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Supporting Information

Janus MoSSe monolayer: A potential wide solar-spectrum water-splitting photocatalyst with low carrier recombination rate

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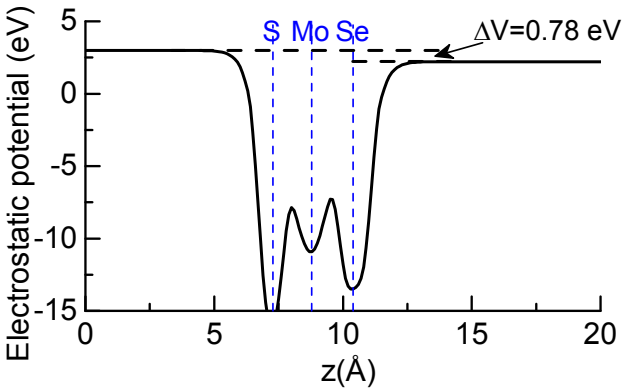


Figure S1. Local electrostatic potential versus atomic layers for pristine MoSSe monolayer.

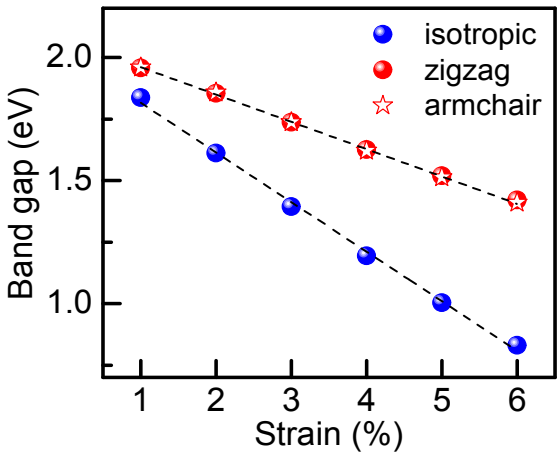
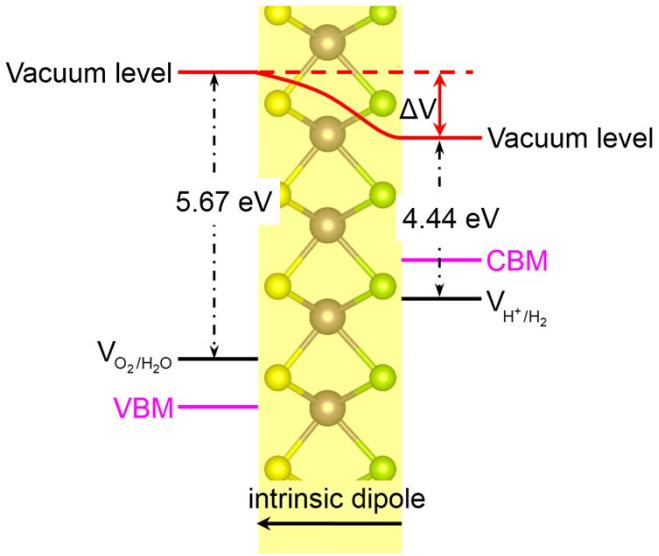


Figure S2. Band gap of MoSSe monolayer as a function of the applied strains. The black dashed lines are linear fitting to the data.



Scheme S1. Schematic plot of energy levels for MoSSe monolayer. ΔV denotes the potential difference between the two sides of MoSSe that is induced by its intrinsic dipole.

Table S1. Calculated elastic modulus C_α, effective masses of carriers in the unit of free-electron mass, and the deformation potential E_α^y for the pristine MoSSe.

	m_x^*	m_y^*	C_x [J/m^2]	C_y [J/m^2]	E_d^x [eV]	E_d^y [eV]
electrons	0.57	0.57	102.54	99.99	8.22	8.43
holes	4.65	4.64	102.54	99.99	3.06	3.09