

Supporting Information for

Exploring the Surface Reconstruction of AgPdIr Nanoalloys with a

Defined IrO₂ – AgPd Heterostructure for Exceptional Formate

Oxidation

Zhen Li,^{ab} Fuyi Chen,^{*ab} Junpeng Wang,^{ab} Chongyang Wang,^{ab} Shuang Shan^{ab} and Longfei Guo^{ab}

a.State Key Laboratory of Solidification Processing, Northwestern Polytechnical University, Xi'an 710072, China. E-mail: fuyichen@nwpu.edu.cn

b.School of Materials Science and Engineering, Northwestern Polytechnical University, Xi'an, 710072, China

Corresponding author at: State Key Laboratory of Solidification Processing, Northwestern Polytechnical University, Xi'an 710072, China.

E-mail address: fuyichen@nwpu.edu.cn.

Table S1 Electrocatalytic Performance Comparison for the Formate Oxidation Reaction (FOR) in Alkaline Media.

Catalyst	Electrolyte	Mass activity (A/mgPd)	Durability remain at 3600s in CA	Reference
IrO ₂ -AgPd	1 M KOH+ 1 M HCOOK	5.21	27%	This work
PdH	1 M KOH+0.5 M HCOOK	0.85	20%	1
PdCu/C	1 M KOH+ 1 M HCOOK	2.0	14%	2
PdP/WO ₃	1 M KOH+1 M HCOOK	0.50	--	3
AgPdCu	1 M KOH+1 M HCOOK	2.73	16%	4
PdRh/C	1 M KOH+1 M HCOOK	4.50	17%	5
PdCe/C	1 M KOH+ 1 M HCOOK	1.10	10%	6
Pd@PdPt	1 M KOH + 0.5 M HCOOK	1.25	20%	7
AgPt	1 M KOH + 0.5 M HCOOK	0.38	55%	8
AuAgPd	1 M KOH+1 M	4.51	29%	9

AgPdRh	HCOOK			
	1 M KOH+1 M	1.85	10%	10
PdPt	HCOOK			
	1 M KOH+0.5	1.65	20%	11
Pd/FeOx/C	M HCOOK			
	1 M KOH+1 M	1.61	--	12
	HCOOK			

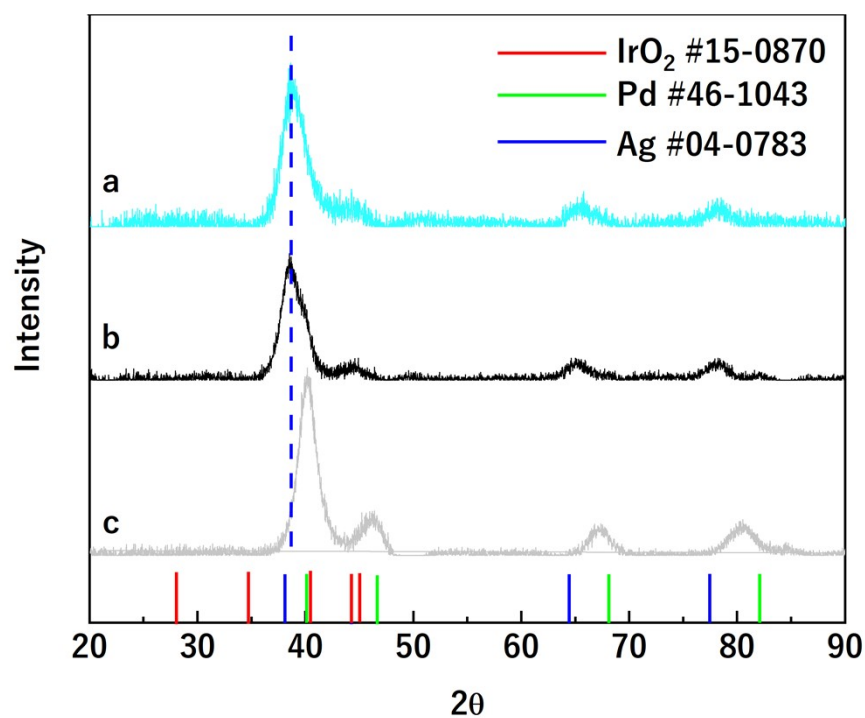


Figure S1. X-ray diffraction (XRD) patterns of the synthesized catalysts: (a) IrO₂-AgPd, (b) AgPd, and (c) IrO₂-Pd.

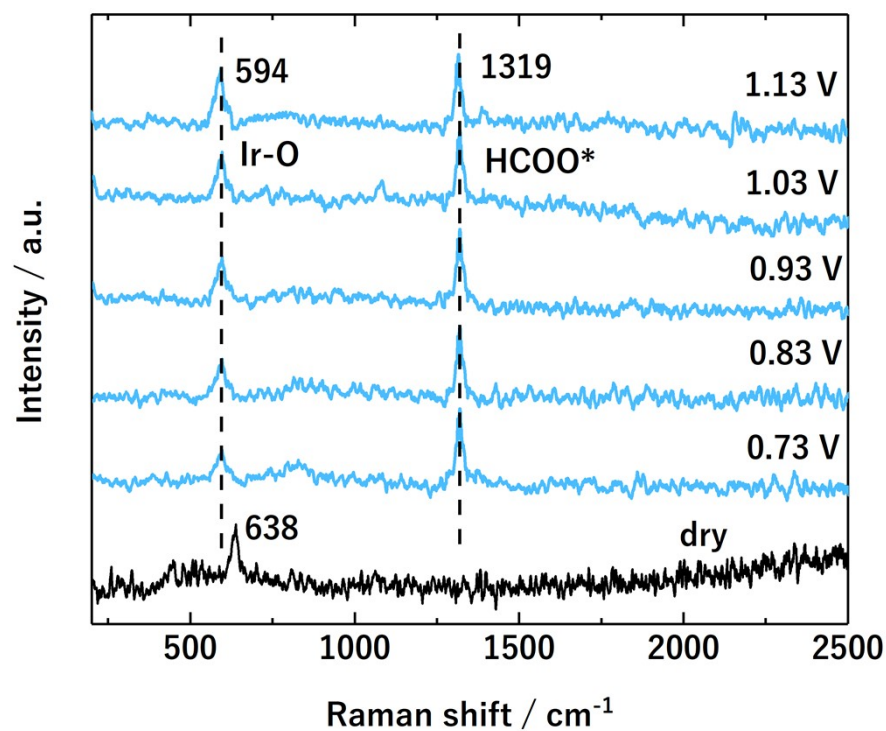


Figure S2 In situ Raman intensities of IrO₂-AgPd during the FOR test in 1M KOH + 1M HCOOK.

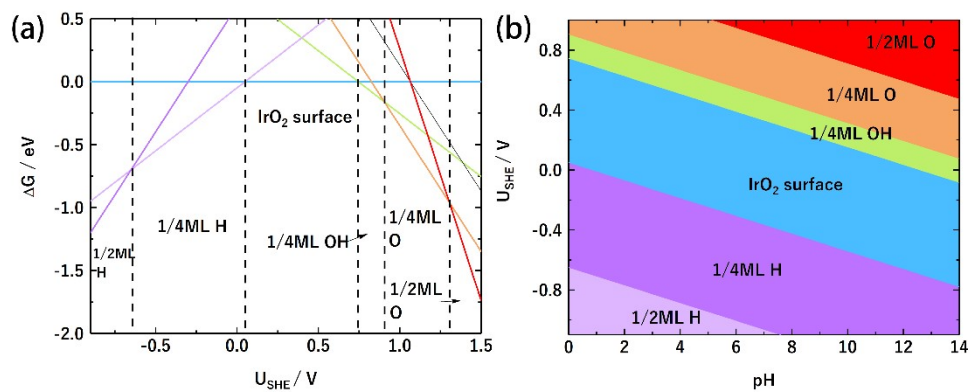


Figure S3. (a) Phase stability diagram and (b) Pourbaix diagram of IrO₂-AgPd.

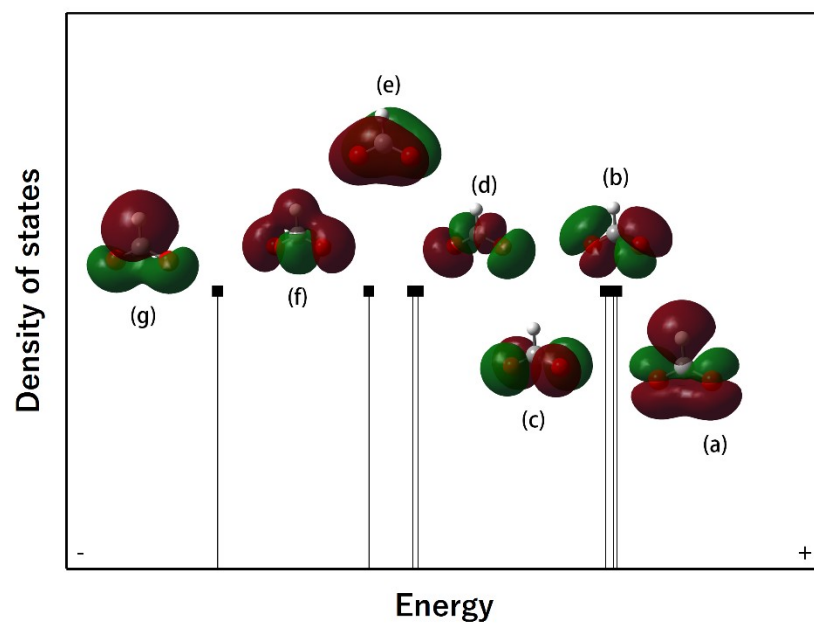


Figure S4. The electronic orbital structure of HCOO^- .

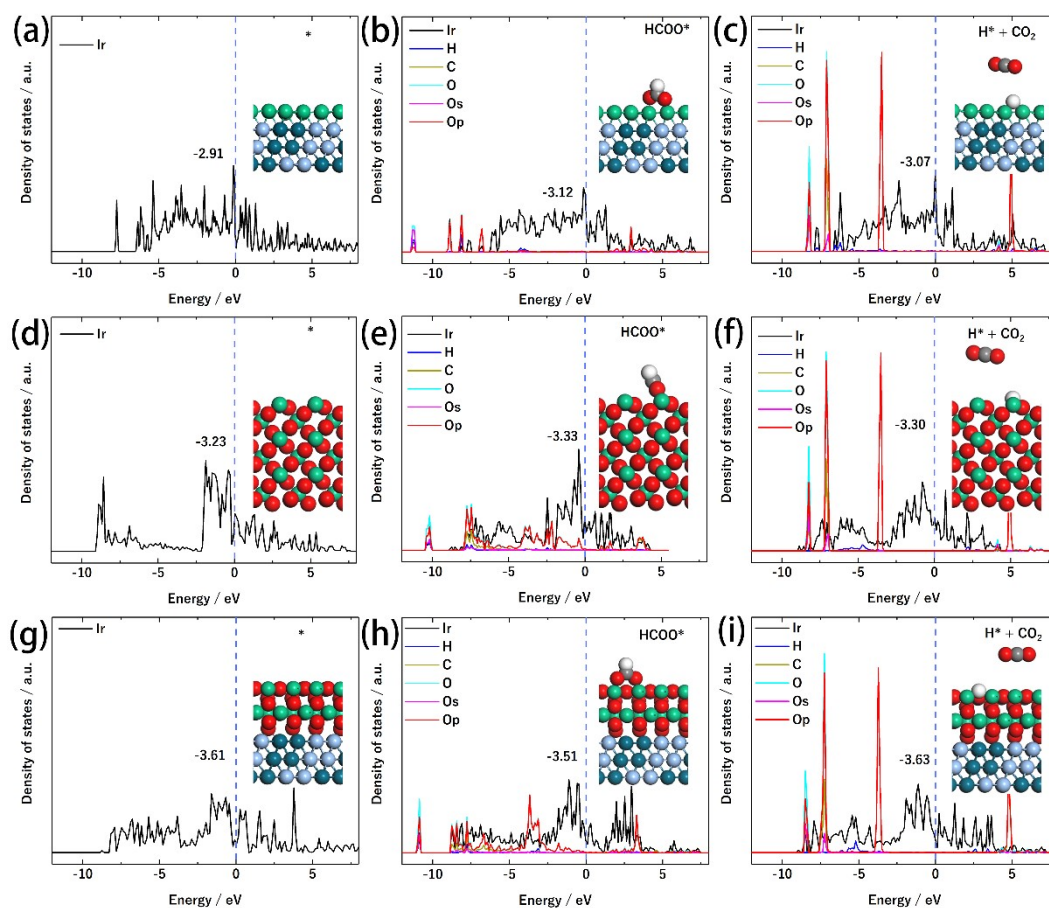


Figure S5. Density of states (DOS) analysis of catalytically active Ir sites during the FOR: (a-c) Projected DOS (PDOS) of surface Ir atoms on Ir-AgPd; (d-f) PDOS of surface Ir atoms on IrO₂(200); (g-i) PDOS of surface Ir atoms on IrO₂(110)-AgPd. The Fermi level is set to 0 eV. Corresponding atomic configurations are shown as insets, with calculated d-band centers.

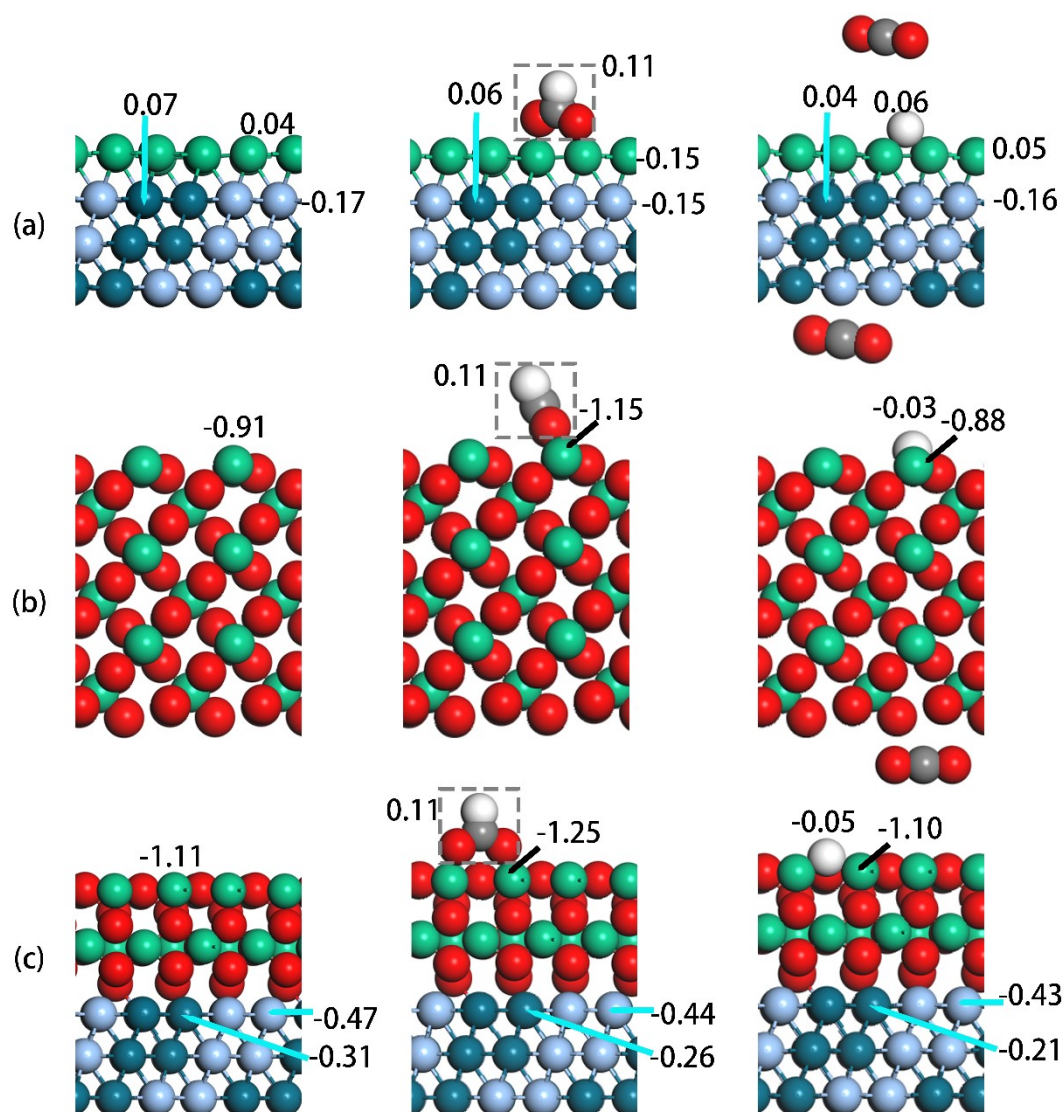


Figure S6. Bader charge analysis of (a) Ir-AgPd, (b) IrO₂(200) and (c) IrO₂(110)-AgPd during FOR.

References

1. H.-Y. Sun, Y. Ding, Y.-Q. Yue, Q. Xue, F.-M. Li, J.-X. Jiang, P. Chen and Y. Chen, *ACS Applied Materials & Interfaces*, 2021, 13, 13149-13157.
2. W. J. Wang, S. Hwang, T. Kim, S. Ha and L. Scudiero, *Electrochimica Acta*, 2021, 387, 138531.
3. S. Kumar, R. Soni and S. Kurungot, *Sustainable Energy & Fuels*, 2021, 5, 4758-4770.
4. Q. Wang, F. Chen, L. Guo, T. Jin, H. Liu, X. Wang, X. Gong and Y. Liu, *Journal of Materials Chemistry A*, 2019, 7, 16122-16135.
5. J. Bai, Q. Xue, Y. Zhao, J.-X. Jiang, J.-H. Zeng, S.-B. Yin and Y. Chen, *ACS Sustainable*

Chemistry & Engineering, 2019, 7, 2830-2836.

6. Q. Tang, F. Chen, T. Jin, L. Guo, Q. Wang and H. Liu, Journal of Materials Chemistry A, 2019, 7, 22996-23007.
7. Y.-C. Jiang, Y. Ding, F.-M. Li, S.-B. Yin, D.-S. Li, X.-F. Li and Y. Chen, Journal of Materials Chemistry A, 2022, 10, 24701-24707.
8. S.-H. Han, H.-M. Liu, J. Bai, X. L. Tian, B. Y. Xia, J.-H. Zeng, J.-X. Jiang and Y. Chen, ACS Applied Energy Materials, 2018, 1, 1252-1258.
9. B. Pan, F. Chen, B. Kou, J. Wang, Q. Tang, L. Guo, Q. Wang, Z. Li, W. Bian and J. Wang, Nanoscale, 2020, 12, 11659-11671.
10. Y. Jin, F. Chen, L. Guo, J. Wang, B. Kou, T. Jin and H. Liu, ACS Applied Materials & Interfaces, 2020, 12, 26694-26703.
11. X.-L. Liu, Y.-C. Jiang, J.-T. Huang, W. Zhong, B. He, P.-J. Jin and Y. Chen, Carbon Energy, 2023, 5, e367.
12. Y. Li, K. Zhang, Y. Ji, Z. Tang, Y. Yao, X. Liu, D. Wang, X. Wang, L. Shi, K. Nie, Z. Yang, J. Xie and Y.-M. Yan, ACS Applied Materials & Interfaces, 2023, 15, 28790-28798.