Supporting Information

Strain mediated oxygen evolution reaction on magnetic two-dimensional monolayers

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Table S1 The 56 magnetic 2D monolayers that are theoretically predicted.

	Ferromagnetic	Antiferromagnetic
Metals	$Co(OH)_2$, CoO_2, ErHCl, ErSeI, EuOBr, EuOI, $FeBr_2$, FeI_2, FeTe, LaCl, NdOBr, PrOBr, ScCl, SmOBr, SmSI, TbBr, TmI_2, TmOI, VS_2, VSe_2, VTe_2, YCl, YbOBr, YbOCl	CoI_2, $CrSe_2$, FeO_2, FeOCl, FeSe, PrOI, VOBr
Semiconductors	CdOCl, $CoBr_2$, $CoCl_2$, CrOBr, CrOCl, CrSBr, $CuCl_2$, ErSCl, HoSI, $LaBr_2$, $NiBr_2$, $NiCl_2$, NiI_2	$CrBr_2$, CrI_2, LaBr, $Mn(OH)_2$, $MnBr_2$, $MnCl_2$, MnI_2, VBr_2, VCl_2, VI_2, $VOBr_2$, $VOCl_2$

Table S2 The overpotential of 8 magnetic 2D monolayers without strain and under the biaxial tensile strains (ε_{xy}) that lead to the lowest overpotentials in OER.

Materials	η (V) / no strain	η (V) / ε_{xy}
CoO_2	0.684	0.372 / 4.0%
FeO_2	1.107	0.600 / 6.0%
FeSe	1.240	1.187 / 5.0%
FeTe	1.048	1.048 / 0.0%
VS_2	1.496	1.214 / 2.0%
VSe_2	0.863	0.796 / 5.0%
VTe_2	0.837	0.491 / 3.0%
$CrSe_2$	1.264	1.002 / 5.0%

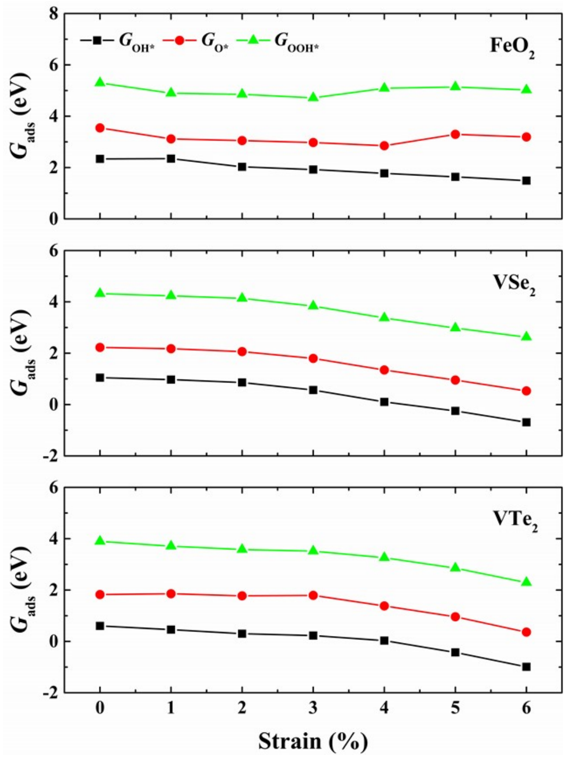

Fig. S1 The Gibbs free energies of adsorbed intermediates (OH*, O* and OOH*) on monolayer FeO_2, VSe_2 and VTe_2 under different biaxial tensile strains.

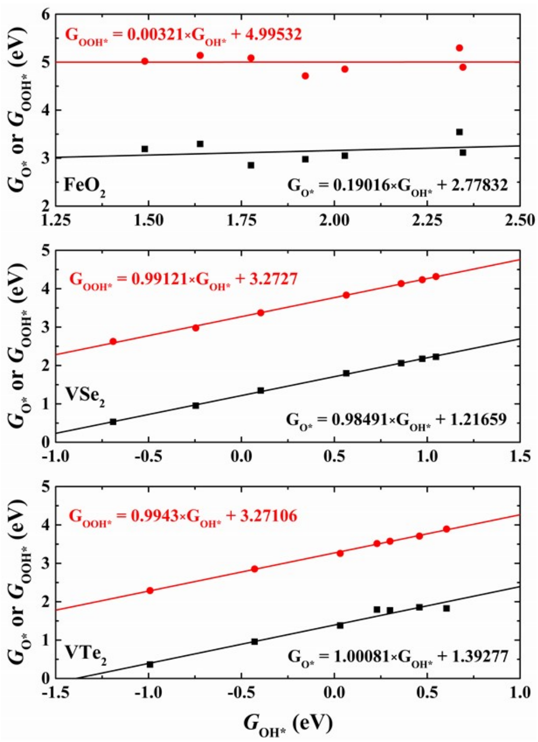

Fig. S2 The scaling relations between G_{OH*} and G_{O*} or G_{OOH*} for monolayer FeO_2, VSe_2 and VTe_2.

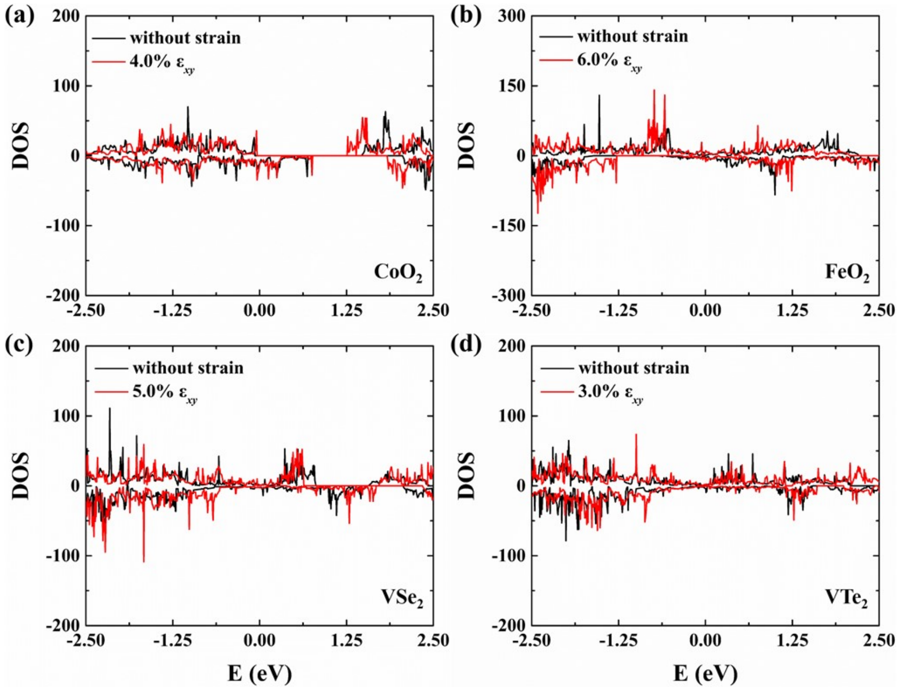

Fig. S3 The DOS of nonmetal atoms (O, Se and Te) for monolayer (a) CoO_2, (b) FeO_2, (c) VSe_2 and (d) VTe_2 without strain and under the biaxial tensile strains that lead to the lowest overpotentials. The Fermi level is set to zero.

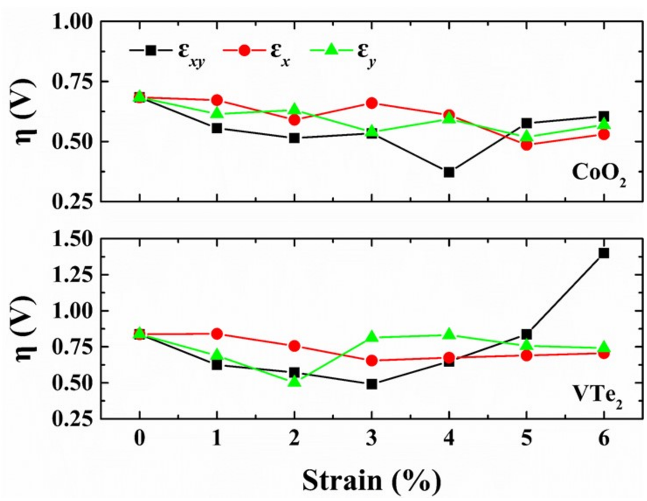

Fig. S4 The overpotentials of monolayer CoO_2 and VTe_2 under uniaxial and biaxial tensile strains.

Based on the same calculation setting, we have calculated the overpotentials of four magnetic 2D monolayers (CoO_2, FeO_2, VSe_2 and VTe_2) by using the PBE+U method. The U parameters adopted for Co, Fe and V atoms in our calculations are 3.3, 4.0 and 3.1 V [Phys. Rev. B 2006, 73, 195107], respectively.

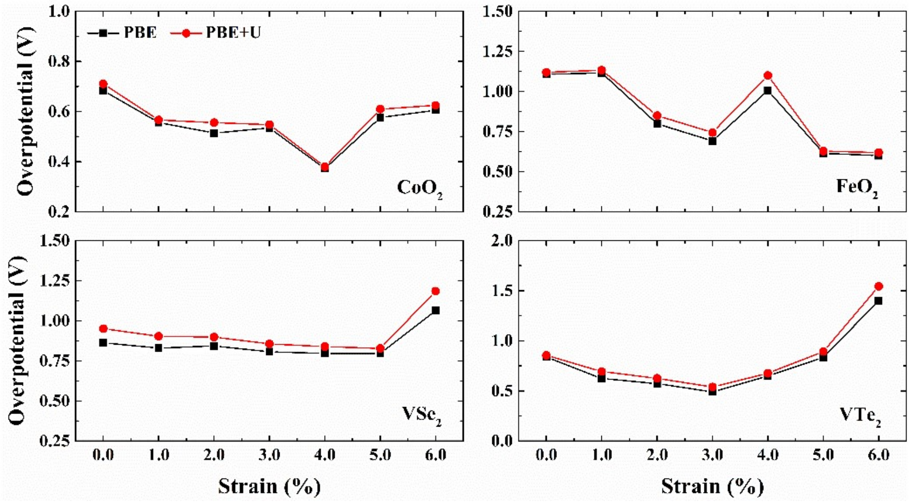

Fig. S5 The overpotentials of monolayer CoO_2, FeO_2, VSe_2 and VTe_2 under different biaxial tensile strains by using the PBE and PBE+U methods.

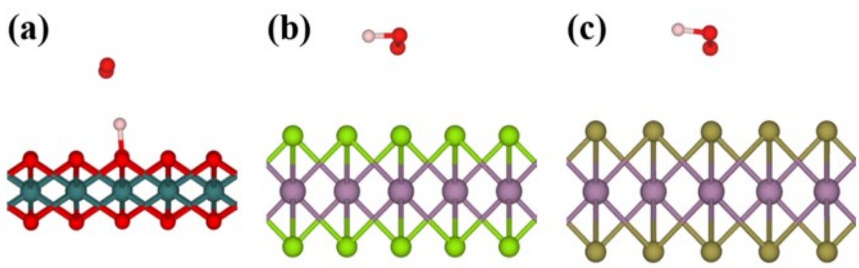

Fig. S6 The relaxed structures of OOH* intermediates on nonmagnetic (a) NiO_2, (b) $MoSe_2$, and (c) $MoTe_2$ monolayers without strain.

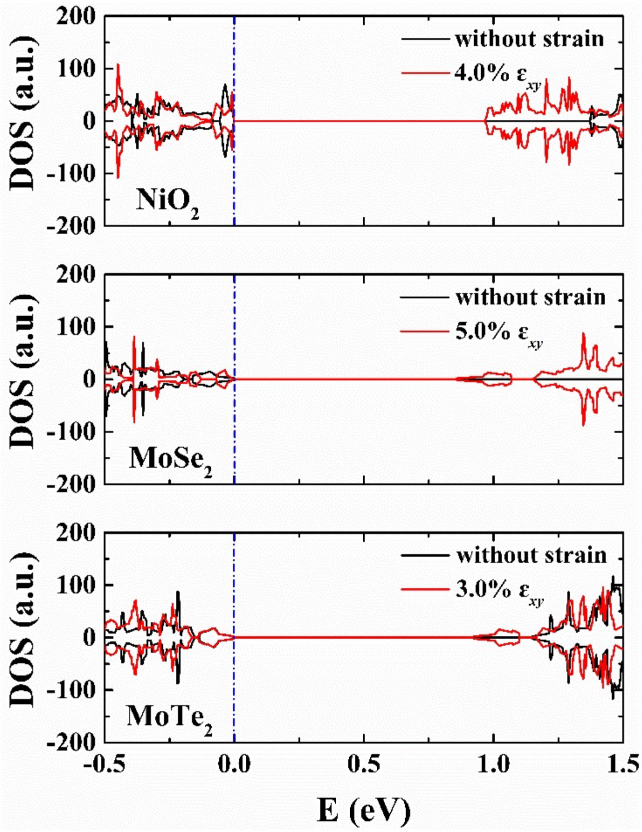

Fig. S7 The DOS (in units of a.u.) of spin-up (top) and spin-down (bottom) for the metal atoms (Ni and Mo) of nonmagnetic 2D monolayers with and without strain.

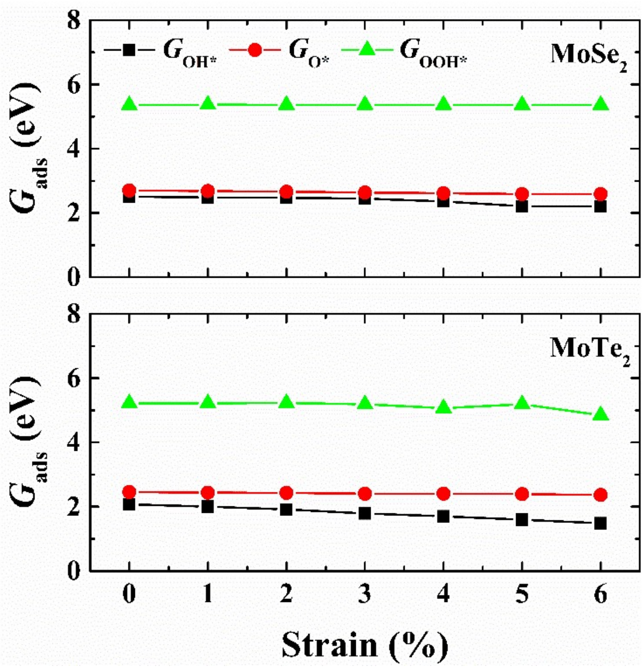

Fig. S8 The Gibbs free energies of the intermediates (OH*, O* and OOH*) on monolayer $MoSe_2$ and $MoTe_2$ under different biaxial tensile strains.