Supporting Information

MoSSe nanotube: A promising photocatalyst with extremely long carrier lifetime

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Table S1. Detailed informations of Janus MoSSe monolayer and nanotube.

Structure	Mo-S (Å)	Mo-Se (Å)	S-Se (Å)	Band gap (eV)	Carrier lifetime (ns)
Monolayer	2.42	2.53	3.23	1.58	0.44[1]
Nanotube	2.38/2.40	2.56/2.58	3.21	1.48	33

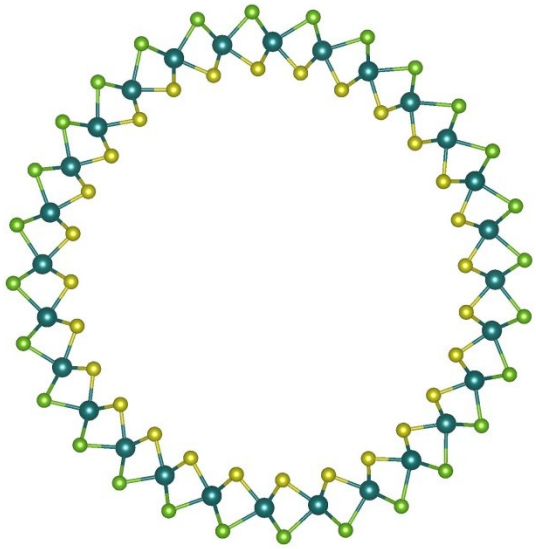

Figure S1. Snapshots of the equilibrium structure of Janus MoSSe nanotube at 300 K.

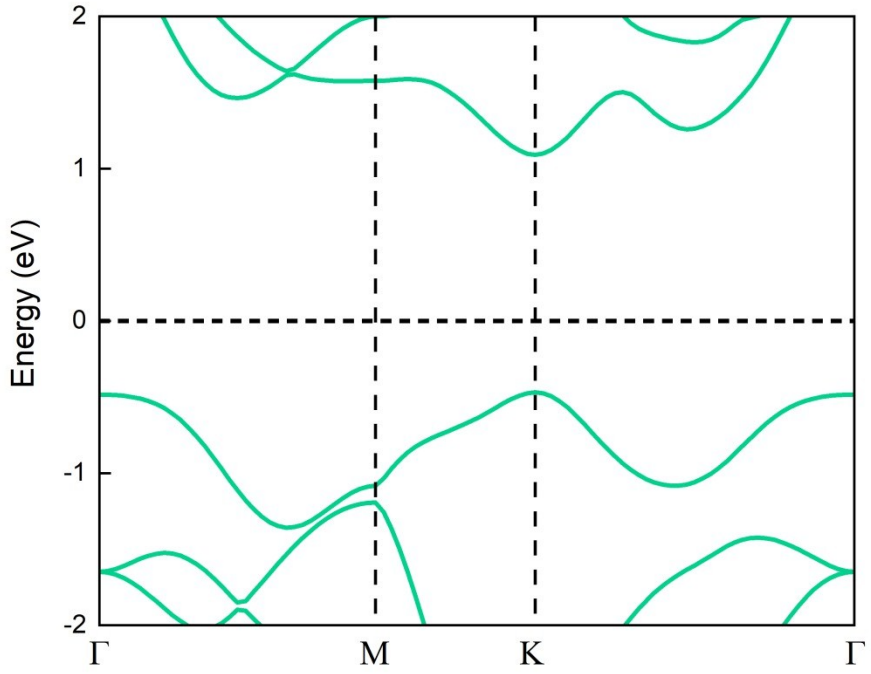

Figure S2. Band structure of MoSSe monolayer.

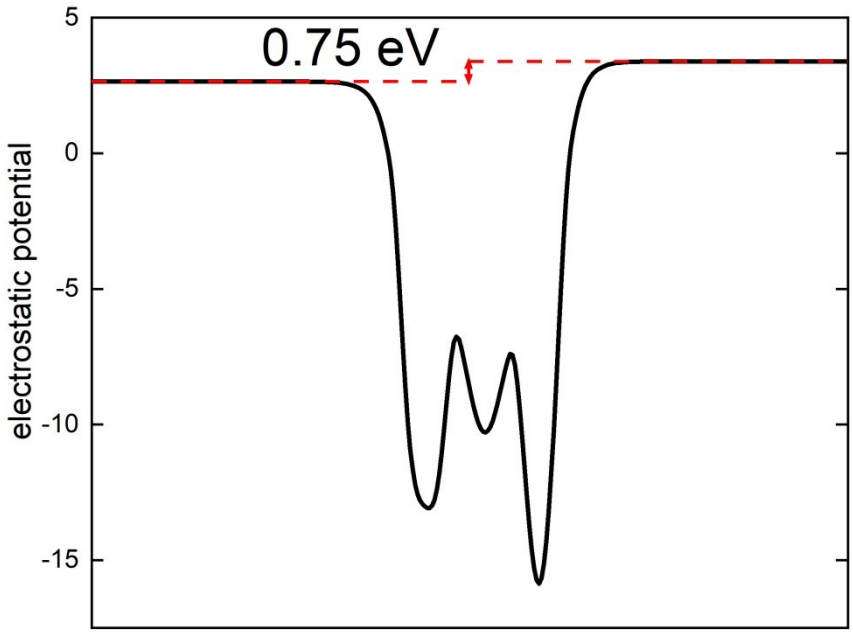

Figure S3. Electrostatic potential of monolayer MoSSe.

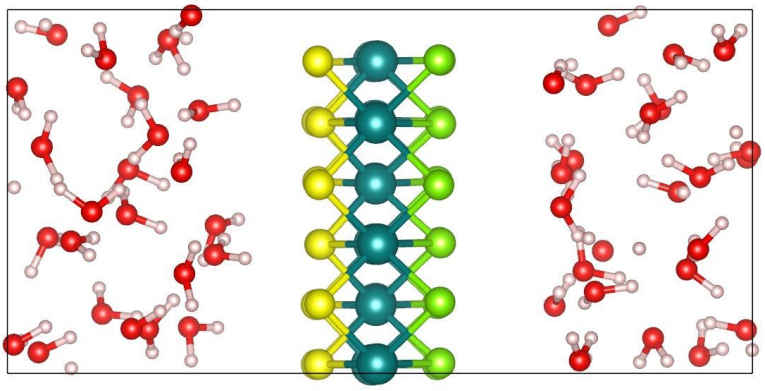

Figure S4. Structure of water/MoSSe monolayer.

A system including 48 H_2O molecules and 12 MoSSe units is constructed to simulate the water/photocatalyst model. Here we perform a MD computation for 3ps at 300K and take final snapshots of the atomic configurations for the following DFT calculations. The geometric structure is shown in Figure S4. The same simulations for MoS_2 and $MoSe_2$ are also performed for comparison. In Figure S5(a), the red and blue lines represent the projected DOS of water on the S surface and Se surface, respectively.

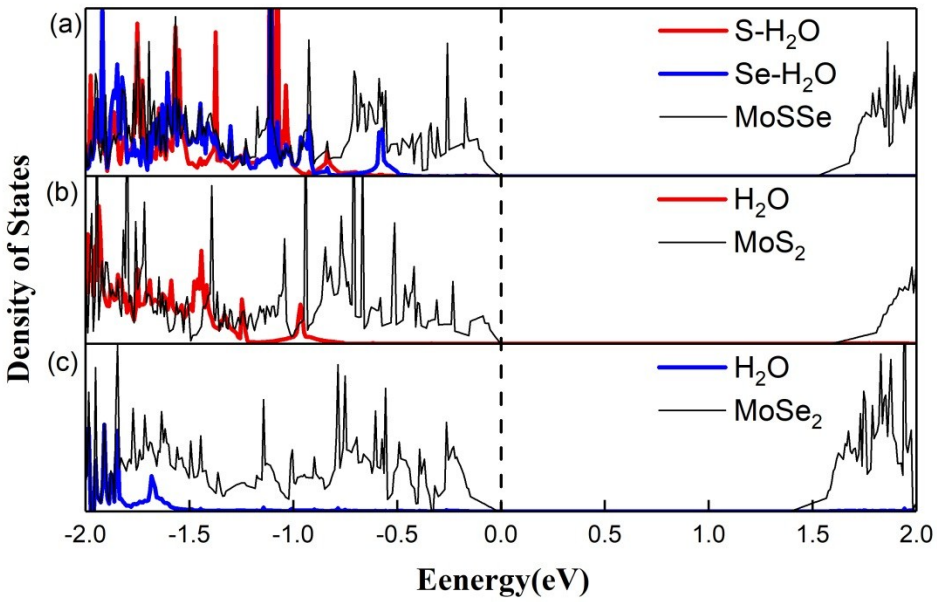

Figure S5. PDOS of (a) water/MoSSe, (b) water/MoS_2 and (c) water/$MoSe_2$. The dash line represents the Fermi level.

Reference

1 H. Jin, T. Wang, Z.-R. Gong, C. Long and Y. Dai, *Nanoscale*, 2018, **10**, 19310–19315.