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Supplementary Materials

First principles study of strain effects on prospective 2D photocatalysts $Sn_2Se_2X_4$ (X = P, As) with ultra-high charge carrier mobility

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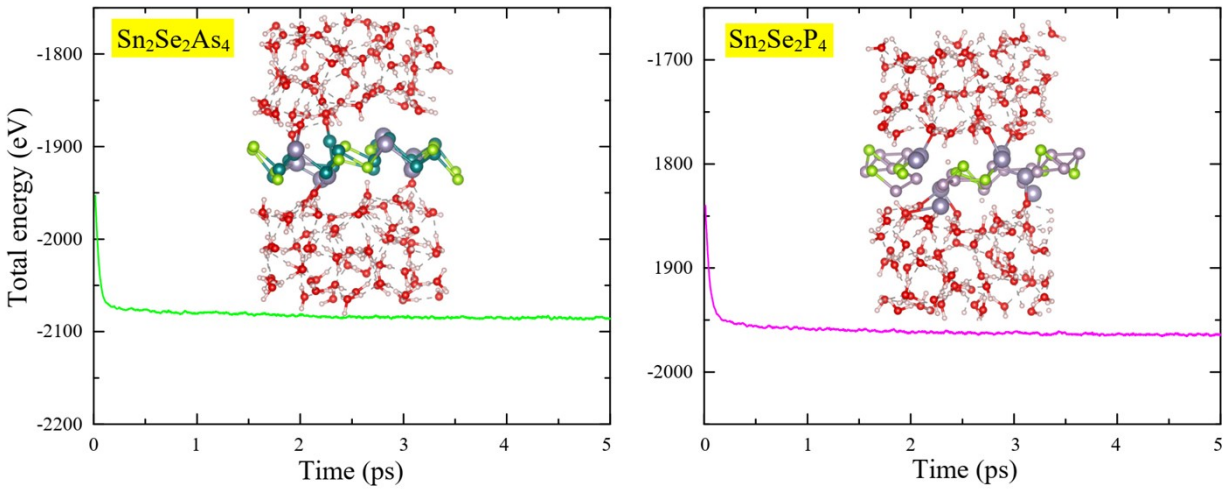

Figure S1. The AIMD energy fluctuations and the snapshot of equilibrium structure of $Sn_2Se_2X_4$ (X = P, As) monolayer in liquid water after annealing at 300 K for 5 ps.

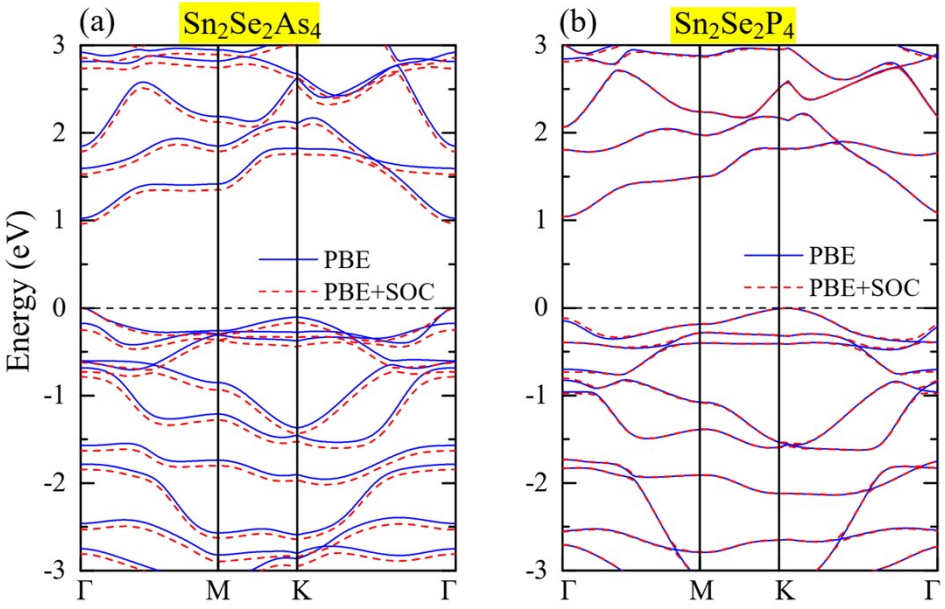

Figure S2. The calculated electronic band structure of the $Sn_2Se_2X_4$ (X = P, As) monolayers with spin-orbital coupling (SOC) (dash red curves), and without SOC (green) extracted from PBE functional.

Table S1. The calculated band gaps E_g^{HSE06} (eV) and the positions of the VBM and CBM of $Sn_2Se_2X_4$ (X = P, As) monolayers.

	$Sn_2Se_2As_4$			$Sn_2Se_2P_4$		
Strains	E_g^{HSE06}	VBM	CBM	E_g^{HSE06}	VBM	CBM
-8%	1.405	-5.891	-4.486	1.231	-5.653	-4.422
-6%	1.538	-5.957	-4.420	1.358	-5.717	-4.358
-4%	1.655	-6.016	-4.361	1.468	-5.771	-4.303
-2%	1.758	-6.067	-4.310	1.556	-5.815	-4.259
0%	1.716	-6.046	-4.330	1.633	-5.854	-4.221
2%	1.659	-6.018	-4.359	1.701	-5.888	-4.187
4%	1.613	-5.995	-4.382	1.655	-5.865	-4.210
6%	1.574	-5.975	-4.402	1.604	-5.839	-4.235
8%	1.538	-5.957	-4.420	1.552	-5.813	-4.261