Supporting Information

Highly efficient and stable photoelectrochemical hydrogen evolution with 2D-NbS_2/Si nanowire heterojunction

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No. of Figures : 10

No. of Graphs : 07

No. of Tables : 02

Optimization of Growth:

Figure S1: a) FESEM image of NbS_2 on Si NW with 20 minutes growth time b) Magnified FESEM image of NbS_2 on Si with 20 minutes growth time

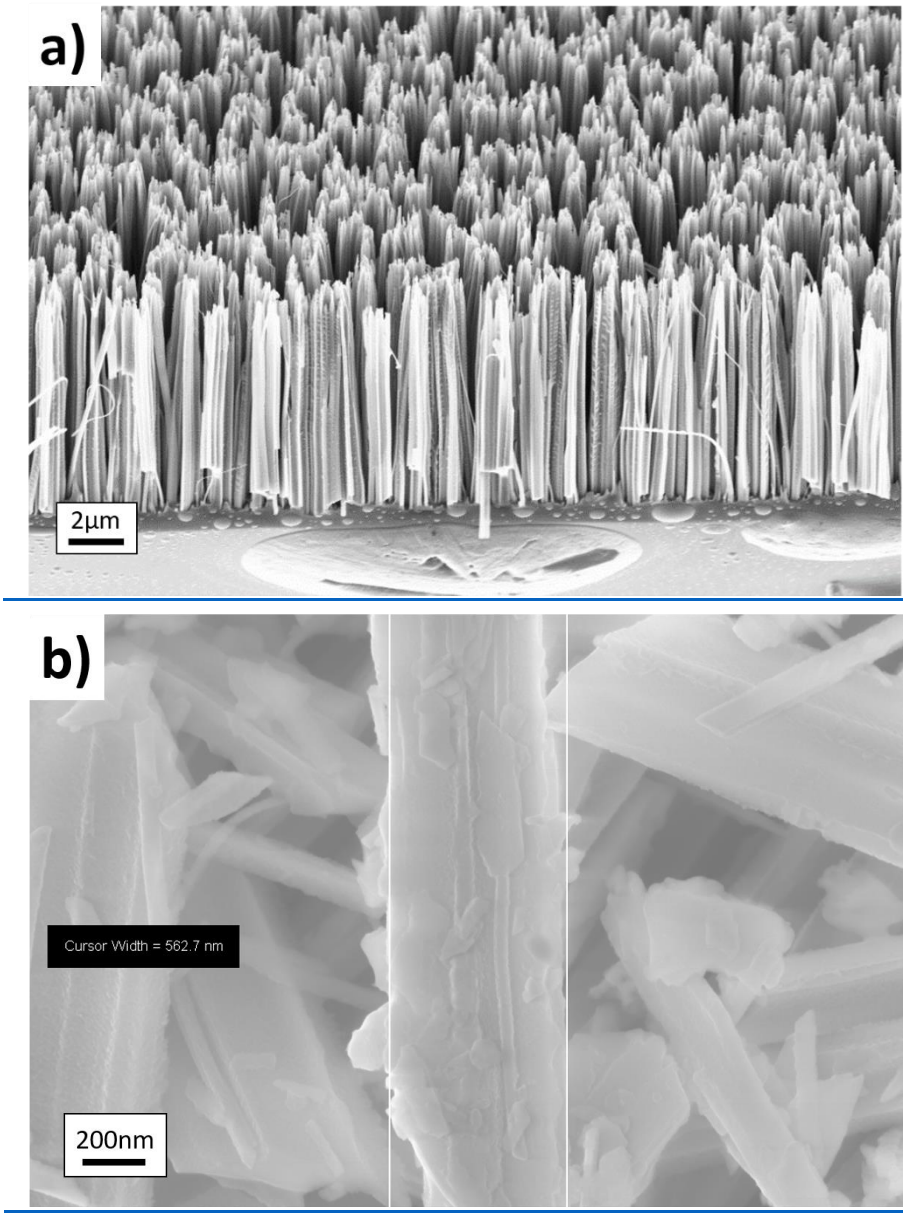
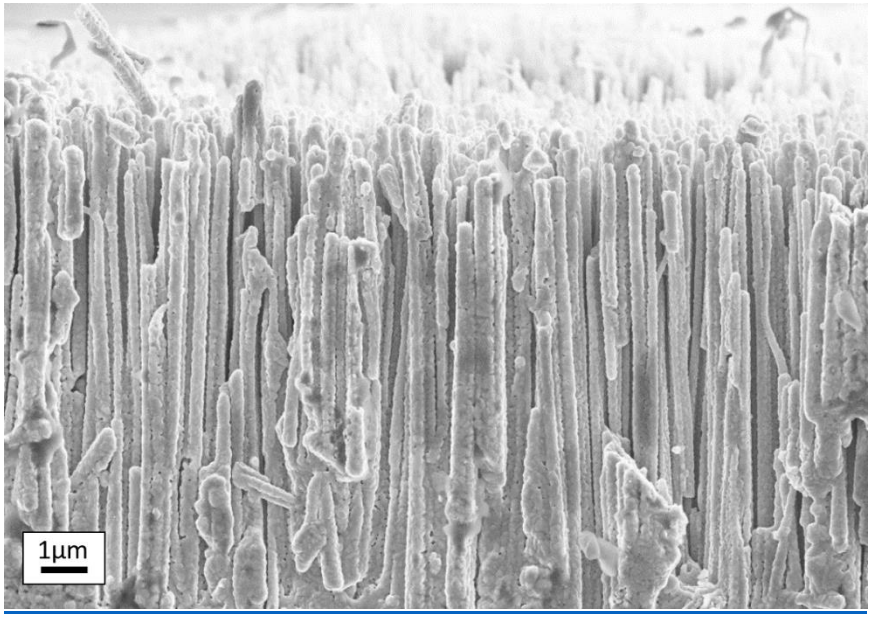


Figure S2 & S3: FESEM image of 40 minutes growth period of NbS_2 on Si NW



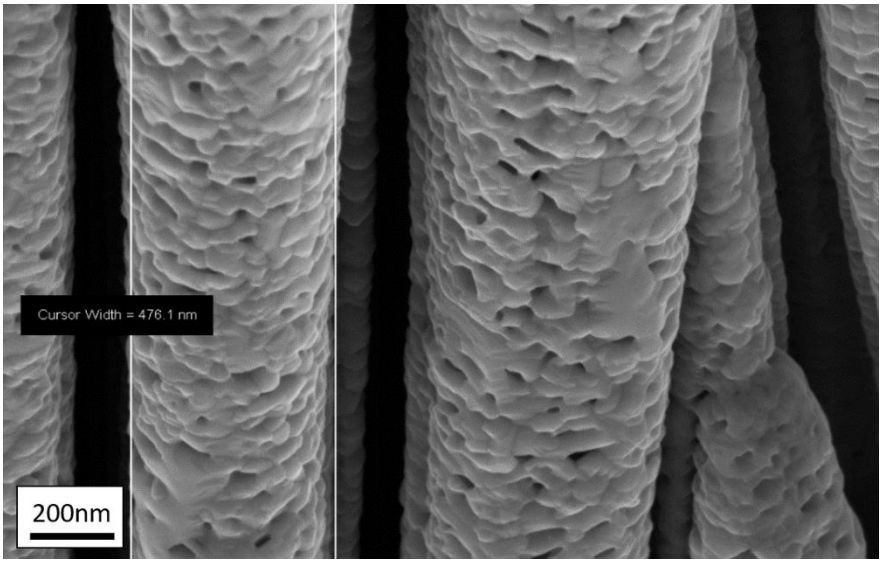


Figure S4: FESEM image of NbS_2 on Si NW with 60 minutes growth time

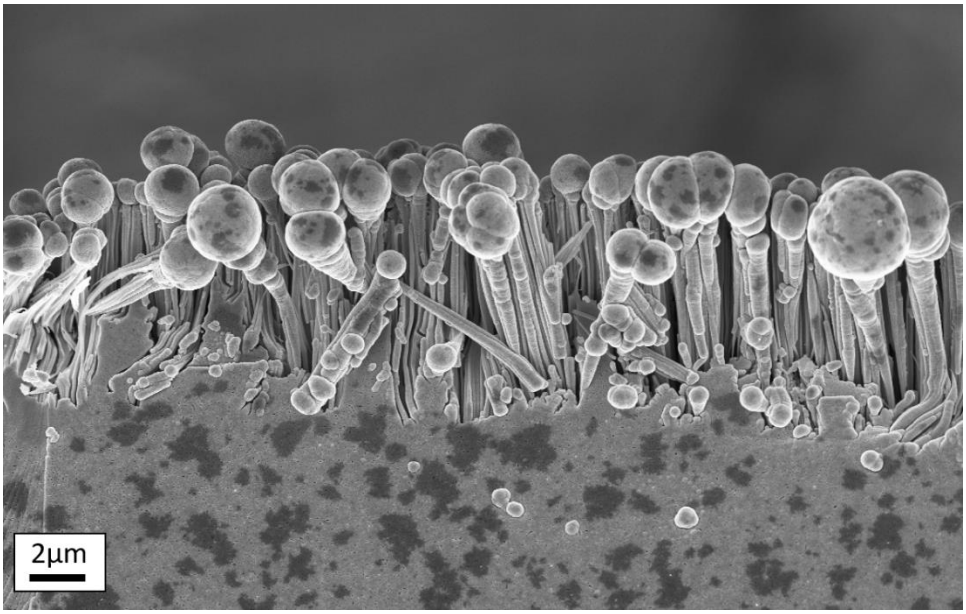


Figure S5: FESEM image of Si NWs

Figure S6: FESEM image of NbS_2 deposited on the Si NWs

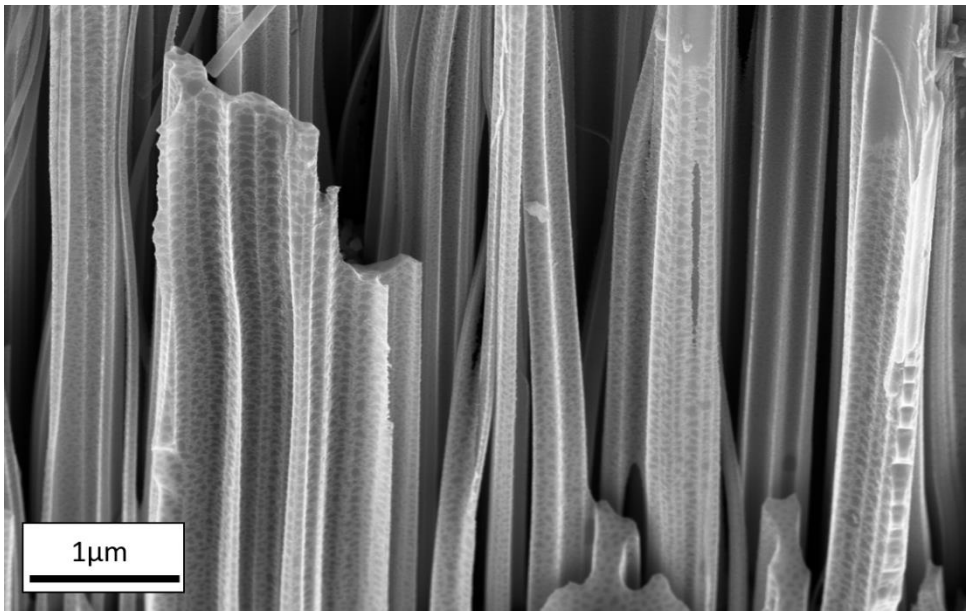


Figure S7: a) and b) corresponds to the AFM image of NbS_2 Nano patches grown in Si substrate.

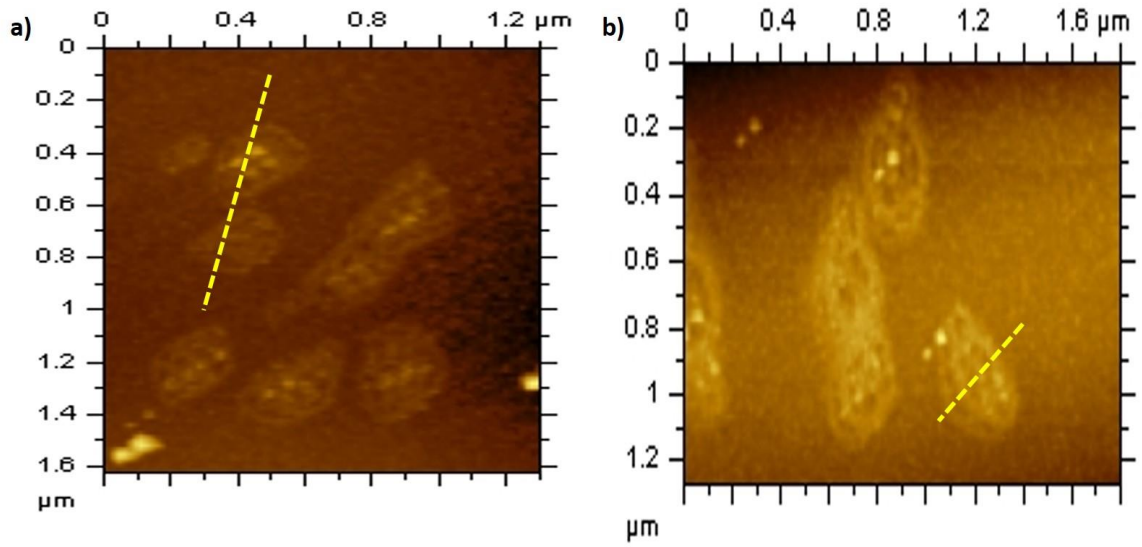


Figure S8: Height profile of NbS_2 grown on Si substrate a) corresponds to height profile of marked in figure S7 a and b) corresponds to the height profile marked in figure S7 b.

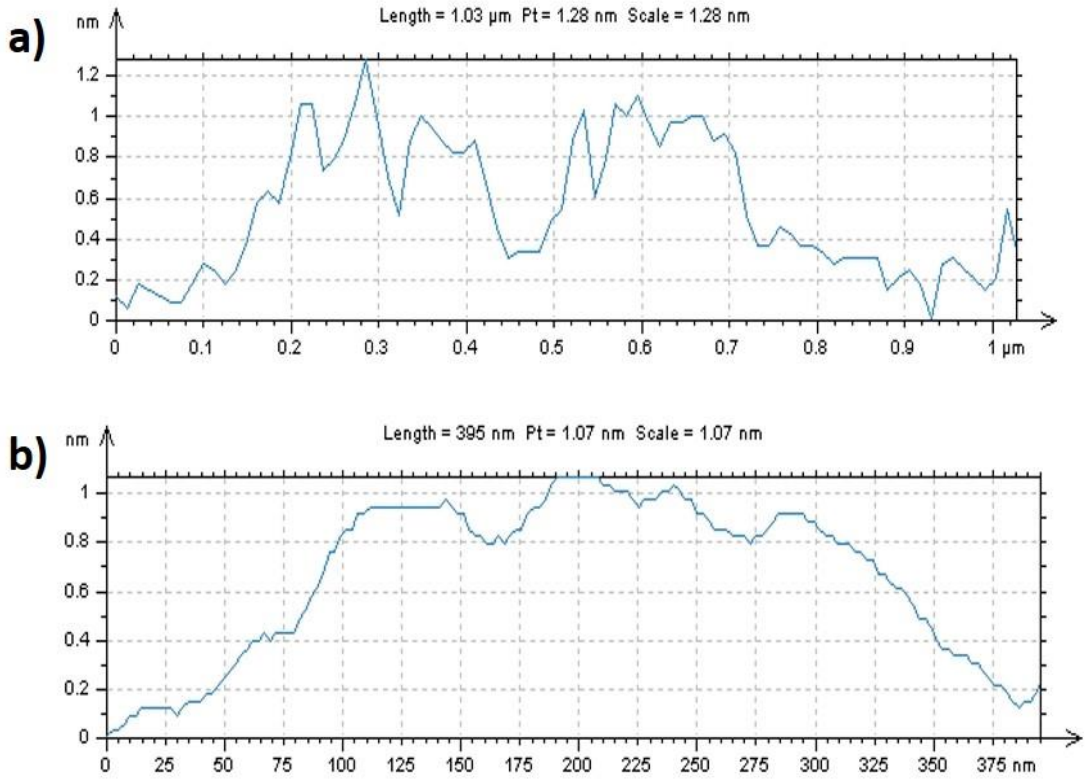


Figure S9: Survey spectrum of NbS_2 on Si NWs:

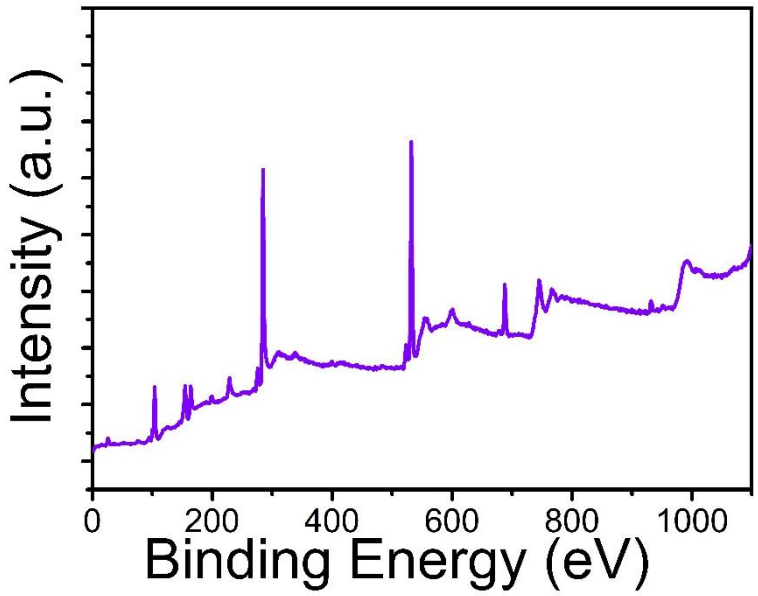


Figure S10: FESEM image of NbS_2 on n++ Si.

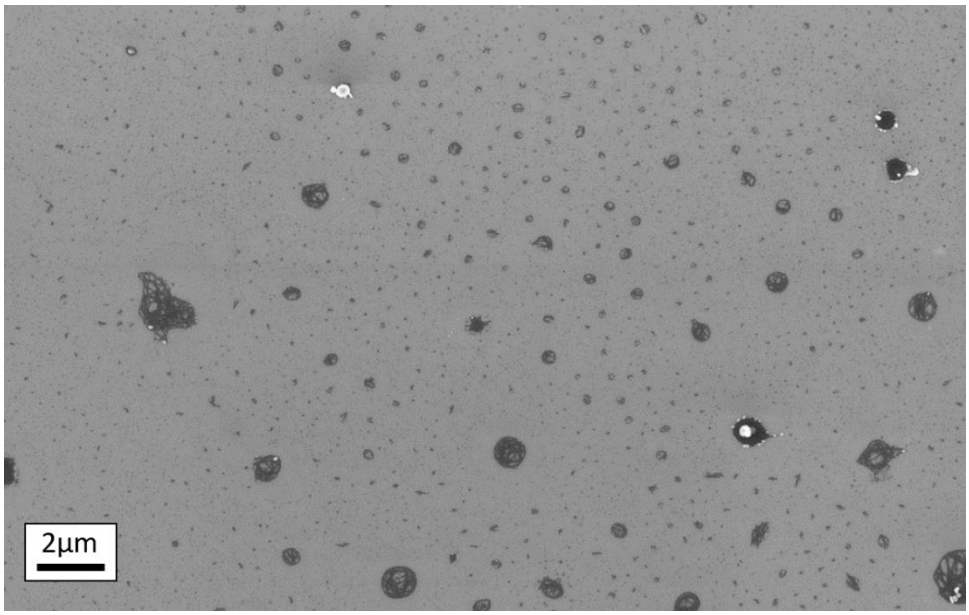


Figure S11: Equivalent circuit of NbS_2/n++ Si.

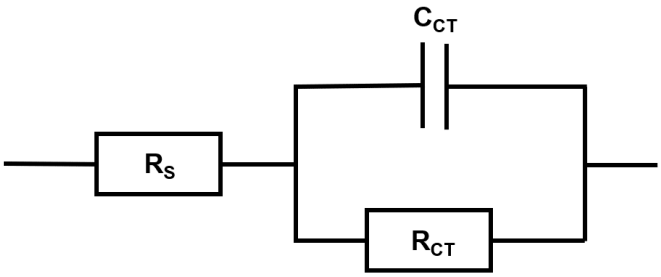


Figure S12: J-V plot of Si, Si NWs, NbS_2/Si and NbS_2/Si NWs recorded under dark condition

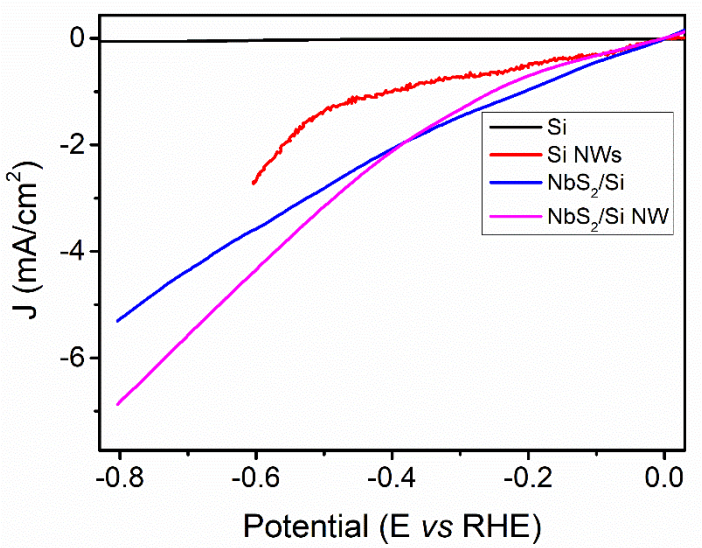


Figure S13: Chopped LSV results of standalone Si NWs

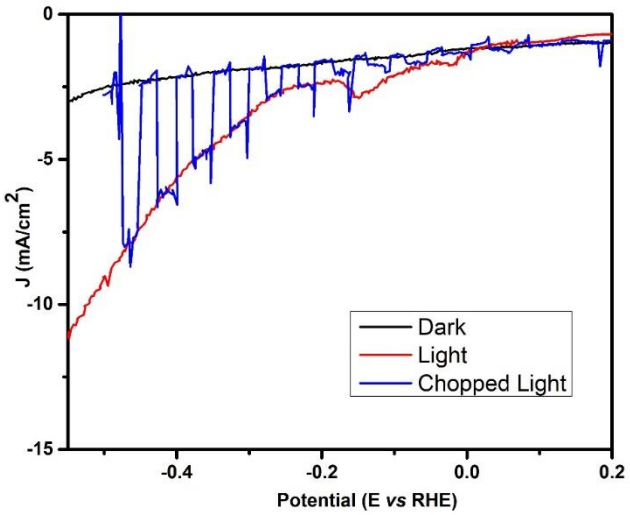


Figure S14: Chopped LSV results of NbS_2 on planar p-Si substrate.

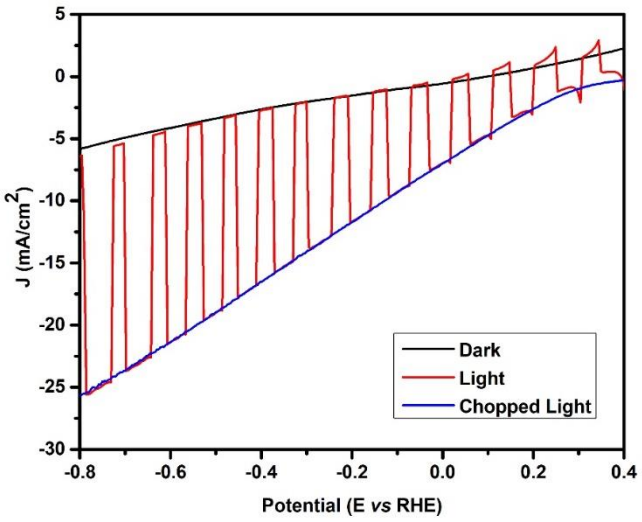


Figure S15: Transient photoresponce of NbS_2/Si NWs at the different applied bias

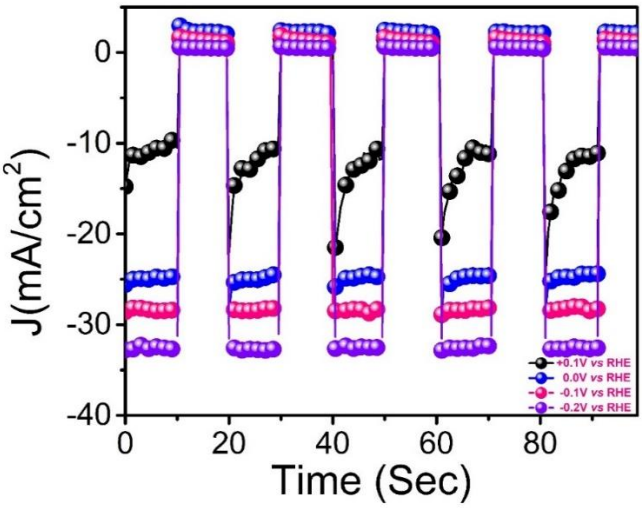


Figure S16: Equivalent circuit of fabricated photoanodes.

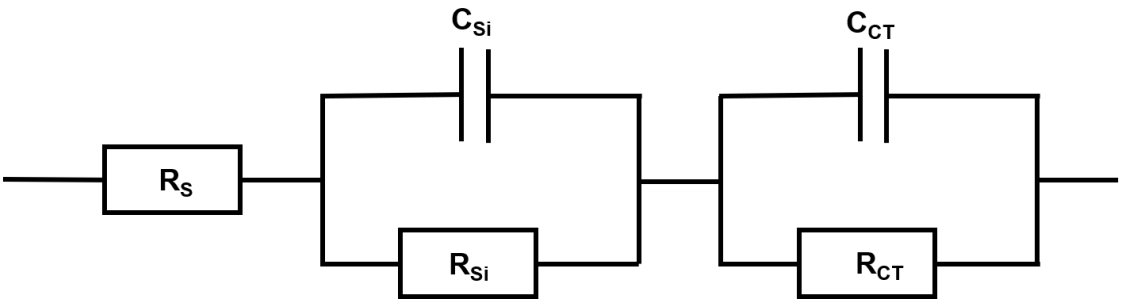


Figure S17: Nyquist plot of fabricated photocathodes under 0.5M $HClO_4$ electrolyte condition along with fitted data.

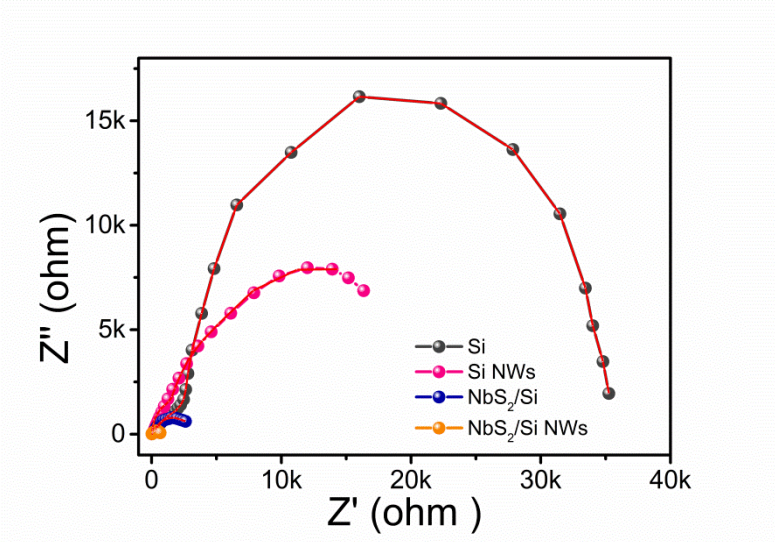


Table S1: The comparison of common electrical characteristics determined from the Nyquist plot of all fabricated photocathodes of PEC analysis.

	R_S (Ω)	R_{Si} (Ω)	R_{CT} (Ω)	C_{CT} (μF)
Si	57	2543	32398	0.231
Si NW	46	1650	18231	7.86
NbS_2/Si	50	100	2500	15.91
NbS_2/Si NW	**48**	**45**	**550**	**97.43**

Table S2: Comparison of PEC performance of reported TMDC/Si NWs heterostructures.

Sl. No	Material	Synthesis Approach	Protective Layer	Turn on Potential (V *vs.* RHE)	J_0 (mA/cm^2)	Ref
1	MoS_2/TiO_2/Si NWs	Chemical Method	TiO_2	~+0.25	-15.0	[1]
2	MoS_2/Si NWs	CVD	NA	+0.26	-16.5	[2]
3	MoS_2/Al_2O_3/ Si NWs	Sputtering	Al_2O_3	+0.4	~32.0	[3]
4	MoS_2/Ag/ Si NWs	Thermal decomposition	NA	+0.62	2.0	[4]
5	MoS_2/Si NWs	Chemical Method	NA	~+0.122	~8.41	[5]
6	MS cluster/Si NWs	Chemical Method	NA	+0.25	-14.3	[6]
7	MoS_2/Si NWs	Chemical Method/ Drop casting	NA	+0.55	-1.8	[7]
8	**NbS_2/Si NWs**	**CVD**	**NA**	**+0.34**	**-26.0**	**This work**

Reference:

[1] L. Zhang, C. Liu, A.B. Wong, J. Resasco, P. Yang, MoS2-wrapped silicon nanowires for photoelectrochemical water reduction, Nano Res. 8 (2014) 281–287. doi:10.1007/s12274-014-0673-y.

[2] D. Hu, J. Xiang, Q. Zhou, S. Su, Z. Zhang, X. Wang, M. Jin, L. Nian, R. Nözel, G. Zhou, Z. Zhang, J. Liu, One-step chemical vapor deposition of MoS_2 nanosheets on SiNWs as photocathodes for efficient and stable solar-driven hydrogen production, Nanoscale. 10 (2018) 3518–3525. doi:10.1039/c7nr09235k.

[3] R. Fan, J. Mao, Z. Yin, J. Jie, W. Dong, L. Fang, F. Zheng, M. Shen, Efficient and Stable Silicon Photocathodes Coated with Vertically Standing Nano-MoS_2 Films for Solar Hydrogen Production, ACS Appl. Mater. Interfaces. 9 (2017)

6123–6129. doi:10.1021/acsami.6b15854.

[4] L. Qiao, M. Liao, J. Wu, Q. Jiang, Y. Zhang, Y. Li, Molybdenum disulfide/silver/p-silicon nanowire heterostructure with enhanced photoelectrocatalytic activity for hydrogen evolution, Int. J. Hydrogen Energy. (2018). doi:10.1016/j.ijhydene.2018.10.090.

[5] C.J. Chen, K.C. Yang, C.W. Liu, Y.R. Lu, C.L. Dong, D.H. Wei, S.F. Hu, R.S. Liu, Silicon microwire arrays decorated with amorphous heterometal-doped molybdenum sulfide for water photoelectrolysis, Nano Energy. 32 (2017) 422–432. doi:10.1016/j.nanoen.2016.12.045.

[6] Y. Hou, Z. Zhu, Y. Xu, F. Guo, J. Zhang, X. Wang, Efficient photoelectrochemical hydrogen production over p-Si nanowire arrays coupled with molybdenum–sulfur clusters, Int. J. Hydrogen Energy. 42 (2017) 2832–2838. doi:10.1016/j.ijhydene.2016.09.106.

[7] Qiao, L., Liao, M., Fang, K., He, X., & Zhang, Y. (2018). Enhancement of Photoelectrochemical Hydrogen Evolution of P-Type Silicon Nanowires Array by Loading MoS2. *Silicon*, 1–8. https://doi.org/10.1007/s12633-018-0014-y