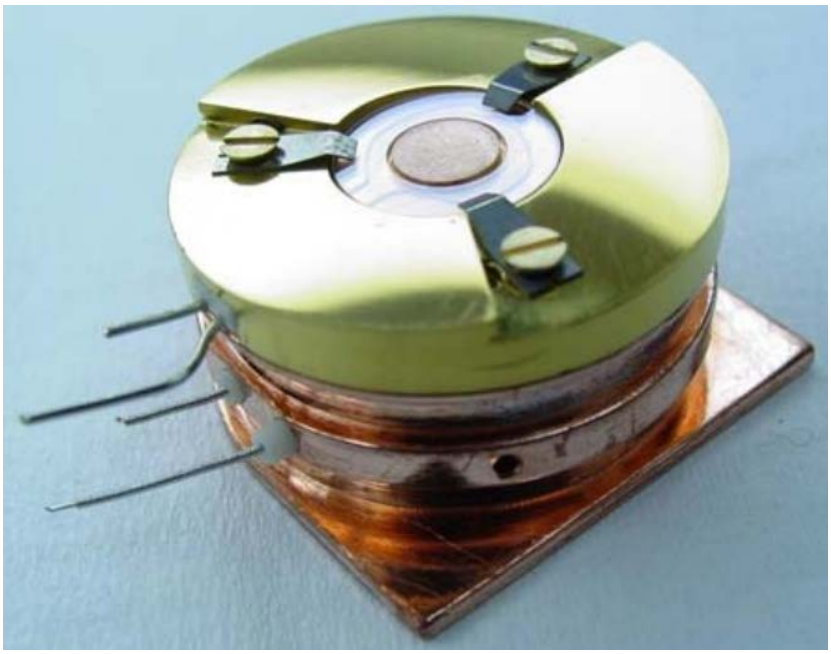

Figure S1. RHK sample holder. A “hat shaped” Ag(100) single crystal is secured under a saphire washer held in with three clips. Sample temperature is monitored using a K-type thermocouple underneath the crystal.

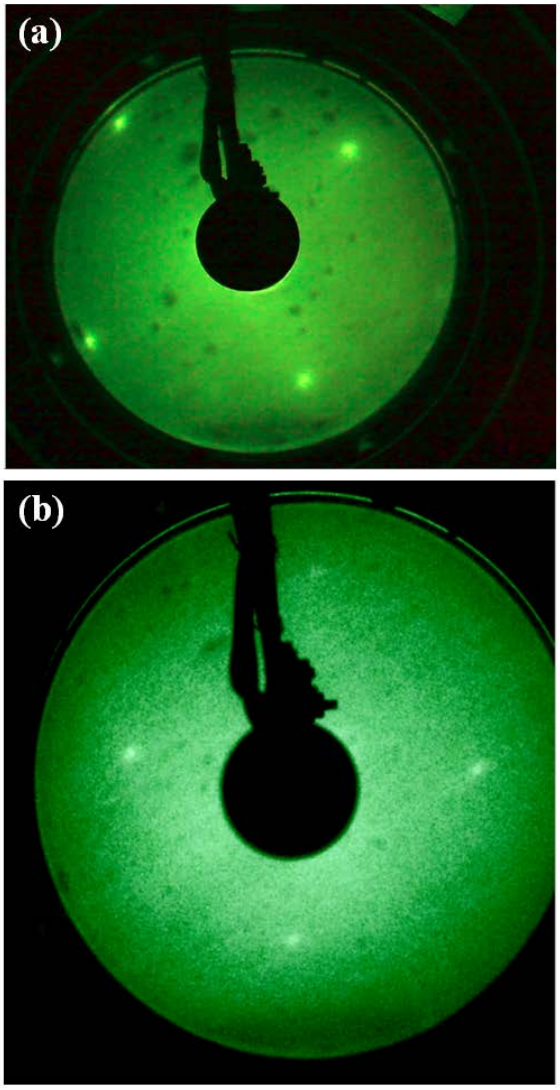

Figure S2. LEED images of (a) clean Ag(100) and (b) MnO film on Ag(100) annealed to 700 K in vacuum.

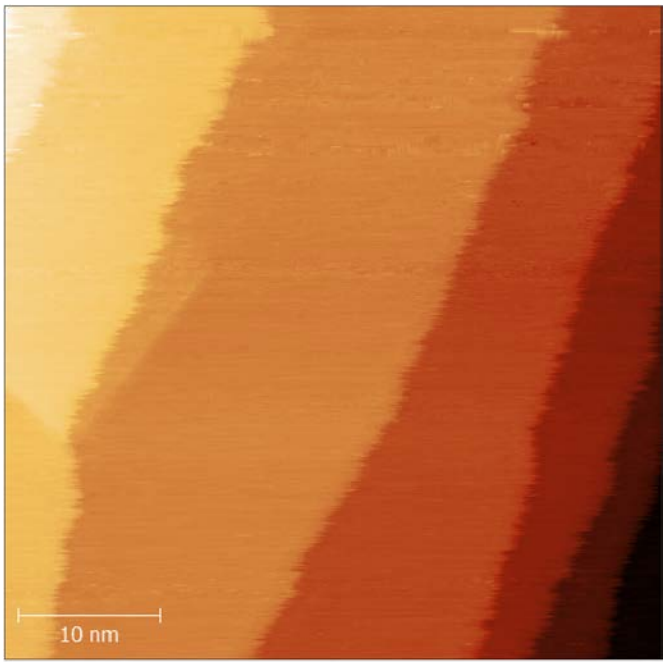

Figure S3. STM of Ag(100) after sputtering and annealling to 700 K. Image collected at 0.96 V and 0.53 nA.

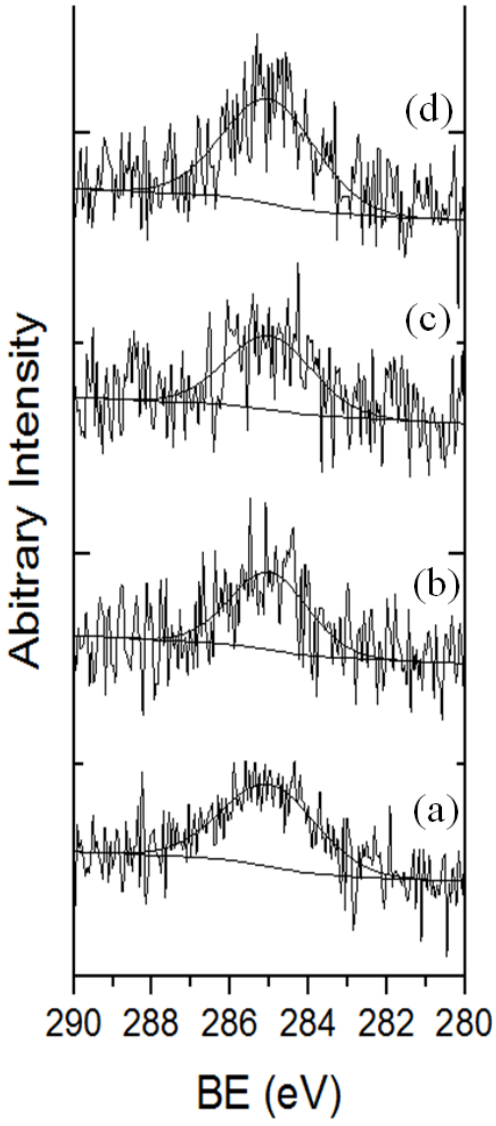

Figure S4. C1s spectra of (a) silver substrate, (b) as deposited MnO film, (c) after exposure to 9.0 x10^{-3} Torr H_2O and (d) after exposure to 2.5 Torr water vapor.

Table S1: Main features of Ag-supported MnO(100)-1x1 and MnO (2x1) monolayers. ΔE_{ad} is the adhesion energy computed with respect to a relaxed monolayer with the lattice parameters of the 2D cell fixed at the Ag(100) values; ΔE_S is the strain energy that is the energy released when in the unsupported MnO film the 2D cell constraints are removed; energies are in eV/MnO unit. The antiferromagnetic (AF) arrangement has been considered (see also Figure 4). Functional and basis sets are reported as described in the manuscript. PW indicates a plane wave basis set.

	MnO(1x1)/Ag(100)		**MnO(2x1)/Ag(100)**	
	E_{ad}	**ΔE_S**	**ΔE_{ad}**	**ΔE_S**
PBE0/B//PBE0/A	-0.33	0.02	-0.42	0.45
HSE06/B//PBE0/A	-0.32	0.02	-0.43	0.47
B3PW91/B//PBE0/A	-0.27	0.02	-0.40	0.44
PBE/B//PBE/A	-0.59	0.02	-0.69	0.16
PBE/PW	-0.47	0.02	-0.67	0.13
PBE+U (U_{eff} = 4 eV)/PW	-0.26	0.07	-0.38	0.41

Table S2: Energetics of the MnO(1x1) and MnO(2x1) supported and unsupported monolayers. Values are in eV per MnO unit. Both ferromagnetic (FM) and antiferromagnetic (AF) arrangements have been considered (see also Figure 4 and text for details). The lattice parameters are fixed at the Ag(100) values. The FM energies have been computed on the AF geometries.

	MnO(1x1)		**MnO(2x1)**	
	AF	**FM**	**AF**	**FM**
PBE0/B//PBE0/A	0	0.08	0.42	0.59
HSE06/B//PBE0/A	0	0.07	0.42	0.58
B3PW91/B//PBE0/A	0	0.09	0.37	0.56
	(1x1)/Ag(100)		**(2x1)/Ag(100)**	
	AF	**FM**	**AF**	**FM**
PBE0/B//PBE0/A	0	0.05	0.33	0.46
HSE06/B//PBE0/A	0	0.03	0.31	0.44
B3PW91/B//PBE0/A	0	0.04	0.25	0.39