Electronic Supplementary Information

The mechanism of enhanced photocatalytic activity for water-splitting of ReS_2 by strain and electric field engineering

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The band structures of the x-axial and z-axial strained ReS_2

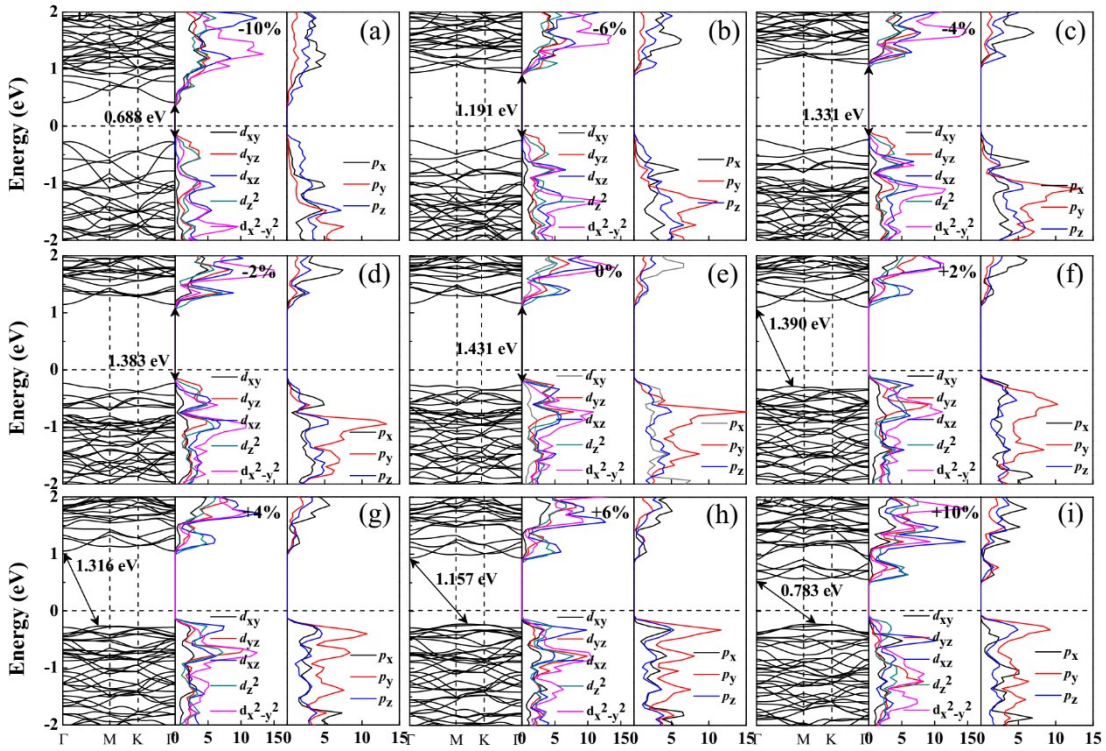

Fig. S1. Band structure and PDOS of ML-ReS_2 at *z*-axial strains of (a) −10%, (b) −6%, (c) −4%, (d) −2%, (e) 0%, (f) 2%, (g) 4%, (h) 6% and (i) 10%.

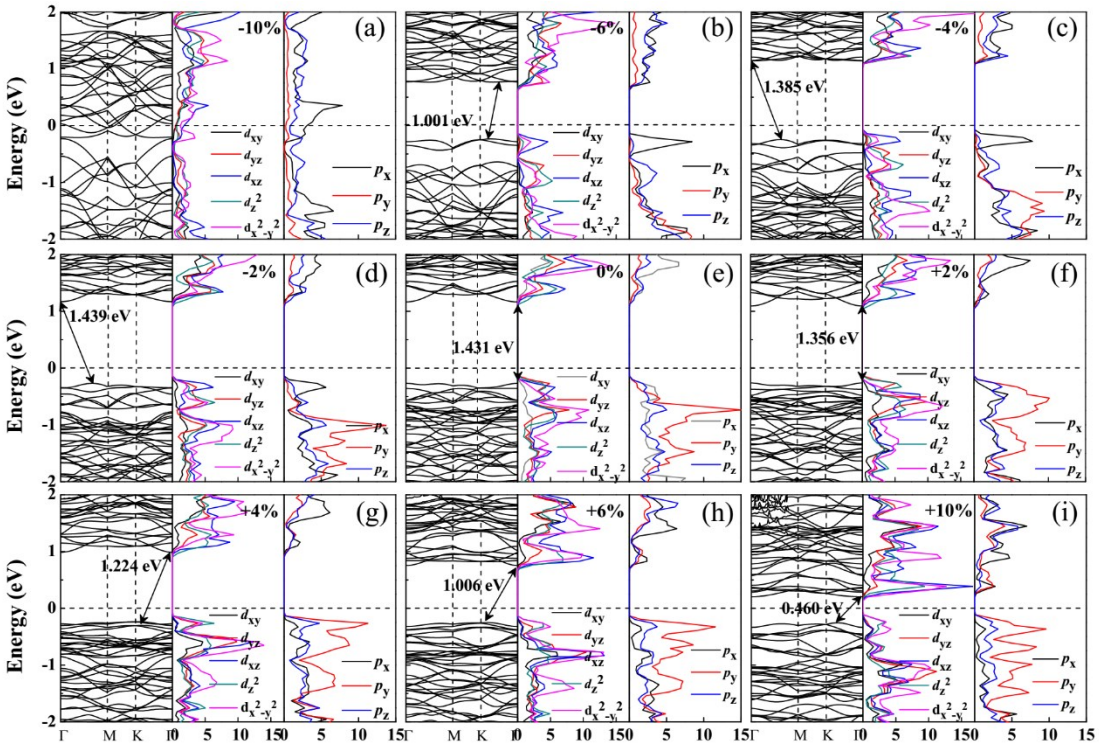

Fig. S2. Band structure and PDOS of ML-ReS_2 at bi-axial strains of (a) −10%, (b) −6%, (c) −4%, (d) −2%, (e) 0%, (f) 2%, (g) 4%, (h) 6% and (i) 10% .

The band edge of uniaxial strained ReS_2

Table S1 The induced dipole density $\mu_\perp/A$ (in D nm^{-2}), change in work function $\Delta W_\perp$ (in eV), band gap E_g (in eV), and VBM and CBM positions E_{VBM} and E_{CBM} (in eV) of ReS_2 at different strain fields.

strain	$\mu_\perp/A$	$\Delta W_\perp$	E_g	E_{VBM}	E_{CBM}
-10%	-0.005	-0.049	0.202	-4.535	-4.327
-8%	-0.007	-0.157	0.658	-4.877	-4.219
-6%	-0.008	-0.210	1.030	-5.196	-4.166
-4%	-0.004	-0.151	1.255	-5.480	-4.225
-2%	-0.007	-0.072	1.389	-5.693	-4.304

x- axial	0	-	-	1.431	-5.807	-4.376
	2%	0.021	0.076	1.318	-5.769	-4.452
	4%	0.004	0.139	1.210	-5.725	-4.515
	6%	0.005	0.223	1.089	-5.687	-4.599
	8%	0.013	0.466	0.808	-5.649	-4.842
	10%	0.010	0.701	0.540	-5.616	-5.077
	-10%	-0.006	-0.047	0.688	-5.017	-4.330
	-8%	-0.005	-0.145	0.951	-5.182	-4.231
	-6%	-0.006	-0.223	1.191	-5.344	-4.153
	-4%	-0.007	-0.200	1.331	-5.506	-4.176
	-2%	-0.004	-0.096	1.383	-5.663	-4.280
z-axial	0	-	-	1.431	-5.807	-4.376
	2%	0.006	0.104	1.390	-5.871	-4.480
	4%	0.008	0.204	1.316	-5.896	-4.580
	6%	0.018	0.306	1.157	-5.839	-4.682
	8%	0.019	0.399	0.973	-5.747	-4.775
	10%	0.006	0.477	0.783	-5.636	-4.854
	-10%	-	-	metal	-	-
	-8%	-0.001	-0.240	0.452	-4.588	-4.136
	-6%	-0.007	-0.356	1.001	-5.021	-4.020
	-4%	-0.006	-0.382	1.385	-5.379	-3.994
	-2%	-0.003	-0.183	1.439	-5.631	-4.193
bi-axial	0	-	-	1.431	-5.807	-4.376
	2%	0.007	0.164	1.356	-5.896	-4.540
	4%	0.007	0.299	1.224	-5.899	-4.675
	6%	0.003	0.409	1.006	-5.791	-4.785
	8%	0.005	0.499	0.785	-5.660	-4.875

10%	0.009	0.676	0.460	-5.512	-5.052