Electronic Supplementary Material (ESI) for CrystEngComm.

Supporting Information

Synergistic Phase and Crystallinity Engineering in Cubic $RuSe_2$ Catalyst toward Efficient Hydrogen Evolution Reaction

Wei Zhan, Nan Li*, Shixiang Zuo, Zhimin Guo, Chenghong Qiang, Zhengping Li and Jiangquan Ma*

Jiangsu Province Advanced Catalysis and Green Manufacturing Collaborative Innovation Center, Changzhou University, Changzhou, Jiangsu Province 213164, China.

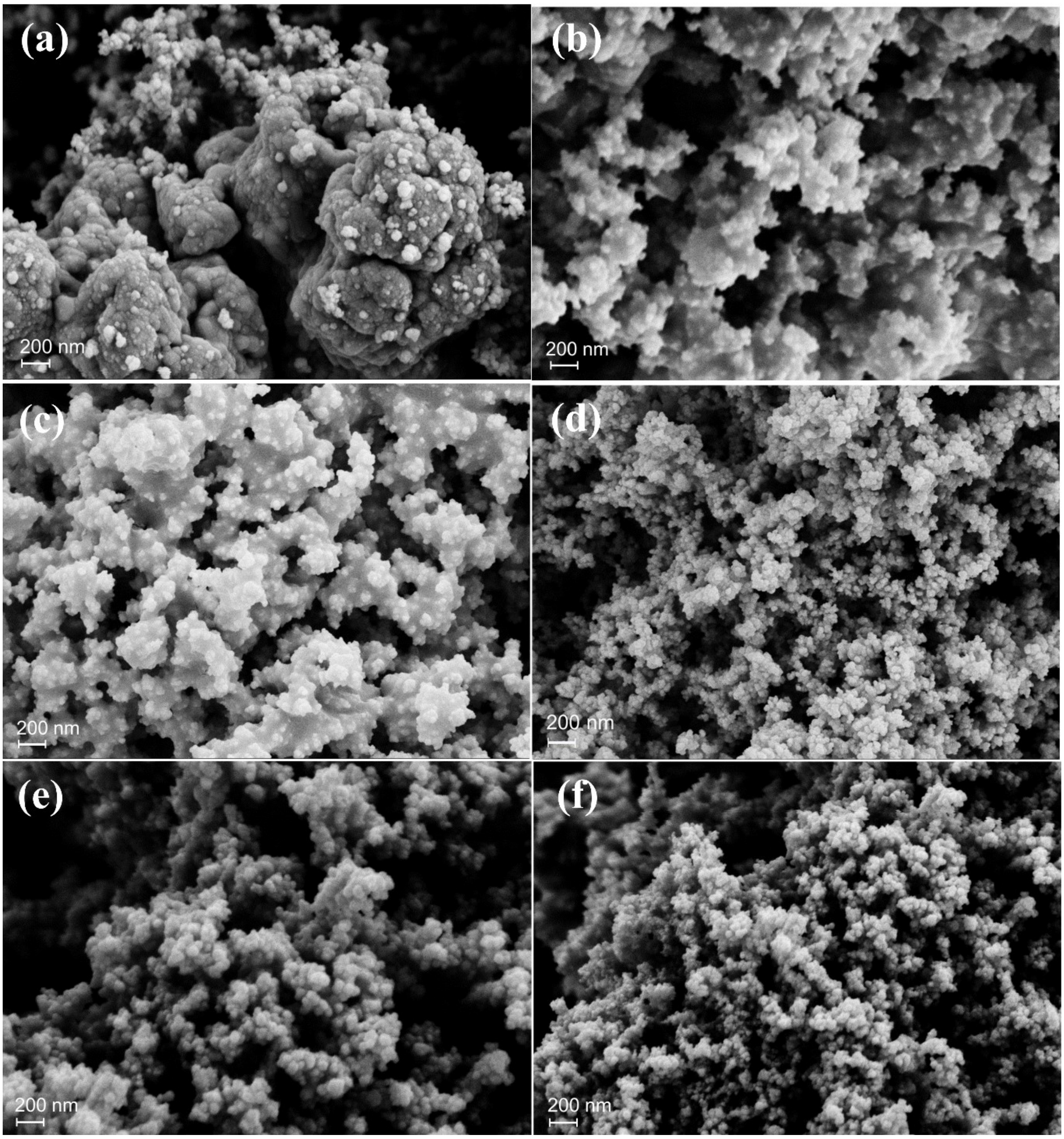

Fig. S1 SEM images of (a) Fresh-$RuSe_2$, (b) $RuSe_2$-200, (c) $RuSe_2$-250, (d) $RuSe_2$-300, (e) $RuSe_2$-400, and (f) $RuSe_2$-600.

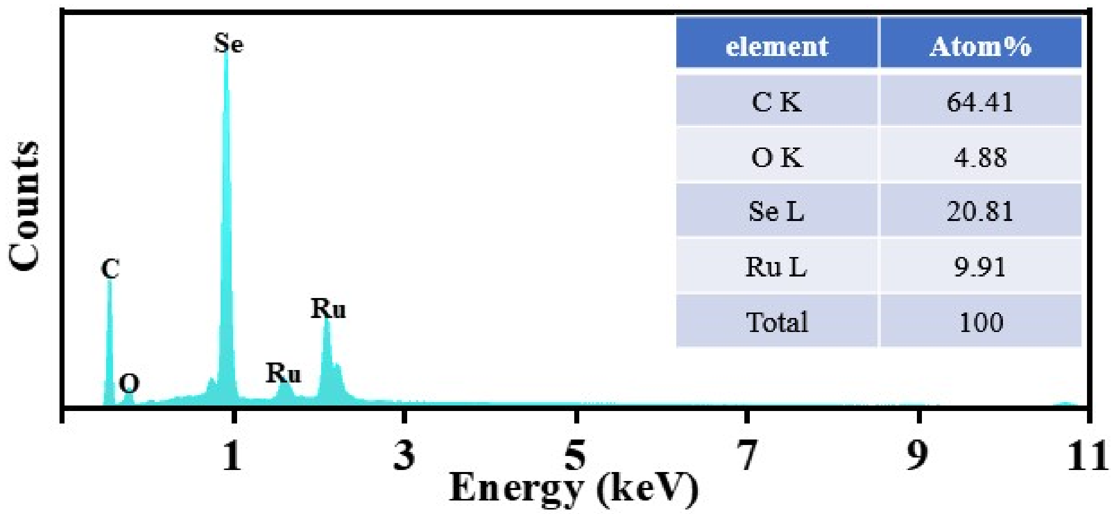

Fig. S2 EDS spectrum of $RuSe_2$-500.

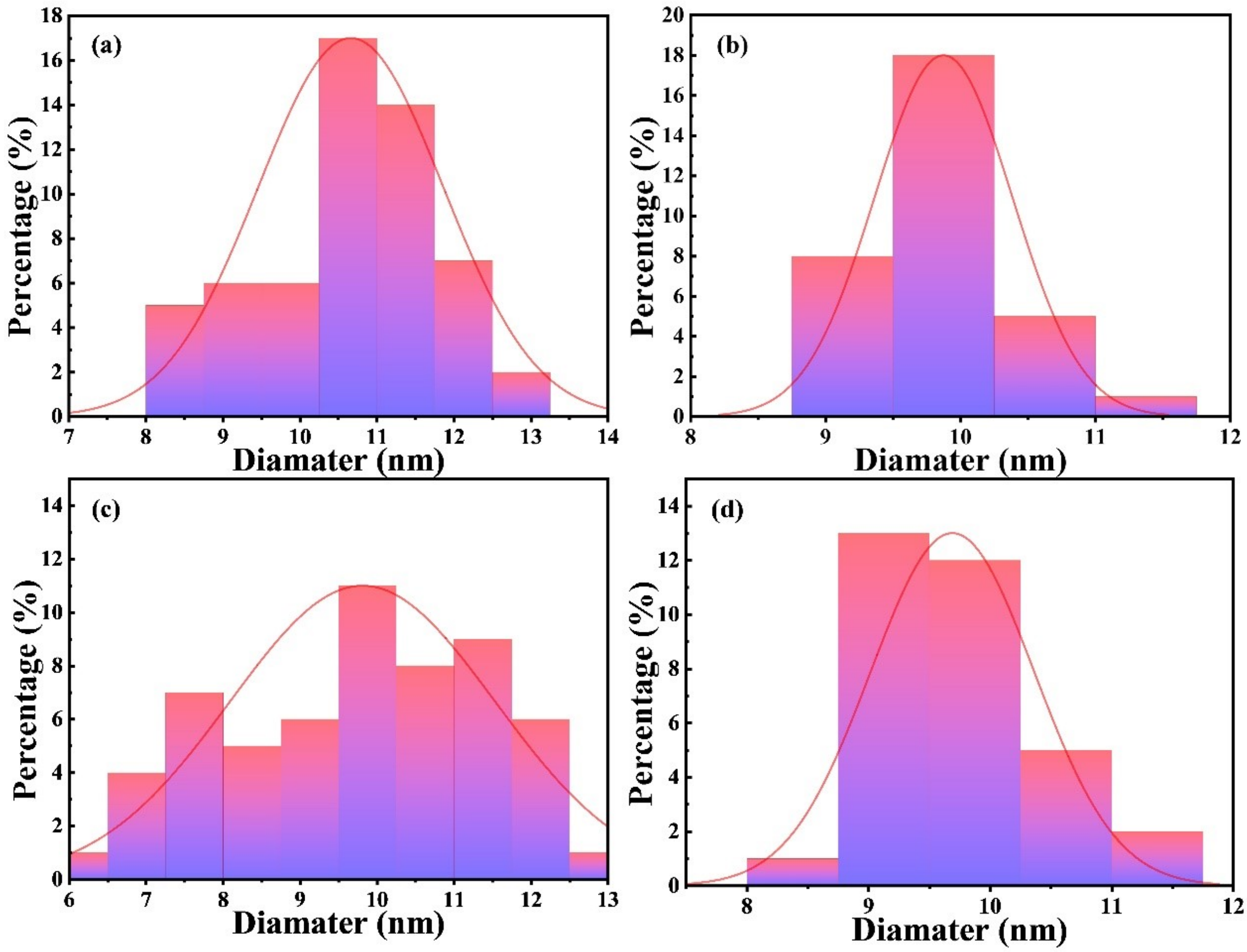

Fig. S3 Particle size distribution of $RuSe_2$-300 (a), $RuSe_2$-400 (b), $RuSe_2$-500 (c), and $RuSe_2$-600 (d). The average diameter is 9.89, 9.87, 9.81 and 9.69 nm, respectively.

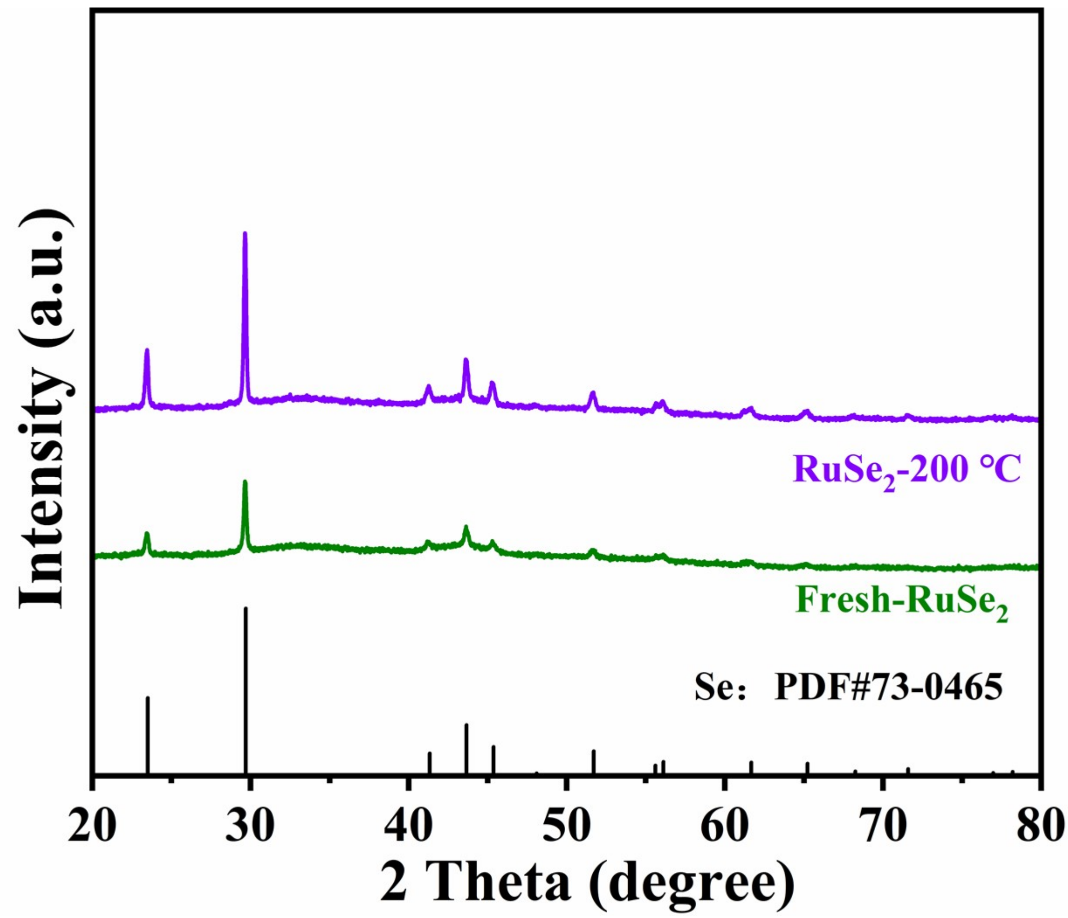

Fig. S4 XRD patterns of Fresh-$RuSe_2$ and $RuSe_2$-200.

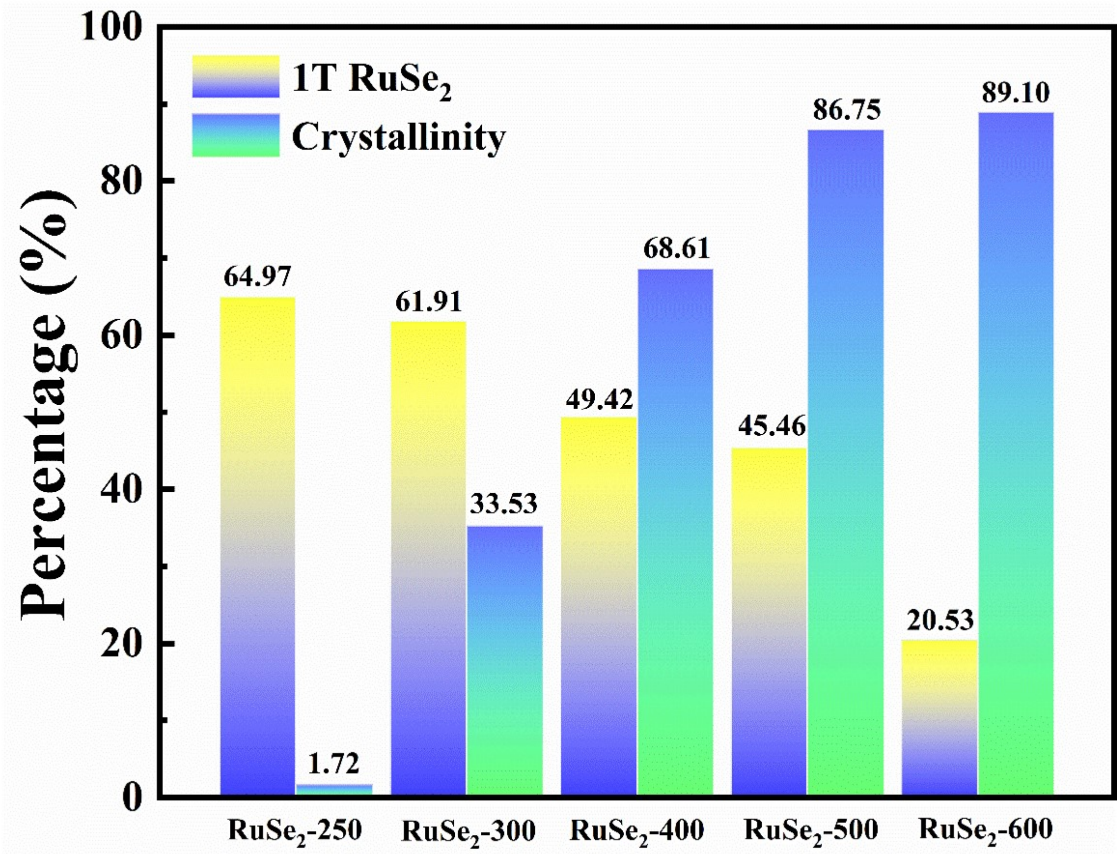

Fig. S5 1T-phase and crystallinity ratios in $RuSe_2$-250, $RuSe_2$-300, $RuSe_2$-400, $RuSe_2$-500 and $RuSe_2$-600.

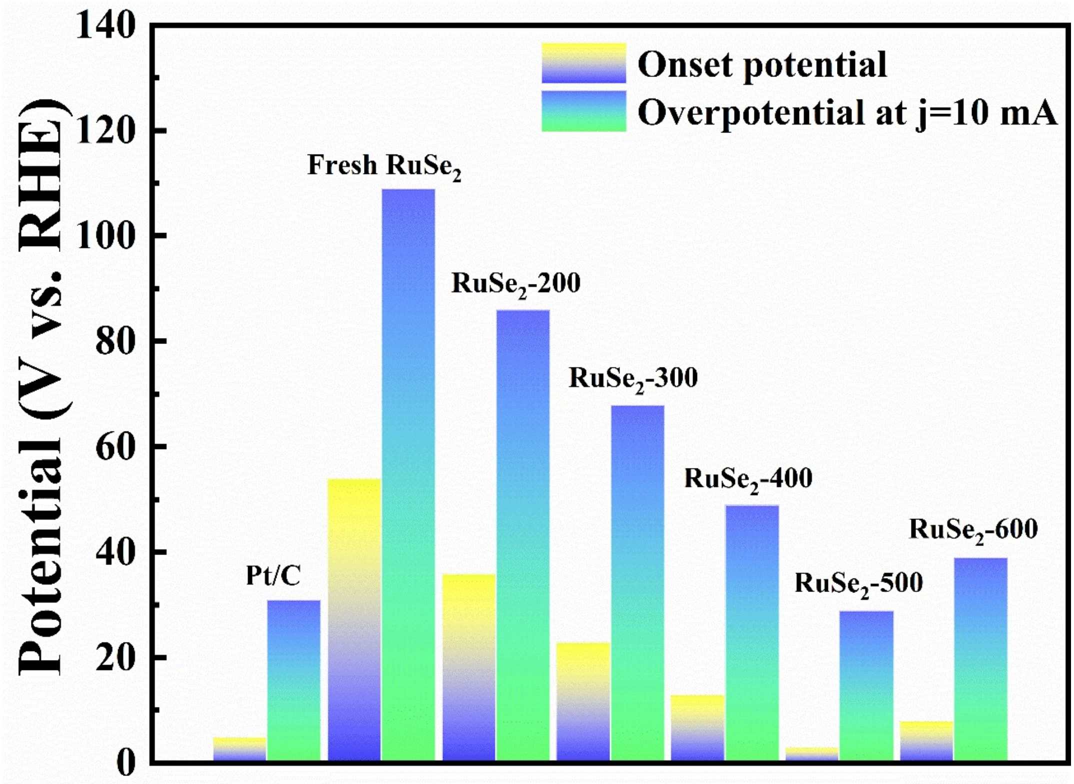

Fig. S6 Onset potential and overpotential at current density of 10 mA·cm^{-2} for Pt/C, Fresh-$RuSe_2$, $RuSe_2$-250, $RuSe_2$-300, $RuSe_2$-400, $RuSe_2$-500 and $RuSe_2$-600.

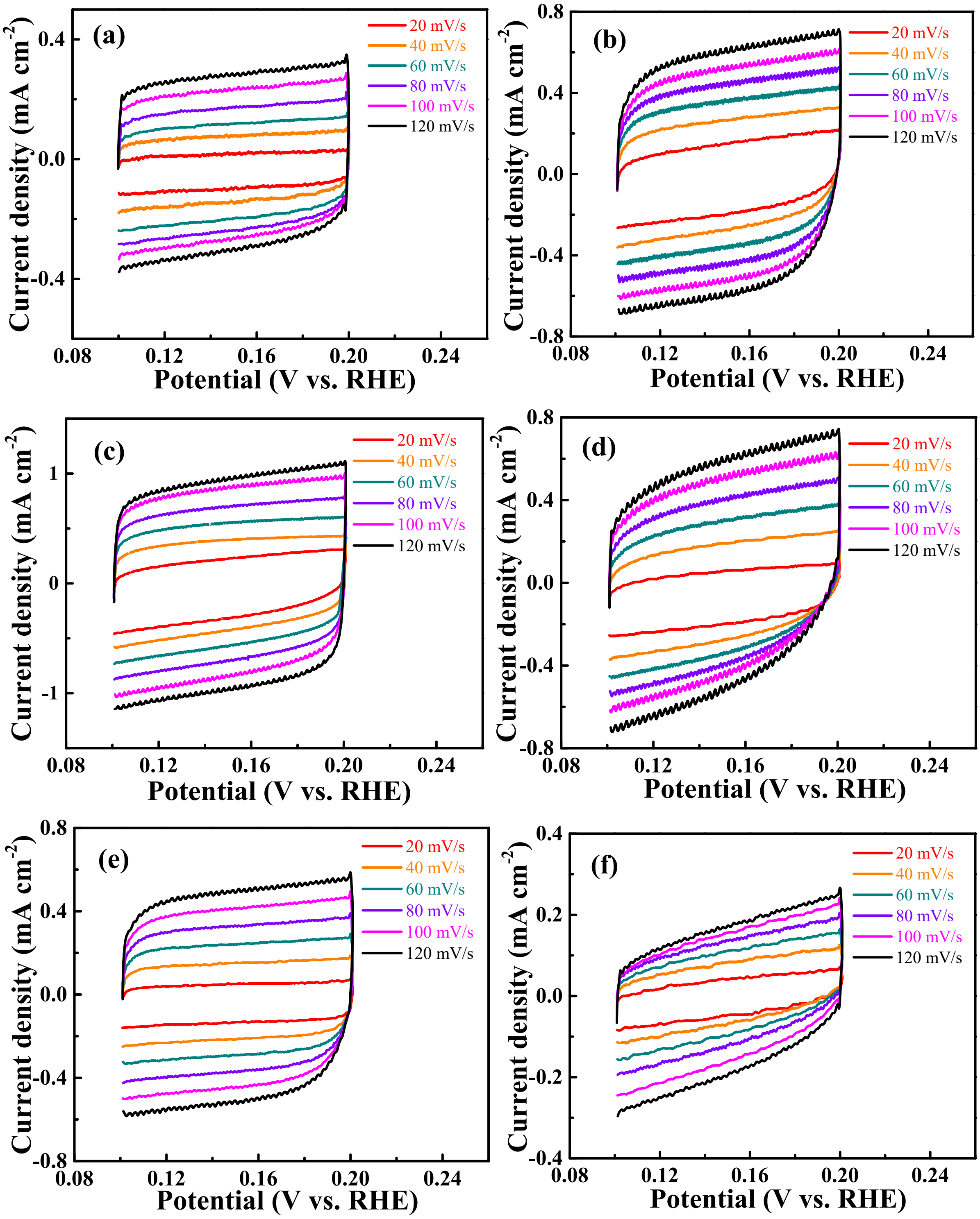

Fig. S7 CV curves of (a) Fresh-$RuSe_2$, (b) $RuSe_2$-250, (c) $RuSe_2$-300, (d) $RuSe_2$-400, (e) $RuSe_2$-500, and (f) $RuSe_2$-600 at various scan rates from 20-120 mV/s.

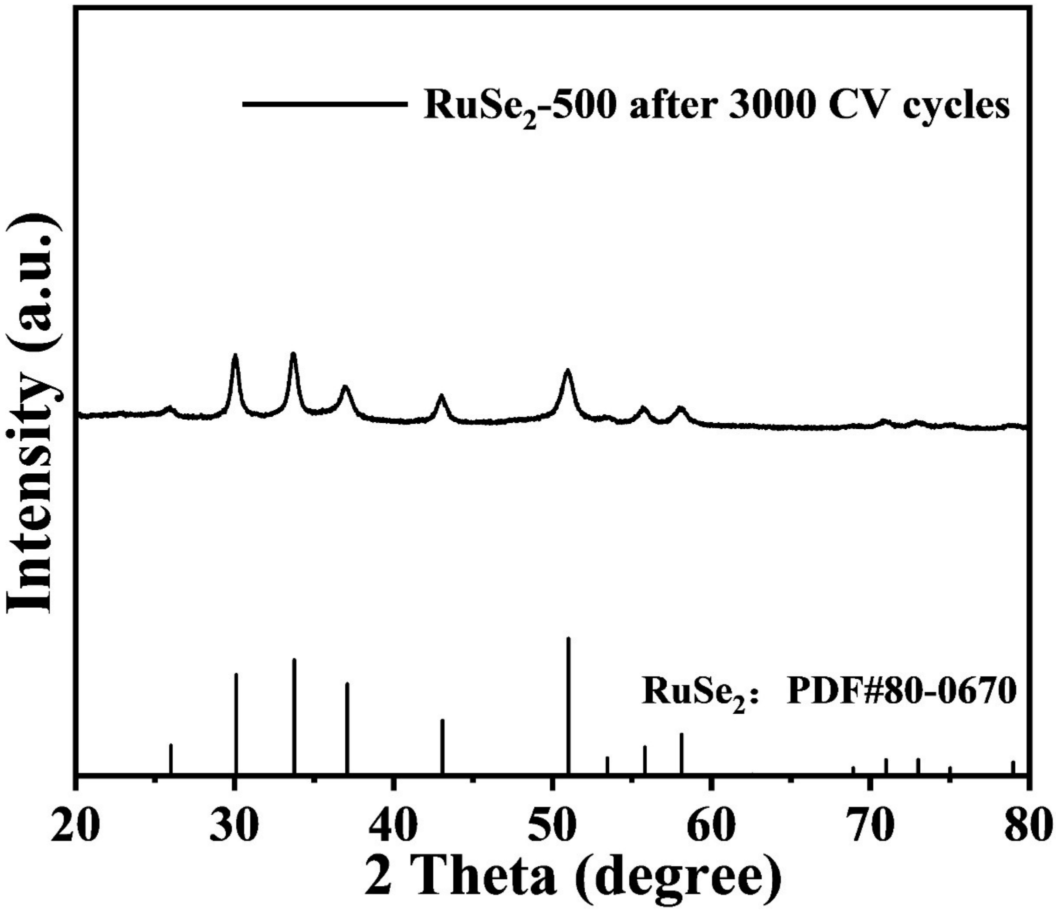

Fig. S8 XRD pattern of $RuSe_2$-500 after long-time stability test.

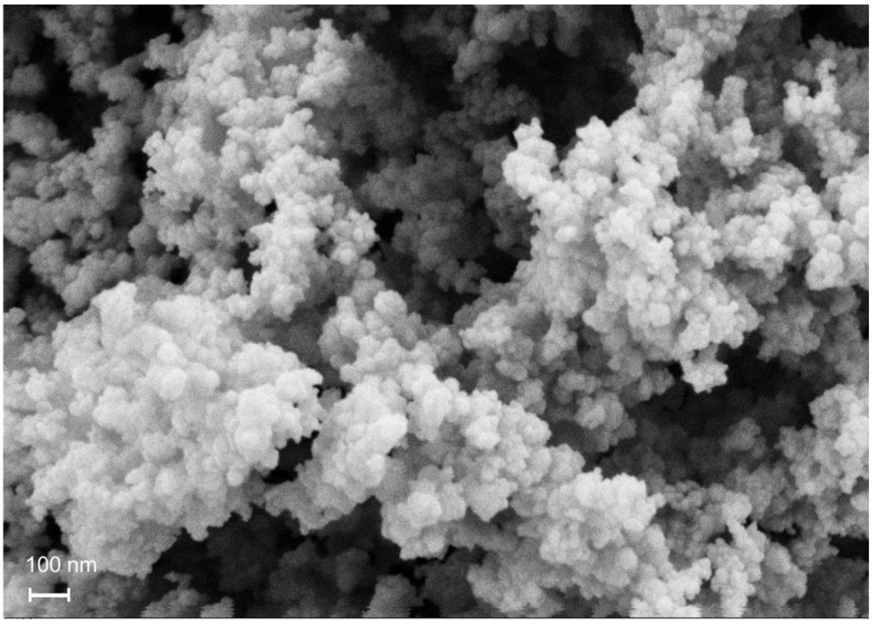

Fig. S9 SEM image of $RuSe_2$-500 after long-time stability test.

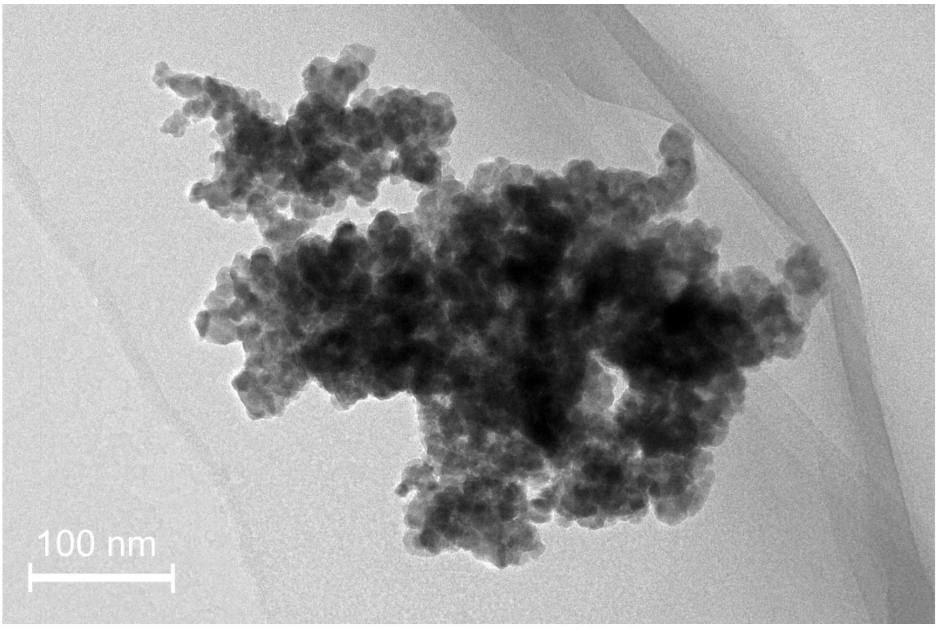

Fig. S10 TEM image of $RuSe_2$-500 after long-time stability test.

Table S1. Data for calculating crystallinity of $RuSe_2$ catalysts.

Catalyst	ΣI_c	ΣI_a	Crystallinity
$RuSe_2$-250	47159.15	2694651.85	1.72%
$RuSe_2$-300	75666.15	150000.85	33.53%
$RuSe_2$-400	365593.19	167263.81	68.61%
$RuSe_2$-500	526038.99	80346.01	86.75%
$RuSe_2$-600	625958.69	76576.32	89.10%

Table S2 Comparison of the features of HER parameters between the present $RuSe_2$-500 and other electrocatalytic materials in the literature.

Catalyst	Mass loading ($mg\ cm^{-2}$)	Substrate	Electrolyte	η (mV) at 10 mA cm^{-2}	Ref
h-$RuSe_2$	0.30	GC	1.0 M KOH	34	S1
Ru_xSe	1	CFP	1.0 M KOH	45	S2
$RuSe_2$/CNT	0.437	RDE	1.0 M KOH	29.5	S3
$Ru_{0.33}Se$@TNA	-	CC	1.0 M KOH	57	S4
$RhSe_2$	0.34	GC	1.0 M KOH	81.6	S5
$PdSe_2$	0.34	GC	1.0 M KOH	138	S6
$IrSe_2$	0.25	GC	1.0 M KOH	72	S7
RuS_2	0.278	GC	1.0 M KOH	78	S8
RuS_x/S-GO	1	CFP	1.0 M KOH	58	S9
RuP_2@NPC	1	GC	1.0 M KOH	52	S10
Ru-MoS_2/CNT	1	CFP	1.0 M KOH	50	S11
$Ru_{0.10}$@2H-MoS_2	0.285	GC	1.0 M KOH	51	S12
Ni-W-600	3	GC	1.0 M KOH	59	S13
$CuCo_2$-P	6.5	CF	1.0 M KOH	49.5	S14
$RuTe_2$	-	GC	1.0 M KOH	34	S15
$RuSe_2$-500	0.275	GC	1.0 M KOH	**29**	This work
Pt/C	0.275	GC	1.0 M KOH	**31**	This work

Supplementary References

S1. Y. M. Zhao, H. J. Cong, P. Li, D. Wu, S. L. Chen, W. Luo, *Angew. Chem., Int. Ed.*, 2021, **60**, 7013-7017.

S2. K. F. Wang, B. Li, W. Wei, J. G. Wang, Q. Shen, P. Qu, *Nanoscale*, 2020, **12**, 23740-23747.

S3. Z. Zhang, C. Jiang, P. Li, K. G. Yao, Z. L. Zhao, J. T. Fan, H. Li, H. J. Wang, *Small*, 2021, **17**, 2007333.

S4. K. F. Wang, Q. Chen, Y. Y. Hu, W. Wei, S. Z. Wang, Q. Shen, P. Qu, *Small*, 2018, **14**, 1802132.

S5. W. W. Zhong, B. B. Xiao, Z. P. Lin, Z. P. Wang, L. G. Huang, S. J. Shen, Q. H. Zhang, L. Gu, *Adv. Mater.*, 2021, **33**, 2007894.

S6. Z. P. Lin, B. B. Xiao, Z. P. Wang, W. Y. Tao, S. J. Shen, L. A. Huang, J. T. Zhang, F. Q. Meng, Q. H. Zhang, L. Gu, W. W. Zhong, *Adv. Funct. Mater.*, 2021, **31**, 2102321.

S7. T. T. Zheng, C. Y. Shang, Z. H. He, X. Y. Wang, C. Cao, H. L. Li, R. Si, B. C. Pan, S. M. Zhou, J. Zeng, *Angew. Chem., Int. Ed.*, 2019, **58**, 14764-14769.

S8. Y. L. Zhu, H. A. Tahini, Y. Wang, Q. Lin, Y. Liang, C. M. Doherty, Y. Liu, X. Y. Li, J. Lu, S. C. Smith, C. Selomulya, X. W. Zhang, Z. P. Shao, H. T. Wang, *J. Mater. Chem. A*, 2019, **7**, 14222-14232.

S9. P. S. Li, X. X. Duan, S. Y. Wang, L. R. Zheng, Y. P. Li, H. H. Duan, Y. Kuang, X. M. Sun, *Small*, 2019, **15**, 1904043.

S10. Z. H. Pu, I. S. Amiinu, Z. K. Kou, W. Q. Li, S. C. Mu, *Angew. Chem., Int. Ed.*, 2017, **56**, 11559-11564.

S11. X. Zhang, F. Zhou, S. Zhang, Y. Y. Liang, R. H. Wang, *Adv. Sci.*, 2019, **6**, 1900090.

S12. J. Wang, W. H. Fang, Y. Hu, Y. H. Zhang, J. Q. Dang, Y. Wu, B. Z. Chen, H. Zhao, Z. X. Li, *Appl. Catal., B*, 2021, **298**, 120490.

S13. Y. K. Li, G. Zhang, H. Huang, W. T. Lu, F. F. Cao, Z. G. Shao, *Small*, 2020, **16**, 2005184.

S14. Y. Cheng, Y. Pei, P. Y. Zhuang, H. Chu, Y. D. Cao, W. Smith, P. Dong, J. F. Shen, M. X. Ye, P. M. Ajayan, *Small*, 2019, **15**, 1904681.

S15. B. Tang, X. D. Yang, Z. H. Kang, L. G. Feng, *Appl. Catal., B*, 2020, **278**, 119281.