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Supplementary Information

Two-Dimensional Janus PtSSe for Photocatalytic Water Splitting under Visible or Infrared Light Spectrum

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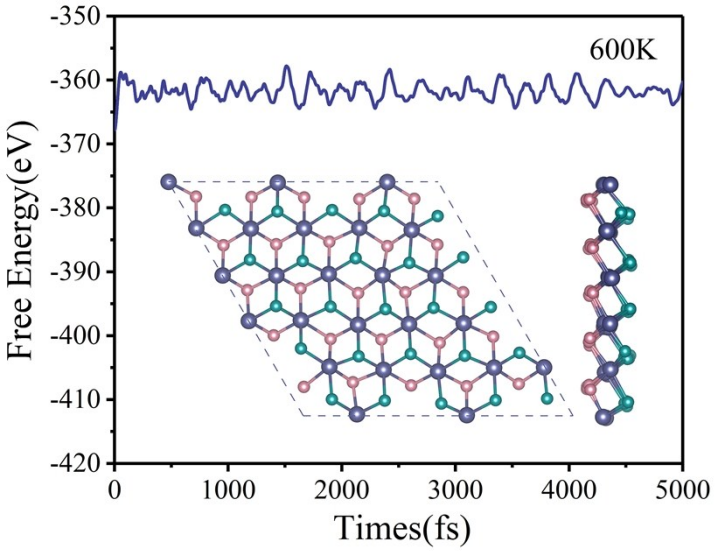

Fig. S1 Variations of total energy of SL PtSSe at 600 K during AIMD simulations. Inset shows snapshots of the equilibrium structure of SL PtSSe at 600 K.

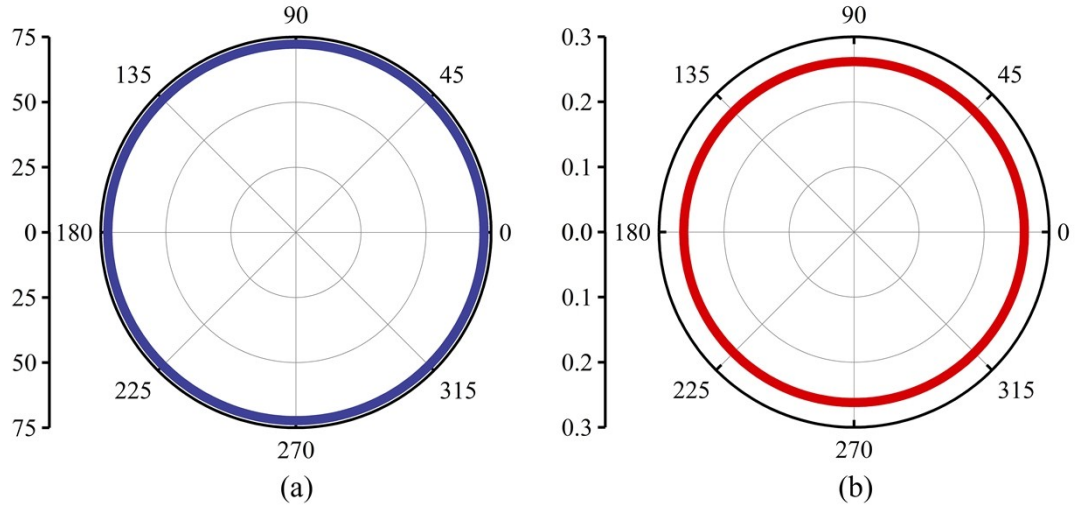

Fig. S2 Young's modulus and Possion's ratio of SL PtSSe as a function of the angle θ.

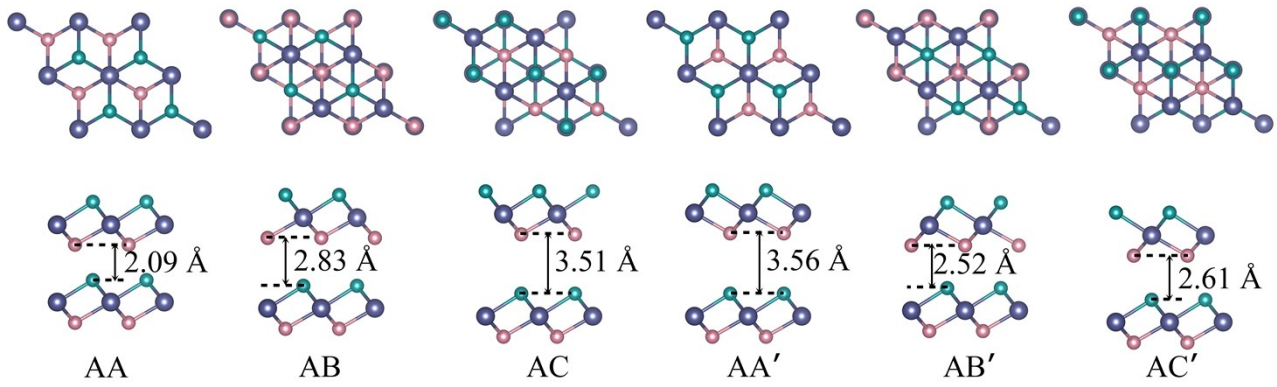

Fig. S3 Optimized crystal structures of DL PtSSe.

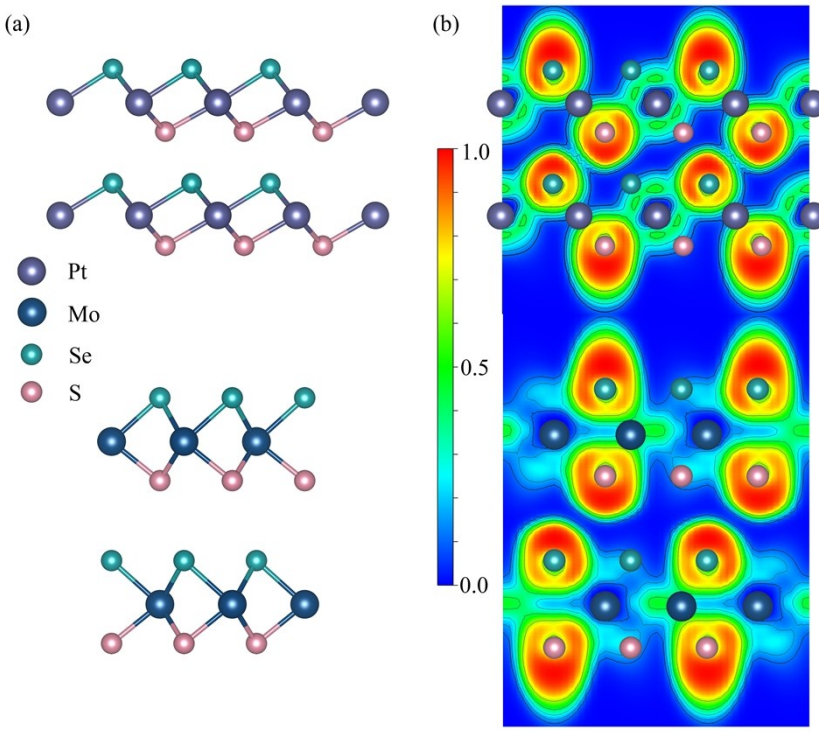

Fig. S4 (a) Crystal structure and (b) ELF of DL PtSSe (with AA stacking) and DL MoSSe.

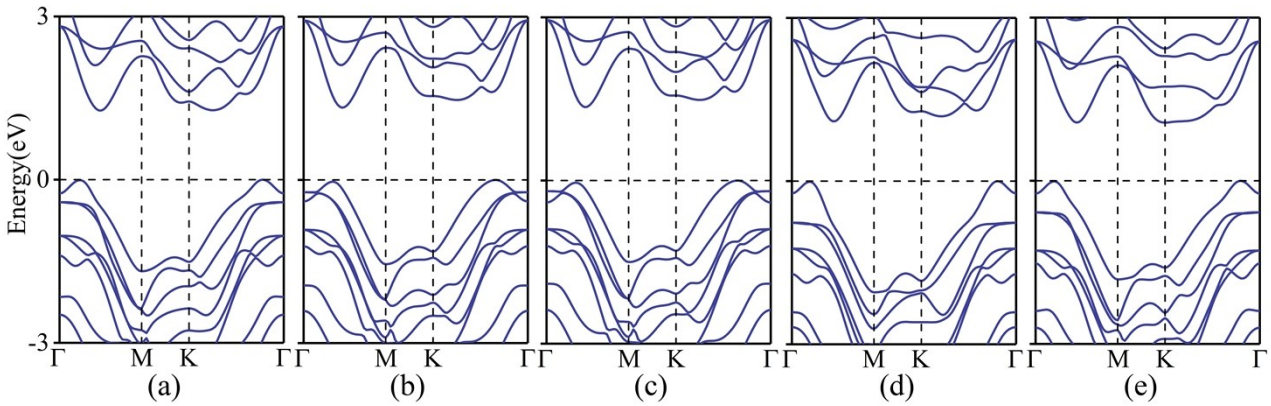

Fig. S5 Band structures of DL PtSSe with AB, AC, AA′, AB′ and AC′ stacking for (a), (b), (c), (d) and (e), respectively. The Fermi level is set to zero.

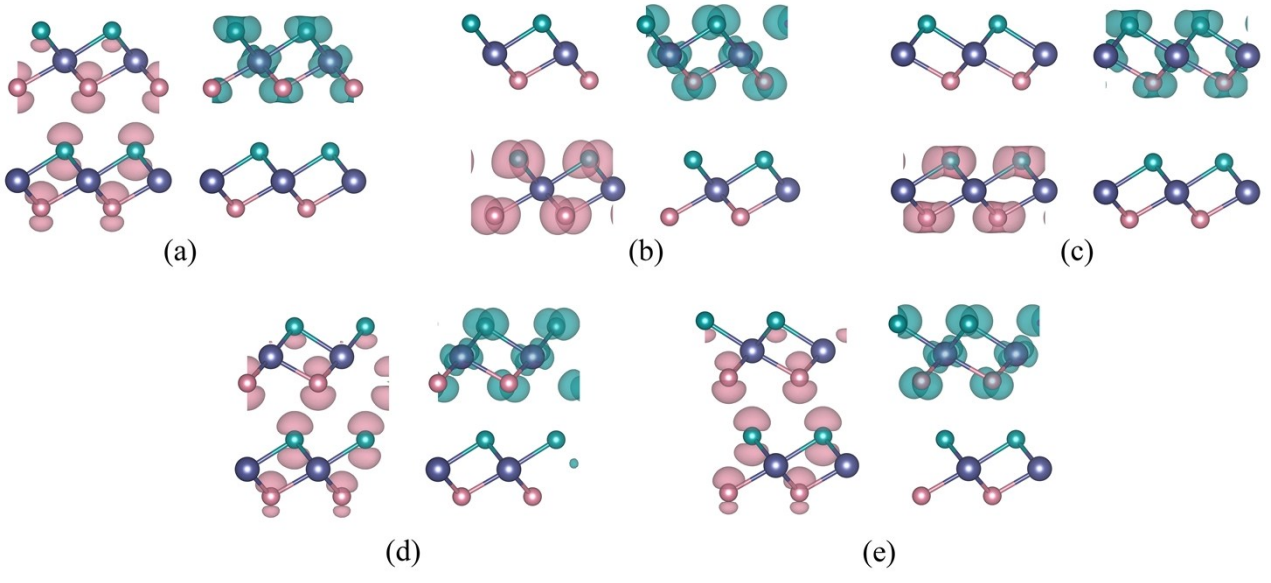

Fig. S6 Charge density of VBM (pink) and CBM (green) of DL PtSSe with AB, AC, AA′, AB′ and

AC′ stacking for (a), (b), (c), (d) and (e), respectively. The value of isosurfaces is 0.07 Bohr^{-3}.

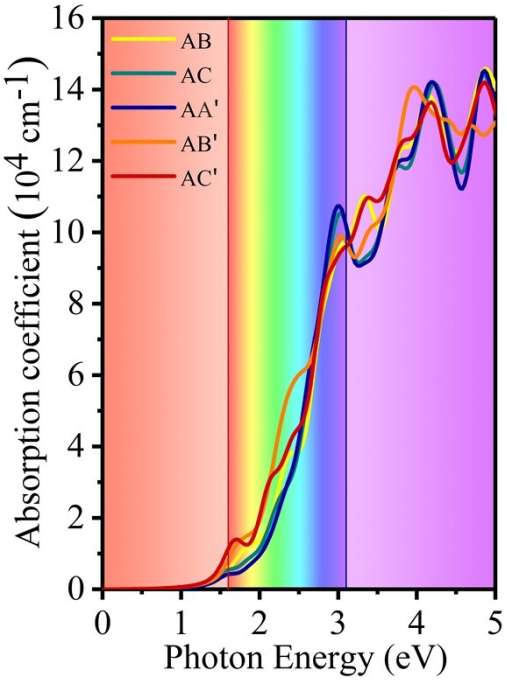

Fig. S7 Optical absorption coefficients of DL PtSSe with with AB, AC, AA′, AB′ and AC′ stacking. The scale of visible light region (1.6~3.1 eV) is in iridescent color.

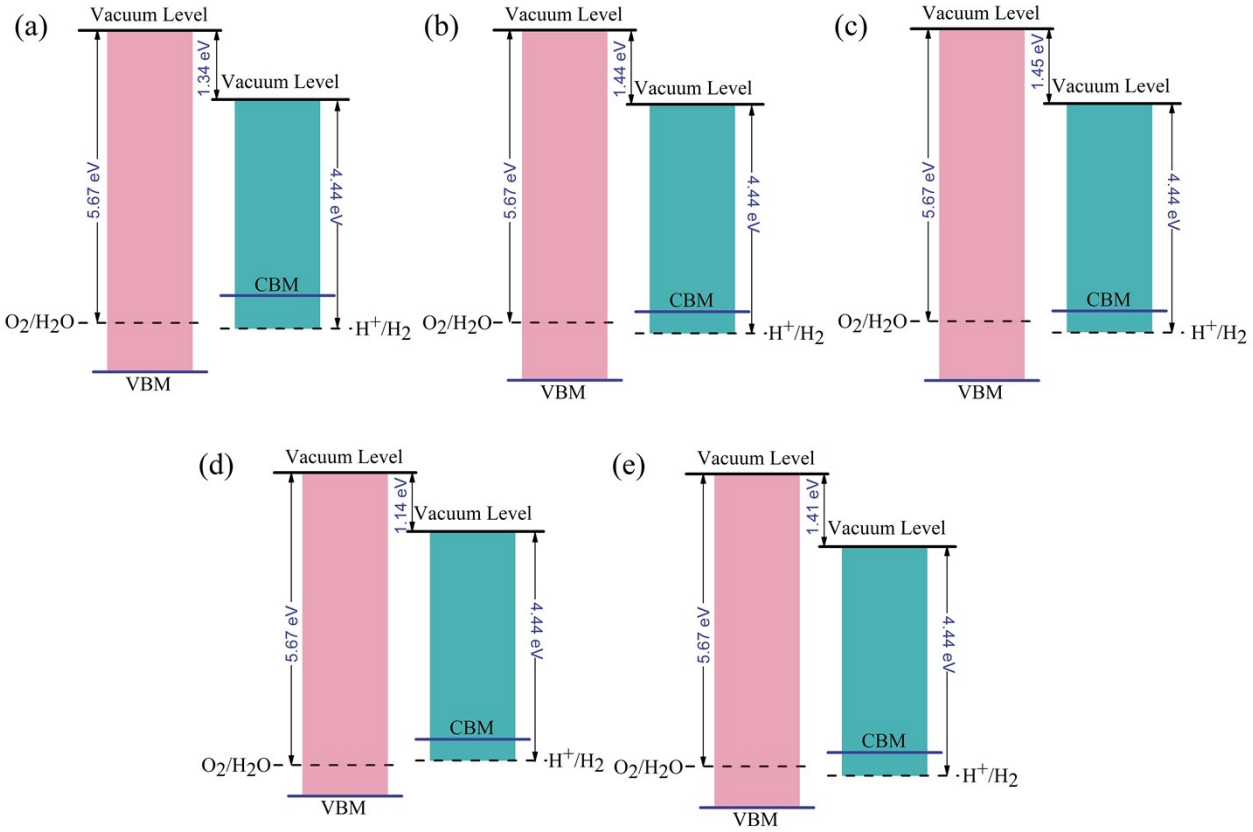

Fig. S8 Band edge alignment with regard to the water redox potentials of DL PtSSe with AB, AC, AA′, AB′ and AC′ stacking for (a), (b), (c), (d) and (e), respectively. The dashed lines indicate the reduction and oxidation potentials of water. The static potential difference is marked in blue.

Table S1 Band gap E_g (eV), electrostatic potential difference $\Delta\Phi$ (eV), energy difference between VBM and the oxidation potential of water ΔE_V (eV), energy difference between CBM and the reduction potential of water ΔE_C (eV) for strained SL PtSSe.

strain	E_g (eV)	$\Delta\Phi$ (eV)	ΔE_V (eV)	ΔE_C (eV)
4%	1.81	0.76	1.14	0.19
2%	2.01	0.76	1.22	0.32
0%	2.19	0.76	1.28	0.44
-2%	2.18	0.76	1.17	0.56
-4%	2.06	0.76	0.95	0.64

Table S2 Interlayer distance d (Å), binding energy E_b (eV), band gap E_g (eV), electrostatic potential difference $\Delta\Phi$ (eV), energy difference between VBM and the oxidation potential of water ΔE_V (eV), energy difference between CBM and the reduction potential of water ΔE_C (eV) for DL PtSSe.

pattern	d (Å)	E_b (eV)	E_g (eV)	$\Delta\Phi$ (eV)	ΔE_V (eV)	ΔE_C (eV)
AA	2.09	2.65	0.65	1.21	0.35	0.28
AB	2.83	2.48	1.27	1.34	0.95	0.64
AC	3.51	2.32	1.33	1.44	1.12	0.42
AA’	3.56	2.32	1.35	1.45	1.15	0.42
AB’	2.52	2.55	1.10	1.14	0.60	0.41
AC’	2.61	2.53	1.07	1.41	0.80	0.45