

Photocatalytic Water Splitting for Hydrogen Production with High Efficiency of Monolayer In₂Te₅: A Theoretical Study

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Table S1 Bader charge transfer from In to each Te atom (unit: *e*).

	Te1	Te2	Te3	Te4	Te5	Te6	Te7	Te8	Te9	Te10
In1	0.274			0.274		0.274				
In2		0.274	0.274					0.274		
In3		0.274			0.274			0.274		
In4				0.274		0.274	0.274			

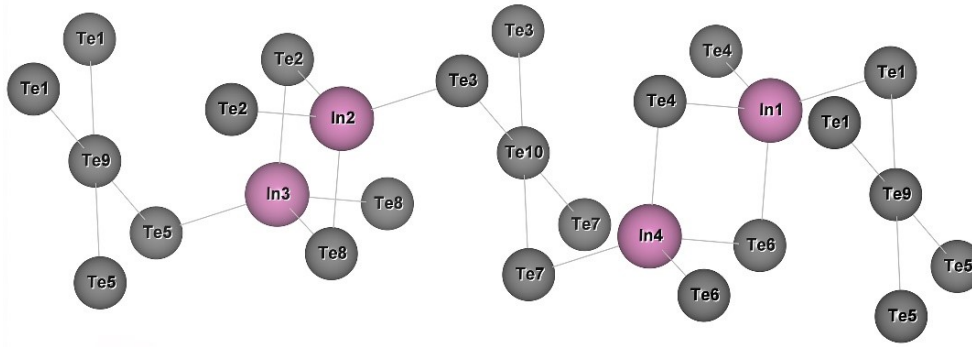


Fig. S1 The ML In_2Te_5 corresponding to Table S1.

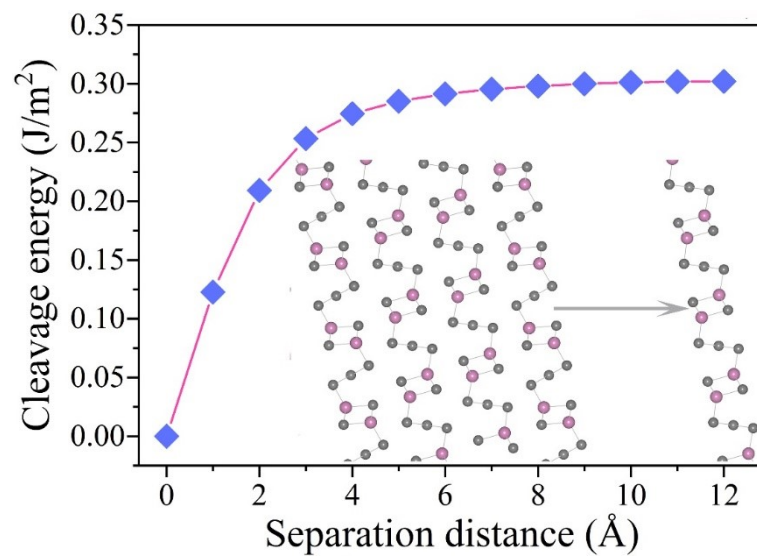


Fig. S2 The calculated cleavage energy varies with separation distance of the ML In_2Te_5 .

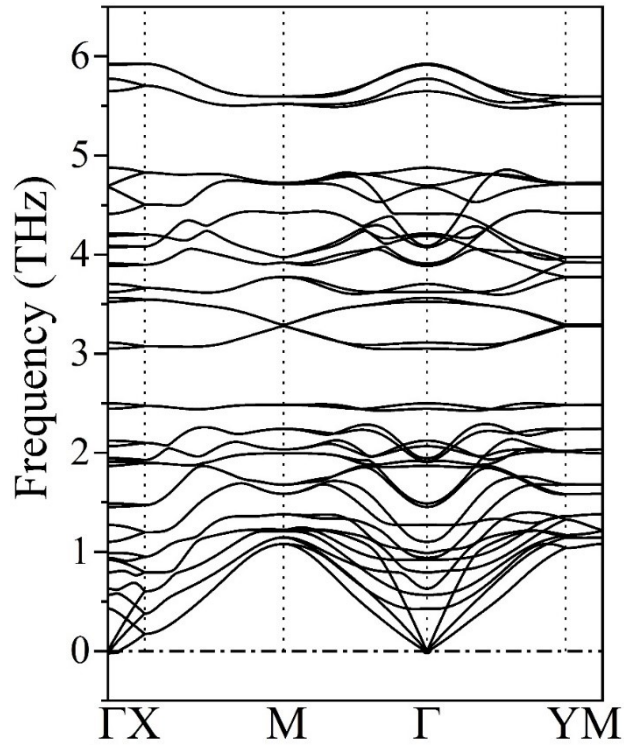


Fig. S3 The calculated phonon spectrum of the ML In_2Te_5 .

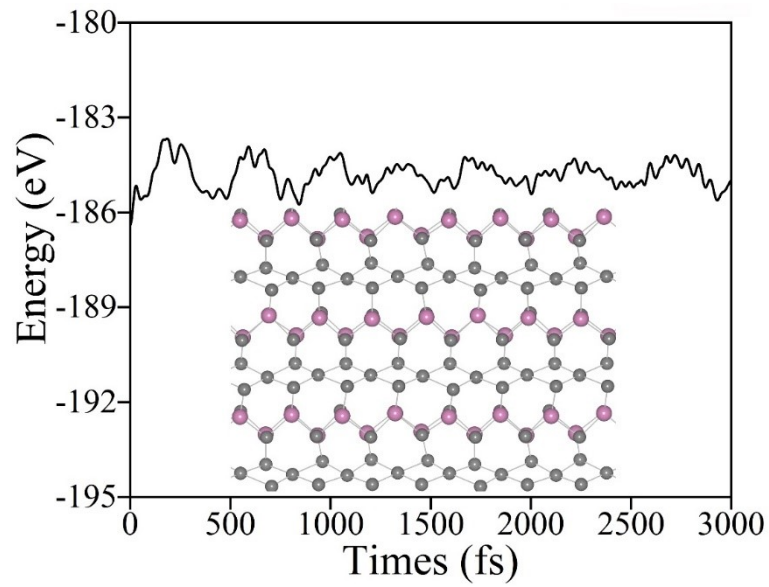


Fig. S4 The time-dependent evolution of total energy for the ML In_2Te_5 .

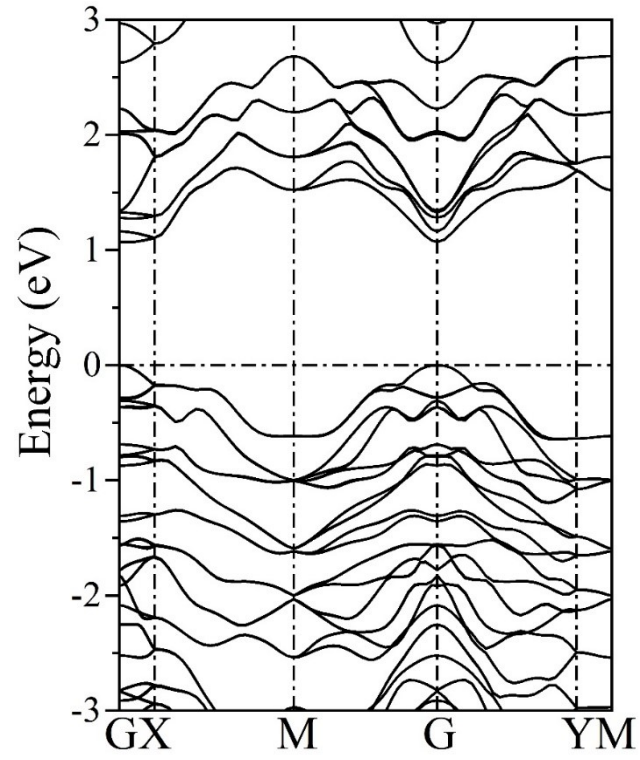


Fig. S5 The calculated band structure with SOC effect based on PBE functional of the ML In₂Te₅.