RGC Ref.: **N_HKUST610/17**
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(please insert ref. above)

The Research Grants Council of Hong Kong
NSFC/RGC Joint Research Scheme
Joint Completion Report

(Please attach a copy of the completion report submitted to the NSFC by the Mainland researcher)

Part A: The Project and Investigator(s)

1. Project Title

Single Atom Based Low Platinum Nano Electrocatalysts: Rational Design, Synthesis, Characterization and Their Applications in Fuel Cells
基於單分子分散的新型低鉑納米電催化劑的設計、合成、表徵及其在燃料電池中的應用

2. Investigator(s) and Academic Department/Units Involved

	Hong Kong Team	Mainland Team
Name of Principal Investigator *(with title)*	Prof. Minhua Shao	Prof. Zidong Wei
Post	Professor	Professor
Unit / Department / Institution	Dept of Chemical and Biological Engineering/ The Hong Kong University of Science and Technology	College of Chemistry and Chemical Engineering/ Chongqing University
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Co-investigator(s) *(with title and institution)*		

3. Project Duration

	Original	Revised	Date of RGC/ Institution Approval *(must be quoted*)
Project Start date	01-01-2018		
Project Completion date	31-12-2021		

Duration *(in month)*	48		
Deadline for Submission of Completion Report	31-12-2022		

Part B: The Completion Report

5. Project Objectives

5.1 Objectives as per original application

1. To develop Fe-N-C based materials by precisely doping N and Fe in carbon structure;

2. To synthesize Pt single atoms supported on or incorporated in Fe-N-C to improve fuel cell performance and durability;

3. To identify active sites, their degradation mechanisms and oxygen reduction reaction pathways in (Pt, Fe)-N-C catalysts through experimental and theoretical approaches.

5.2 Revised Objectives

Date of approval from the RGC: N.A.

Reasons for the change: N.A.

1.
2.
3. ....

6. Research Outcome

Major findings and research outcome
(maximum 1 page; please make reference to Part C where necessary)

1. A facile and universal secondary-atom-assisted strategy was proposed to prepare atomic iron sites with high density hosted on porous nitrogen-doped carbon nanowires (Fe-NCNWs). The secondary metals can significantly improve the activity of Fe-N-C catalysts. Iron ions surrounded by secondary metal ions (Al, Mg,

and Zn) were directly converted to the atomic Fe-N_x moieties rather than nanosized iron compounds. Furthermore, the secondary metal compounds produced in the high-temperature pyrolysis acted as templates for the formation of nanopores, increasing the surface area to host atomic Fe-N_x moieties. On the basis of the above secondary-metal-assisted strategy, we further introduced P doping to modulate the coordination environment of isolated Fe atoms, determining that P doping can also improve the activity of Fe-N-C catalysts. (J.-C. L, et al., ACS Catalysis, 2019, 9, 5929-5934)

2. Highly ORR-active single atom dispersed Fe-N-C electrocatalyst derived from metal organic framework was successfully synthesized. The optimal Zn/Fe ratio was 0.95/0.05 in the precursor for both acidic and alkaline solutions. An onset potential (E_{onset}) of 0.95 V and half-wave potential ($E_{1/2}$) of 0.81 V were observed in the 0.1 M $HClO_4$ solution. The half-wave potential was only lowered by 16 mV after 10000 cycles. It is worth noting that the stability of this catalyst is comparable to or better than the best ones reported in the literature. (F. Xiao, et al., Nano Energy, 2019, 61: 60-68)
3. The Pt-Fe-N-C electrocatalyst was optimized through the impregnation and ball milling method by taking advantage of the hierarchical porous structure in the Fe-N-C support. The electrocatalyst consisting of 0.21 $wt\%_{Pt}$ and 2 $wt\%_{Fe}$. Scanning transmission electron microscopy characterization showed that particles below 2 nm size were homogeneously dispersed on the graphitized carbon support consisted with rich Pt and Fe single atoms. There is no noticeable activity and surface area decay for Pt-Fe-N-C indicating from a negligible change in the half potential and CV curves before and after 70,000 potential cycles at 0.6-1.0 V in an O_2-saturated 0.1 M $HClO_4$. The activity and durability of the Pt-Fe-N-C catalyst was also tested in a single fuel cell. The corresponding peak power density of Pt-Fe-N-C cathode could reach 0.75 W cm^{-2} at 0.35 V, which was 50% higher than that of Fe-N-C (0.50 W cm^{-2} at 0.30 V). (F.Xiao, et al., Nano Energy, 2020, 77, 105192) The performance and durability of Pt-Fe-N-C can be further improved by NH_3 treatment. Pt mass activity of the hybrid catalyst is 3.7 times higher than that of commercial Pt/C in a fuel cell. More importantly, the fuel cell with an ultra-low Pt loading in the cathode (0.015 mgPt cm^{-2}) shows excellent durability, with 97 % activity retention after 100,000 cycles and no noticeable current drop at 0.6 V for over 200 h (F. Xiao, et al., Nature Catalysis, under revision). These results highlight the importance of the synergistic effects among active sites in hybrid electrocatalysts and provide an alternative way to design more active and durable low-Pt electrocatalysts for electrochemical devices.

Potential for further development of the research and the proposed course of action *(maximum half a page)*

Our synthesis methods of Fe-N-C and Pt-Fe-N-C have been patented. This breakthrough could largely reduce the catalyst cost of proton exchange fuel cell and lead to great progress on the clean energy technology development. These electrocatalysts can be commercialized in the near future after addressing the scale-up problems.

7. The Layman's Summary

(describe in layman's language the nature, significance and value of the research project, in no more than 200 words)

Proton exchange membrane fuel cells are clean energy conversion devices that have attracted significant attention for potential use in electric vehicles. The high cost of platinum -based electrocatalysts for oxygen reduction reactions in the cathode of PEMFCs has hindered its widespread adoption. This project develops a novel class of catalyst consisting of single-atom Pt, Fe and N doped carbon structures in collaboration with Chongqing University. In such a material, Pt and Fe atoms are uniformly dispersed in carbon without forming other compounds that are less active in oxygen reduction reactions. The density of active sites are significantly increased as a result. These catalysts enhance both the stability and ORR activity of carbon-based non-precious metal catalysts.

Part C: Research Output

8. Peer-reviewed journal publication(s) arising directly from this research project

(Please attach a copy of each publication and/or the letter of acceptance if not yet submitted in the previous progress report(s). All listed publications must acknowledge RGC's funding support by quoting the specific grant reference.)

Please fill in the following table for each publication.

i. **The Latest Status of Publication**	**Published**	**Accepted but not yet published^**	**Under Review^**	**Under Preparation^** (optional)
	√			
^ For not-yet-published publication, items (vi) to (xxvi) can be left blank if information is not yet available.				
ii. **Author(s)** *(denote the corresponding author with an asterisk*)*	F. Xiao, Y.-C. Wang, Z.-P. Wu, G.Y. Chen, F. Yang, S.Q. Zhu, K. Siddharth, Z.J. Kong, A.L. Lu, J.-C. Li, C.-J. Zhong*, Z.-Y. Zhou*, M.H. Shao*			
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	M.H.Shao	0000-0003-4496-0057	kemshao@ust.hk	
iv. **Title (in published language)**	Recent Advances in Electrocatalysts for Proton Exchange Membrane Fuel Cells and Alkaline Membrane Fuel Cells			
v. **Title in other language (if any)**				
vi. **Full name of journal/book**	Advanced Materials			
vii. **Volume**	33			
viii. **Issue number**	50			
ix. **Pages**	N/A			
x. **Article Number**	2006292			
xi. **Other necessary publishing details (if any)**				
xii. **Year of publication / Year of acceptance**	2021			

xiii. **Original language of the publication**	English
xiv. **Publisher or equivalent**	Wiley-VCH Verlag GmbH & Co. KGaA
xv. **Digital object identifier (DOI)**	10.1002/adma.202006292
xvi. **Abstract (as set out in the journal article)**	The rapid progress of proton exchange membrane fuel cells (PEMFCs) and alkaline exchange membrane fuel cells (AMFCs) has boosted the hydrogen economy concept via diverse energy applications in the past decades. For a holistic understanding of the development status of PEMFCs and AMFCs, recent advancements in electrocatalyst design and catalyst layer optimization, along with cell performance in terms of activity and durability in PEMFCs and AMFCs, are summarized here. The activity, stability, and fuel cell performance of different types of electrocatalysts for both oxygen reduction reaction and hydrogen oxidation reaction are discussed and compared. Research directions on the further development of active, stable, and low-cost electrocatalysts to meet the ultimate commercialization of PEMFCs and AMFCs are also discussed.
xvii. **Open access status** *(Immediate open access / Embargoed open access / Non-open access)*	*Non-open access*
xviii. **Embargo end date (month, year) (if any)**	
xix. **Accessible from the institutional repository** *(Yes or No)*	Yes
xx. **Hyperlink to the publication (the link to institutional repository if preferred) (if any)**	https://repository.ust.hk/ir/Record/1783.1-108859
xxi. **Other affordable means for access (if any)** *(Individual article purchase offered by the publisher / Access through the university libraries (on membership) / Contacting the corresponding author(s))*	
xxii. **Article Processing Charge (APC) for publishing the article in an open access journal*** *(Required / Not required / Not applicable)*	Not required
xxiii. **Total amount of associated APC* (in Hong Kong dollars, if any)**	
xxiv. **Amount of associated APC paid by university* (or universities, in case it is borne by more than one university) (in Hong Kong dollars, if any)**	
xxv. **Copyright retained by author(s)** *(Yes or No)*	No
xxvi. **Number(s) and jurisdiction(s) of the granted patents associated with the article (if any)**	
xxvii. **Submitted to RGC (indicate the year ending of the relevant progress report)**	2021
xxviii. **Attached to this report** *(Yes or No)*	yes
xxix. **Acknowledged the support of RGC** *(Yes or No)*	yes

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ii. **Author(s)** *(denote the corresponding author with an asterisk*)*	F. Xiao, Q. Wang, G.-L. Xu, X.P. Qin, I.H. Hwang, C.-J. Sun, M. Liu, W. Hua, H.-W. Wu, S.Q. Zhu, J.-C. Li, J.G. Wang, Y.M. Zhu, D.J. Wu, Z.D. Wei, M. Gu*, K. Amine*, M.H. Shao*			
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iv. **Title (in published language)**	Durable Electrocatalysts Consisting of Atomically Dispersed Pt and Fe Sites and Pt-Fe Nanoparticles for Proton Exchange Membrane Fuel Cells			
v. **Title in other language (if any)**				
vi. **Full name of journal/book**	Nature catalysis			
vii. **Volume**				
viii. **Issue number**				
ix. **Pages**				
x. **Article Number**				
xi. **Other necessary publishing details (if any)**				
xii. **Year of publication / Year of acceptance**				
xiii. **Original language of the publication**				
xiv. **Publisher or equivalent**				
xv. **Digital object identifier (DOI)**				
xvi. **Abstract (as set out in the journal article)**				
xvii. **Open access status** *(Immediate open access / Embargoed open access / Non-open access)*				
xviii. **Embargo end date (month, year) (if any)**				
xix. **Accessible from the institutional repository** *(Yes or No)*	No			
xx. **Hyperlink to the publication (the link to institutional repository if preferred) (if any)**				
xxi. **Other affordable means for access (if any)** *(Individual article purchase offered by the publisher / Access through the university libraries (on membership) / Contacting the corresponding author(s))*				
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xxviii. **Attached to this report** *(Yes or No)*	yes
xxix. **Acknowledged the support of RGC** *(Yes or No)*	yes

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ii. **Author(s)** *(denote the corresponding author with an asterisk*)*	J.-C. Li, X.P. Qin, F. Xiao, C.H. Liang, M.J. Xu, Y. Meng, E. Sarnello, L. Fang, T. Li, S. Ding, Z.Y. Lyu, S.Q. Zhu, X.P. Pan, P.-X. Hou, C. Liu*, Y.H. Lin*, M.H. Shao*			
iii. **Contact information of the corresponding author(s)**	Name	ORCID (if any)	Email	
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	Y.H. Lin	0000-0003-3791-7587	yuehe.lin@wsu.edu	
	M.H.Shao	0000-0003-4496-0057	kemshao@ust.hk	
iv. **Title (in published language)**	Highly dispersive cerium atoms on carbon nanowires as oxygen reduction reaction electrocatalysts for Zn-air batteries			
v. **Title in other language (if any)**				
vi. **Full name of journal/book**	Nano Letters			
vii. **Volume**	21			
viii. **Issue number**	10			
ix. **Pages**	4508–4515			
x. **Article Number**	N/A			
xi. **Other necessary publishing details (if any)**				
xii. **Year of publication / Year of acceptance**	2021			
xiii. **Original language of the publication**	English			
xiv. **Publisher or equivalent**	American Chemical Society			
xv. **Digital object identifier (DOI)**	10.1021/acs.nanolett.1c01493			
xvi. **Abstract (as set out in the journal article)**	Highly efficient noble-metal-free electrocatalysts for oxygen reduction reaction (ORR) are essential to reduce the costs of fuel cells and metal–air batteries. Herein, a single-atom Ce–N–C catalyst, constructed of atomically dispersed Ce anchored on N-doped porous carbon nanowires, is proposed to boost the ORR. This catalyst has a high Ce content of 8.55 wt % and a high activity with ORR half-wave potentials of 0.88 V in alkaline media and 0.75 V in acidic electrolytes, which are comparable to widely studied Fe–N–C catalysts. A Zn–air battery based on this material shows excellent performance and durability. Density functional theory calculations reveal that atomically dispersed Ce with adsorbed hydroxyl species (OH) can significantly reduce the energy barrier of the rate-determining step resulting in an improved ORR activity.			

xvii. **Open access status** *(Immediate open access / Embargoed open access / Non-open access)*	*Non-open access*
xviii. **Embargo end date (month, year) (if any)**	
xix. **Accessible from the institutional repository** *(Yes or No)*	yes
xx. **Hyperlink to the publication (the link to institutional repository if preferred) (if any)**	https://repository.ust.hk/ir/Record/1783.1-111219
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xxii. **Article Processing Charge (APC) for publishing the article in an open access journal*** *(Required / Not required / Not applicable)*	Not required
xxiii. **Total amount of associated APC* (in Hong Kong dollars, if any)**	
xxiv. **Amount of associated APC paid by university* (or universities, in case it is borne by more than one university) (in Hong Kong dollars, if any)**	
xxv. **Copyright retained by author(s)** *(Yes or No)*	No
xxvi. **Number(s) and jurisdiction(s) of the granted patents associated with the article (if any)**	
xxvii. **Submitted to RGC (indicate the year ending of the relevant progress report)**	2021
xxviii. **Attached to this report** *(Yes or No)*	yes
xxix. **Acknowledged the support of RGC** *(Yes or No)*	yes

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ii. **Author(s)** *(denote the corresponding author with an asterisk*)*	J. Li, Q.Y. Zhou, M.F. Yue, S.G. Chen, J.H. Deng, X.Y. Ping, J. Li, Q. Liao, M.H. Shao, Z.D. Wei*			
iii. **Contact information of the corresponding author(s)**	Name	ORCID (if any)	Email	
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iv. **Title (in published language)**	Cross-linked multi-atom Pt catalyst for highly efficient oxygen reduction catalysis			
v. **Title in other language (if any)**				
vi. **Full name of journal/book**	Applied Catalysis B: Environmental			
vii. **Volume**	284			
viii. **Issue number**	N/A			
ix. **Pages**	N/A			
x. **Article Number**	119728			
xi. **Other necessary publishing details (if any)**				
xii. **Year of publication / Year of acceptance**	2021			
xiii. **Original language of the publication**	English			
xiv. **Publisher or equivalent**	Elsevier Ltd			
xv. **Digital object identifier (DOI)**	10.1016/j.apcatb.2020.119728			
xvi. **Abstract (as set out in the journal article)**	Although single-atom catalysts (SACs) are drawing wide attention because they offer properties that differ from those of conventional nanoparticle (NP)-based catalysts, the lack of neighboring metal centers to cooperate in catalysis limits their actual application in many important chemical processes. Here, we report the synthesis of multi-atom Pt catalyst that consists of cross-linked Pt-Pt metal centers stabilized by atomically dispersed ZnFe-*N*-C support through Pt-N bonds. XAFS analysis reveals that each Pt atom in the multi-atom Pt catalyst coordinates with ~2.6 N atoms and ~4.3 Pt atoms. This novel catalyst combines the merits of SACs and NPs, resulting in 100 % exposure of surface Pt atoms and excellent stability and fuel cell performance. With an ultralow Pt loading of 0.035 mg cm^{-2} at the cathode, the fuel cell delivers a 1.02 W cm^{-2} maximal power output. DFT calculations revealed that the strongly coupled Pt-N bond is critical for stabilizing the cross-linked Pt.			
xvii. **Open access status** *(Immediate open access / Embargoed open access / Non-open access)*	*Non-open access*			
xviii. **Embargo end date (month, year) (if any)**				

xix. **Accessible from the institutional repository** *(Yes or No)*	yes
xx. **Hyperlink to the publication (the link to institutional repository if preferred) (if any)**	https://repository.ust.hk/ir/Record/1783.1-109402
xxi. **Other affordable means for access (if any)** *(Individual article purchase offered by the publisher / Access through the university libraries (on membership) / Contacting the corresponding author(s))*	
xxii. **Article Processing Charge (APC) for publishing the article in an open access journal*** *(Required / Not required / Not applicable)*	Not required
xxiii. **Total amount of associated APC* (in Hong Kong dollars, if any)**	
xxiv. **Amount of associated APC paid by university* (or universities, in case it is borne by more than one university) (in Hong Kong dollars, if any)**	
xxv. **Copyright retained by author(s)** *(Yes or No)*	No
xxvi. **Number(s) and jurisdiction(s) of the granted patents associated with the article (if any)**	
xxvii. **Submitted to RGC (indicate the year ending of the relevant progress report)**	2021
xxviii. **Attached to this report** *(Yes or No)*	yes
xxix. **Acknowledged the support of RGC** *(Yes or No)*	yes

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iv. **Title (in published language)**	Solid-state synthesis of highly dispersed nitrogen-coordinated single iron atom electrocatalysts for proton exchange membrane fuel cells			
v. **Title in other language (if any)**				
vi. **Full name of journal/book**	Nano Letters			
vii. **Volume**	21			
viii. **Issue number**	8			
ix. **Pages**	3633-3639			
x. **Article Number**	N/A			
xi. **Other necessary publishing details (if any)**				
xii. **Year of publication / Year of acceptance**	2021			
xiii. **Original language of the publication**	English			
xiv. **Publisher or equivalent**	American Chemical Society			
xv. **Digital object identifier (DOI)**	10.1021/acs.nanolett.1c00702			

xvi. **Abstract (as set out in the journal article)**	Fe–N–C with atomically dispersed Fe single atoms is the most promising candidate to replace platinum for the oxygen reduction reaction (ORR) in fuel cells. However, the conventional synthesis procedures require quantities solvents and metal precursors, sluggish adsorption process, and tedious washing, resulting in limited metal doping and uneconomical for large-scale production. For the first time, Fe_2O_3 is adopted as the Fe precursor to derive abundant single Fe atoms dispersed on carbon surfaces. The Fe–N–C catalyst synthesized by this simple method shows an excellent ORR activity with half-wave potentials of 0.82 and 0.90 V in acidic and alkaline solutions, respectively. A single fuel cell with an optimized Fe–N–C cathode shows a high peak power density of 0.84 W cm^{-2}. The solid-state transformation synthesis method developed in this study may shed light on mass production of single-atom-based catalysts.
xvii. **Open access status** *(Immediate open access / Embargoed open access / Non-open access)*	*Non-open access*
xviii. **Embargo end date (month, year) (if any)**	
xix. **Accessible from the institutional repository** *(Yes or No)*	yes
xx. **Hyperlink to the publication (the link to institutional repository if preferred) (if any)**	https://repository.ust.hk/ir/Record/1783.1-109890
xxi. **Other affordable means for access (if any)** *(Individual article purchase offered by the publisher / Access through the university libraries (on membership) / Contacting the corresponding author(s))*	
xxii. **Article Processing Charge (APC) for publishing the article in an open access journal*** *(Required / Not required / Not applicable)*	Not required
xxiii. **Total amount of associated APC* (in Hong Kong dollars, if any)**	
xxiv. **Amount of associated APC paid by university* (or universities, in case it is borne by more than one university) (in Hong Kong dollars, if any)**	
xxv. **Copyright retained by author(s)** *(Yes or No)*	No
xxvi. **Number(s) and jurisdiction(s) of the granted patents associated with the article (if any)**	
xxvii. **Submitted to RGC (indicate the year ending of the relevant progress report)**	2021
xxviii. **Attached to this report** *(Yes or No)*	yes
xxix. **Acknowledged the support of RGC** *(Yes or No)*	yes

i. **The Latest Status of Publication**	**Published**	**Accepted but not yet published^**	**Under Review^**	**Under Preparation^** (optional)
	√			
^ For not-yet-published publication, items (vi) to (xxvi) can be left blank if information is not yet available.				
ii. **Author(s)** *(denote the corresponding author with an asterisk*)*	Q.L. Zhao*, Y.A. Wang, W.H. Lai, F. Xiao, Y.X. Lyu, C.Z. Liao, M.H. Shao*			
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	M.H.Shao	0000-0003-4496-0057	kemshao@ust.hk	
iv. **Title (in published language)**	Approaching a high-rate and sustainable production of hydrogen peroxide: oxygen reduction on Co-N-C single-atom electrocatalysts in simulated seawater			
v. **Title in other language (if any)**				
vi. **Full name of journal/book**	Energy and Environmental Science			
vii. **Volume**	14			
viii. **Issue number**	10			
ix. **Pages**	5444-5456			
x. **Article Number**	N/A			
xi. **Other necessary publishing details (if any)**				
xii. **Year of publication / Year of acceptance**	2021			
xiii. **Original language of the publication**	English			
xiv. **Publisher or equivalent**	The Royal Society of Chemistry			
xv. **Digital object identifier (DOI)**	10.1039/D1EE00878A			
xvi. **Abstract (as set out in the journal article)**	Electrochemical production of H_2O_2 from O_2 using simulated seawater provides a promising alternative to the energy-intensive industrial anthraquinone process. In this study, a flow cell system is built for electrocatalytic production of H_2O_2 under an air atmosphere in simulated seawater using cobalt single-atom catalysts (Co SACs). The Co SACs can achieve a high H_2O_2 production rate of 3.4 mol $g_{catalyst}^{-1}$ h^{-1} under an air flow at a current density of 50 mA cm_{geo}^{-2} and long-term stability over 24 h in 0.5 M NaCl. It is found that Co–N_5 rather than the Co–N_4 structure in Co SACs is the main active site for H_2O_2 formation in the two-electron oxygen reduction reaction (ORR) pathway. It also shows high chloride-endurability without inhibition of the ORR process in simulated seawater. The fast production of H_2O_2 on Co–N_5 sites in a flow cell provides a promising path of electrocatalytic oxygen reduction in simulated seawater, eventually converting ubiquitous air and seawater towards energy sustainability.			

xvii. **Open access status** *(Immediate open access / Embargoed open access / Non-open access)*	*Non-open access*
xviii. **Embargo end date (month, year) (if any)**	
xix. **Accessible from the institutional repository** *(Yes or No)*	yes
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xxi. **Other affordable means for access (if any)** *(Individual article purchase offered by the publisher / Access through the university libraries (on membership) / Contacting the corresponding author(s))*	
xxii. **Article Processing Charge (APC) for publishing the article in an open access journal*** *(Required / Not required / Not applicable)*	Not required
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xxviii. **Attached to this report** *(Yes or No)*	yes
xxix. **Acknowledged the support of RGC** *(Yes or No)*	yes

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ii. **Author(s)** *(denote the corresponding author with an asterisk*)*	Y.X. Wang, H.Y. Su, Y.H. He, L.G. Li, S.Q. Zhu (equal contribution), H. Shen, P.F. Xie, X.B. Fu, G.Y. Zhou, C. Feng, D.K. Zhao, F. Xiao, X.J. Zhu, Y.C. Zeng, M.H. Shao*, S.W. Chen*, G. Wu*, J. Zeng*, C. Wang*			
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iv. **Title (in published language)**	Advanced electrocatalysts with single-metal-atom active sites			
v. **Title in other language (if any)**				
vi. **Full name of journal/book**	Chemical Reviews			
vii. **Volume**	120			
viii. **Issue number**	21			
ix. **Pages**	12217–12314			
x. **Article Number**	N/A			
xi. **Other necessary publishing details (if any)**				
xii. **Year of publication / Year of acceptance**	2020			
xiii. **Original language of the publication**	English			
xiv. **Publisher or equivalent**	American Chemical Society			
xv. **Digital object identifier (DOI)**	10.1021/acs.chemrev.0c00594			

xvi. **Abstract (as set out in the journal article)**	Electrocatalysts with single metal atoms as active sites have received increasing attention owing to their high atomic utilization efficiency and exotic catalytic activity and selectivity. This review aims to provide a comprehensive summary on the recent development of such single-atom electrocatalysts (SAECs) for various energy-conversion reactions. The discussion starts with an introduction of the different types of SAECs, followed by an overview of the synthetic methodologies to control the atomic dispersion of metal sites and atomically resolved characterization using state-of-the-art microscopic and spectroscopic techniques. In recognition of the extensive applications of SAECs, the electrocatalytic studies are dissected in terms of various important electrochemical reactions, including hydrogen evolution reaction (HER), oxygen evolution reaction (OER), oxygen reduction reaction (ORR), carbon dioxide reduction reaction (CO2RR), and nitrogen reduction reaction (NRR). Examples of SAECs are deliberated in each case in terms of their catalytic performance, structure–property relationships, and catalytic enhancement mechanisms. A perspective is provided at the end of each section about remaining challenges and opportunities for the development of SAECs for the targeted reaction.
xvii. **Open access status** *(Immediate open access / Embargoed open access / Non-open access)*	*Non-open access*
xviii. **Embargo end date (month, year) (if any)**	
xix. **Accessible from the institutional repository** *(Yes or No)*	yes
xx. **Hyperlink to the publication (the link to institutional repository if preferred) (if any)**	https://repository.ust.hk/ir/Record/1783.1-107280
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xxii. **Article Processing Charge (APC) for publishing the article in an open access journal*** *(Required / Not required / Not applicable)*	Not required
xxiii. **Total amount of associated APC* (in Hong Kong dollars, if any)**	
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xxv. **Copyright retained by author(s)** *(Yes or No)*	No
xxvi. **Number(s) and jurisdiction(s) of the granted patents associated with the article (if any)**	

xxvii. **Submitted to RGC (indicate the year ending of the relevant progress report)**	2021
xxviii. **Attached to this report** *(Yes or No)*	yes
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ii. **Author(s)** *(denote the corresponding author with an asterisk*)*	X.L. Gao, G.L. Zhou, H. Wang, J.Z. Yin*, L.L. Zhang*, F. Xiao, K. Siddharth, S.Q. Zhu, M.H. Shao*			
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iv. **Title (in published language)**	Defect engineering of molybdenum-based materials for electrocatalysis			
v. **Title in other language (if any)**				
vi. **Full name of journal/book**	Catalysts			
vii. **Volume**	10			
viii. **Issue number**	11			
ix. **Pages**	N/A			
x. **Article Number**	1301			
xi. **Other necessary publishing details (if any)**				
xii. **Year of publication / Year of acceptance**	2020			
xiii. **Original language of the publication**	English			
xiv. **Publisher or equivalent**	MDPI			
xv. **Digital object identifier (DOI)**	10.3390/catal10111301			
xvi. **Abstract (as set out in the journal article)**	Molybdenum-based electrocatalysts have been widely applied in electrochemical energy conversion reactions. The essential roles of defects, including doping, vacancies, grain boundaries, and dislocations in improving various electrocatalytic performances have been reported. This review describes the latest development of defect engineering in molybdenum-based materials for hydrogen evolution, oxygen reduction, oxygen evolution, and nitrogen reduction reactions. The types of defects, preparation methods, characterization techniques, and applications of molybdenum-based defect materials are elucidated. Finally, challenges and future research directions for these types of materials are also discussed.			
xvii. **Open access status** *(Immediate open access / Embargoed open access / Non-open access)*	*open access*			
xviii. **Embargo end date (month, year) (if any)**				

xix. **Accessible from the institutional repository** *(Yes or No)*	yes
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xxii. **Article Processing Charge (APC) for publishing the article in an open access journal*** *(Required / Not required / Not applicable)*	Not required
xxiii. **Total amount of associated APC* (in Hong Kong dollars, if any)**	
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xxv. **Copyright retained by author(s)** *(Yes or No)*	No
xxvi. **Number(s) and jurisdiction(s) of the granted patents associated with the article (if any)**	
xxvii. **Submitted to RGC (indicate the year ending of the relevant progress report)**	2021
xxviii. **Attached to this report** *(Yes or No)*	yes
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ii. **Author(s)** *(denote the corresponding author with an asterisk*)*	F. Xiao , G-L. Xu, C.-J. Sun, I. Hwang, M.J. Xu, H.-W. Wu, Z.D. Wei, X.Q. Pan, K. Amine*, M.H. Shao*			
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iv. **Title (in published language)**	Durable hybrid electrocatalysts for proton exchange membrane fuel cells			
v. **Title in other language (if any)**				
vi. **Full name of journal/book**	Nano Energy			
vii. **Volume**	77			
viii. **Issue number**	N/A			
ix. **Pages**	N/A			
x. **Article Number**	105192			
xi. **Other necessary publishing details (if any)**				
xii. **Year of publication / Year of acceptance**	2020			
xiii. **Original language of the publication**	English			
xiv. **Publisher or equivalent**	Elsevier Ltd			
xv. **Digital object identifier (DOI)**	10.1016/j.nanoen.2020.105192			
xvi. **Abstract (as set out in the journal article)**	The low durability of carbon-based non-precious metal electrocatalysts hinders their practical applications in proton exchange membrane fuel cells (PEMFCs). In this study, we rationally design a hybrid Pt-Fe-N-C electrocatalyst with unprecedented durability. It consists of abundant Pt and Fe single atoms homogeneously dispersed on the nitrogen-doped carbon support and a small amount of Pt-Fe alloy nanoparticles. A PEMFC with Pt-Fe-N-C as the cathode shows a larger peak power density (0.75 W cm^{-2}) than that with Fe-N-C as the cathode (0.50 W cm^{-2}). The remarkable durability of Pt-Fe-N-C is reflected from no noticeable drop in the half-wave potential after 70000 potential cycles between 0.6 and 1.0 V in the liquid cell, and 80% current retention after 85 h of potential hold at 0.4 V in the fuel cell. This work demonstrates the feasibility of improving the durability of Fe-N-C material via ultra-low Pt doping and makes non-precious metal electrocatalysts be close to achieving commercial metrics.			

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xviii. **Embargo end date (month, year) (if any)**	
xix. **Accessible from the institutional repository** *(Yes or No)*	yes
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xxv. **Copyright retained by author(s)** *(Yes or No)*	No
xxvi. **Number(s) and jurisdiction(s) of the granted patents associated with the article (if any)**	
xxvii. **Submitted to RGC (indicate the year ending of the relevant progress report)**	2021
xxviii. **Attached to this report** *(Yes or No)*	yes
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ii. **Author(s)** *(denote the corresponding author with an asterisk*)*	Y. Yao , S.Q. Zhu , H.J. Wang, H. Li, M.H. Shao*			
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iv. **Title (in published language)**	A spectroscopic study of electrochemical nitrogen and nitrate reduction on rhodium surfaces			
v. **Title in other language (if any)**				
vi. **Full name of journal/book**	Angewandte Chemie International Edition			
vii. **Volume**	59			
viii. **Issue number**	26			
ix. **Pages**	10479-10483			
x. **Article Number**	N/A			
xi. **Other necessary publishing details (if any)**				
xii. **Year of publication / Year of acceptance**	2020			
xiii. **Original language of the publication**	English			
xiv. **Publisher or equivalent**	Wiley-VCH Verlag GmbH & Co. KGaA			
xv. **Digital object identifier (DOI)**	10.1002/anie.202003071			
xvi. **Abstract (as set out in the journal article)**	Rh is a promising electrocatalyst for the nitrogen reduction reaction (NRR) given its suitable nitrogen-adsorption energy and low overpotential. However, the NRR pathway on Rh surfaces remains unknown. In this study, we employ surface-enhanced infrared-absorption spectroscopy (SEIRAS) and differential electrochemical mass spectrometry (DEMS) to study the reaction mechanism of NRR on Rh. N_2H_x ($0 \leq x \leq 2$) is detected with a N=N stretching mode at $\approx 2020\ cm^{-1}$ by SEIRAS and a signal at $m/z=29$ by DEMS. A new two-step reaction pathway on Rh surfaces is proposed that involves an electrochemical process with a two-electron transfer to form N_2H_2 and its subsequent decomposition in the electrolyte producing NH_3. Our results also indicate that nitrate reduction and the NRR share the same reaction intermediate N_2H_x.			
xvii. **Open access status** *(Immediate open access / Embargoed open access / Non-open access)*	*Non-open access*			
xviii. **Embargo end date (month, year) (if any)**				
xix. **Accessible from the institutional repository** *(Yes or No)*	yes			
xx. **Hyperlink to the publication (the link to institutional repository if preferred) (if any)**	https://repository.ust.hk/ir/Record/1783.1-103618			

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xxii. **Article Processing Charge (APC) for publishing the article in an open access journal*** *(Required / Not required / Not applicable)*	Not required
xxiii. **Total amount of associated APC* (in Hong Kong dollars, if any)**	
xxiv. **Amount of associated APC paid by university* (or universities, in case it is borne by more than one university) (in Hong Kong dollars, if any)**	
xxv. **Copyright retained by author(s)** *(Yes or No)*	No
xxvi. **Number(s) and jurisdiction(s) of the granted patents associated with the article (if any)**	
xxvii. **Submitted to RGC (indicate the year ending of the relevant progress report)**	2021
xxviii. **Attached to this report** *(Yes or No)*	yes
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ii. **Author(s)** *(denote the corresponding author with an asterisk*)*	Y. Yao, J. Wang, U.B. Shahid, M. Gu, H.J. Wang, H. Li*, M.H. Shao*			
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iv. **Title (in published language)**	Electrochemical synthesis of ammonia from nitrogen under ambient conditions: current status and challenges			
v. **Title in other language (if any)**				
vi. **Full name of journal/book**	Electrochemical Energy Reviews			
vii. **Volume**	3			
viii. **Issue number**	2			
ix. **Pages**	239–270			
x. **Article Number**	N/A			
xi. **Other necessary publishing details (if any)**				
xii. **Year of publication / Year of acceptance**	2020			
xiii. **Original language of the publication**	English			
xiv. **Publisher or equivalent**	Springer Nature			
xv. **Digital object identifier (DOI)**	10.1007/s41918-019-00061-3			

xvi. **Abstract (as set out in the journal article)**	The electrochemical synthesis of ammonia under mild conditions has attracted significant interest in recent years because it can allow for the direct conversion of renewable electricity to chemical energy in the form of ammonia, which is an ideal medium for energy storage and transportation. And in contradistinction to the Haber–Bosch process, the electrochemical synthesis of ammonia is a much more environmentally friendly process that can operate under mild conditions with zero carbon dioxide (CO_2) emission. However, this process is severely hindered by poor ammonia formation rates and Faradaic efficiency due to the competing hydrogen evolution reaction. Based on this, a review focused on the current status and challenges of the electrochemical synthesis of ammonia is imperative to promulgate this key process and promote future research. And therefore, this review will systematically survey the recent progress of the electrochemical synthesis of ammonia; and different from previous reviews, this review will include not only advances in electrocatalysts, but also in reactors, electrolytes and reaction mechanisms. In addition, future research directions and strategies to improve the performance of ammonia electrochemical synthesis systems are proposed with the aim of shedding light on the future direction of ammonia synthesis through nitrogen electrochemical reduction.
xvii. **Open access status** *(Immediate open access / Embargoed open access / Non-open access)*	*Non-open access*
xviii. **Embargo end date (month, year) (if any)**	
xix. **Accessible from the institutional repository** *(Yes or No)*	yes
xx. **Hyperlink to the publication (the link to institutional repository if preferred) (if any)**	https://repository.ust.hk/ir/Record/1783.1-102513
xxi. **Other affordable means for access (if any)** *(Individual article purchase offered by the publisher / Access through the university libraries (on membership) / Contacting the corresponding author(s))*	
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xxv. **Copyright retained by author(s)** *(Yes or No)*	No

xxvi. **Number(s) and jurisdiction(s) of the granted patents associated with the article (if any)**	
xxvii. **Submitted to RGC (indicate the year ending of the relevant progress report)**	2021
xxviii. **Attached to this report** *(Yes or No)*	yes
xxix. **Acknowledged the support of RGC** *(Yes or No)*	yes

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ii. **Author(s)** *(denote the corresponding author with an asterisk*)*	S.J. Yi, X.P. Qin , C.H. Liang , J.S. Li, R. Rajagopalan, Z.J. Zhang, J.Y. Song, Y.G. Tang, F.Y. Cheng, H.Y. Wang ,*, M.H. Shao*			
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iv. **Title (in published language)**	Insights into $KMnO_4$ etched N-rich carbon nanotubes as advanced electrocatalysts for Zn-air batteries			
v. **Title in other language (if any)**				
vi. **Full name of journal/book**	Applied Catalysis B: Environmental			
vii. **Volume**	264			
viii. **Issue number**	N/A			
ix. **Pages**	N/A			
x. **Article Number**	118537			
xi. **Other necessary publishing details (if any)**				
xii. **Year of publication / Year of acceptance**	2020			
xiii. **Original language of the publication**	English			
xiv. **Publisher or equivalent**	Elsevier Ltd			
xv. **Digital object identifier (DOI)**	10.1016/j.apcatb.2019.118537			
xvi. **Abstract (as set out in the journal article)**	Increasing the number of active sites is critical for developing N-doped carbon electrocatalysts towards oxygen reduction reaction (ORR) in fuel cells and metal-air batteries applications. Herein, we prepared N-doped carbon nanotubes (N-CNT) with enriched pyridinic N and abundant defects resulted from the etching of $KMnO_4$ of the precursor (polypyrrole). It was observed that the content of pyridinic N could be well controlled by regulating the etching time. The resultant catalyst displayed a superior ORR activity compared commercial Pt/C in an alkaline solution, which was further confirmed by home-made Zn-air batteries. Density functional theory (DFT) computations showed that the superior catalytic activity originated from the second nearest carbon atom to the pyridinic-N at the edge. This work provides a simple etching approach to alter the N configuration and the amount of defects in N-doped CNT, which can be extended to many other energy conversion materials.			

xvii. **Open access status** *(Immediate open access / Embargoed open access / Non-open access)*	*Non-open access*
xviii. **Embargo end date (month, year) (if any)**	
xix. **Accessible from the institutional repository** *(Yes or No)*	yes
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xxiii. **Total amount of associated APC* (in Hong Kong dollars, if any)**	
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xxv. **Copyright retained by author(s)** *(Yes or No)*	No
xxvi. **Number(s) and jurisdiction(s) of the granted patents associated with the article (if any)**	
xxvii. **Submitted to RGC (indicate the year ending of the relevant progress report)**	2019
xxviii. **Attached to this report** *(Yes or No)*	yes
xxix. **Acknowledged the support of RGC** *(Yes or No)*	yes

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ii. **Author(s)** *(denote the corresponding author with an asterisk*)*	J.-C. Li , H. Zhong, M.J. Xu , T. Li, L.G. Wang, Q.R Shi, S. Feng, Z.Y. Lyu, D. Liu, D. Du, S.P. Beckman, X.Q. Pan, Y.H. Lin*, M.H. Shao*			
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iv. **Title (in published language)**	Boosting the activity of Fe-Nx moieties in Fe-N-C electrocatalysts via phosphorus doping for oxygen reduction reaction			
v. **Title in other language (if any)**	P掺杂提高Fe–N–C催化剂中Fe–Nx活性基团的氧还原催化活性			
vi. **Full name of journal/book**	Science China Materials			
vii. **Volume**	63			
viii. **Issue number**	6			
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x. **Article Number**	N/A			
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xii. **Year of publication / Year of acceptance**	2020			
xiii. **Original language of the publication**	English			
xiv. **Publisher or equivalent**	Springer Nature			
xv. **Digital object identifier (DOI)**	10.1007/s40843-019-1207-y			
xvi. **Abstract (as set out in the journal article)**	The Fe-N-C material is a promising non-noble-metal electrocatalyst for oxygen reduction reaction (ORR). Further improvement on the ORR activity is highly desired in order to replace Pt/C in acidic media. Herein, we developed a new-type of single-atom Fe-N-C electrocatalyst, in which Fe-N_x active sites were modified by P atoms. The half-wave potential of the optimized material reached 0.858 V, which is 23 mV higher than that of the pristine one in a 0.1 mol L^{-1} $HClO_4$ solution. Density functional theory (DFT) calculations revealed that P doping can reduce the thermodynamic over potential of the rate determining step and consequently improve the ORR activity.			
xvii. **Open access status** *(Immediate open access / Embargoed open access / Non-open access)*	*Non-open access*			
xviii. **Embargo end date (month, year) (if any)**				
xix. **Accessible from the institutional repository** *(Yes or No)*	yes			

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xxiii. **Total amount of associated APC* (in Hong Kong dollars, if any)**	
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xxv. **Copyright retained by author(s)** *(Yes or No)*	No
xxvi. **Number(s) and jurisdiction(s) of the granted patents associated with the article (if any)**	
xxvii. **Submitted to RGC (indicate the year ending of the relevant progress report)**	2019
xxviii. **Attached to this report** *(Yes or No)*	yes
xxix. **Acknowledged the support of RGC** *(Yes or No)*	yes

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ii. **Author(s)** *(denote the corresponding author with an asterisk*)*	F. Xiao , X.P. Qin , M.J. Xu , S.Q. Zhu , L.L. Zhang , Y.M. Hong, S.-I. Choi, Q.W. Chang , Y. Xu , X.Q, Pan*, M.H. Shao*			
iii. **Contact information of the corresponding author(s)**	Name	ORCID (if any)	Email	
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iv. **Title (in published language)**	Impact of heat treatment on the electrochemical properties of carbon-supported octahedral Pt-Ni nanoparticles			
v. **Title in other language (if any)**				
vi. **Full name of journal/book**	ACS Catalysis			
vii. **Volume**	9			
viii. **Issue number**	12			
ix. **Pages**	11189–11198			
x. **Article Number**	N/A			
xi. **Other necessary publishing details (if any)**				
xii. **Year of publication / Year of acceptance**	2019			
xiii. **Original language of the publication**	English			
xiv. **Publisher or equivalent**	American Chemical Society			
xv. **Digital object identifier (DOI)**	10.1021/acscatal.9b03206			

xvi. **Abstract (as set out in the journal article)**	Thermal annealing is commonly used to remove surface contaminants and redistribute elements in alloys. In this study, Pt–Ni alloy nanoparticles supported on carbon black are selected as a model catalyst to understand the relationship between the annealing conditions (temperature and atmosphere) and the electrocatalytic performance for oxygen reduction, hydrogen evolution, and ethanol oxidation reactions. The impacts of thermal treatment temperature and atmosphere on structures, compositions, and in turn electrocatalytic activities are systematically studied. Interestingly, an ultrathin carbon layer can be formed on the nanoparticle surface by heat treatment in Ar atmosphere at temperatures higher than 350 °C, which significantly decreases its activity toward oxygen reduction and ethanol oxidation reactions. This carbon coating, however, is absent in other atmospheres including N_2, air, 7% H_2/Ar, and vacuum. Aberration-corrected scanning transmission electron microscopic characterizations with atomic-level resolutions confirm the formation of a Ni-enriched surface on Pt–Ni/C after treatment in Ar, which plays a critical role in catalyzing the growth of stable carbon layers from the surrounding carbons. Further density functional theory calculation results suggest that the absence of a carbon layer in N_2 may originate from the stable N–C bond formed during heat treatment and passivation effect of adsorbed N_2. It illustrates different effects of inert gases on carbon layer formation by combining experimental and computational approaches. These results may shed light on the proper design of postheat treatment protocols for carbon-supported catalysts and may also provide a feasible method to coat carbon layers on nanoparticle surfaces for various energy storage and conversion applications.
xvii. **Open access status** *(Immediate open access / Embargoed open access / Non-open access)*	*Non-open access*
xviii. **Embargo end date (month, year) (if any)**	
xix. **Accessible from the institutional repository** *(Yes or No)*	yes
xx. **Hyperlink to the publication (the link to institutional repository if preferred) (if any)**	https://repository.ust.hk/ir/Record/1783.1-100800
xxi. **Other affordable means for access (if any)** *(Individual article purchase offered by the publisher / Access through the university libraries (on membership) / Contacting the corresponding author(s))*	

xxii. **Article Processing Charge (APC) for publishing the article in an open access journal*** *(Required / Not required / Not applicable)*	Not required
xxiii. **Total amount of associated APC* (in Hong Kong dollars, if any)**	
xxiv. **Amount of associated APC paid by university* (or universities, in case it is borne by more than one university) (in Hong Kong dollars, if any)**	
xxv. **Copyright retained by author(s)** *(Yes or No)*	No
xxvi. **Number(s) and jurisdiction(s) of the granted patents associated with the article (if any)**	
xxvii. **Submitted to RGC (indicate the year ending of the relevant progress report)**	2019
xxviii. **Attached to this report** *(Yes or No)*	yes
xxix. **Acknowledged the support of RGC** *(Yes or No)*	yes

i. **The Latest Status of Publication**	**Published**	**Accepted but not yet published^**	**Under Review^**	**Under Preparation^** (optional)
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^ For not-yet-published publication, items (vi) to (xxvi) can be left blank if information is not yet available.				
ii. **Author(s)** *(denote the corresponding author with an asterisk*)*	Y. Yao, H.J. Wang, X.-Z. Yuan, H. Li,* M.H. Shao*			
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iv. **Title (in published language)**	Electrochemical nitrogen reduction reaction on ruthenium			
v. **Title in other language (if any)**				
vi. **Full name of journal/book**	ACS Energy Letters			
vii. **Volume**	4			
viii. **Issue number**	6			
ix. **Pages**	1336–1341			
x. **Article Number**	N/A			
xi. **Other necessary publishing details (if any)**				
xii. **Year of publication / Year of acceptance**	2019			
xiii. **Original language of the publication**	English			
xiv. **Publisher or equivalent**	American Chemical Society			
xv. **Digital object identifier (DOI)**	10.1021/acsenergylett.9b00699			
xvi. **Abstract (as set out in the journal article)**	Ruthenium is a good catalyst for ammonia synthesis in the Haber–Bosch process and a promising electrocatalyst for electrochemical N_2 reduction reaction (NRR). However, the NRR pathway on Ru is unclear because of the lack of information on reaction intermediates. Surface-enhanced infrared absorption spectroscopy combined with electrochemical measurements is employed to study the NRR mechanisms on Ru thin film. During the nitrogen reduction, the $*N_2H_x$ ($0 \leq x \leq 2$) was detected with the band of N=N stretching (~1940 cm^{-1}) at potentials below 0.2 V in an N_2-satureated $HClO_4$ solution. The coverage of $*N_2H_x$ on the Ru surface was significantly increased with the potential decreasing from 0.2 to −0.4 V. The formed $*N_2H_x$ species could be oxidized at potentials higher than −0.1 V. In an N_2-satureated KOH solution, no N-related infrared absorption band was observed on Ru surfaces, indicating that the adsorption of nitrogen molecules on Ru surfaces is very weak.			
xvii. **Open access status** *(Immediate open access / Embargoed open access / Non-open access)*	*Non-open access*			

xviii. **Embargo end date (month, year) (if any)**	
xix. **Accessible from the institutional repository** *(Yes or No)*	yes
xx. **Hyperlink to the publication (the link to institutional repository if preferred) (if any)**	https://repository.ust.hk/ir/Record/1783.1-97486
xxi. **Other affordable means for access (if any)** *(Individual article purchase offered by the publisher / Access through the university libraries (on membership) / Contacting the corresponding author(s))*	
xxii. **Article Processing Charge (APC) for publishing the article in an open access journal*** *(Required / Not required / Not applicable)*	Not required
xxiii. **Total amount of associated APC* (in Hong Kong dollars, if any)**	
xxiv. **Amount of associated APC paid by university* (or universities, in case it is borne by more than one university) (in Hong Kong dollars, if any)**	
xxv. **Copyright retained by author(s)** *(Yes or No)*	No
xxvi. **Number(s) and jurisdiction(s) of the granted patents associated with the article (if any)**	
xxvii. **Submitted to RGC (indicate the year ending of the relevant progress report)**	2019
xxviii. **Attached to this report** *(Yes or No)*	yes
xxix. **Acknowledged the support of RGC** *(Yes or No)*	yes

i. **The Latest Status of Publication**	**Published**	**Accepted but not yet published^**	**Under Review^**	**Under Preparation^** (optional)
	√			
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ii. **Author(s)** *(denote the corresponding author with an asterisk*)*	Z.X. Huang, X.P. Qin , G.Z. Li, W.C., Yao, J. Liu, N.G. Wang, K. Ithisuphalap, G. Wu*, M.H. Shao*, Z.C. Shi*			
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	M.H.Shao	0000-0003-4496-0057	kemshao@ust.hk	
iv. **Title (in published language)**	Co_3O_4 nanoparticles anchored on nitrogen-doped partially exfoliated multiwall carbon nanotubes as an enhanced oxygen electrocatalyst for the rechargeable and flexible solid-state Zn-air battery			
v. **Title in other language (if any)**				
vi. **Full name of journal/book**	ACS Applied Energy Materials			
vii. **Volume**	2			
viii. **Issue number**	6			
ix. **Pages**	4428-4438			
x. **Article Number**				
xi. **Other necessary publishing details (if any)**				
xii. **Year of publication / Year of acceptance**	2019			
xiii. **Original language of the publication**	English			
xiv. **Publisher or equivalent**	American Chemical Society			
xv. **Digital object identifier (DOI)**	10.1021/acsaem.9b00675			

xvi. **Abstract (as set out in the journal article)**	This work presents a desirable bifunctional catalyst—Co_3O_4 nanoparticles anchored on nitrogen-doped partially exfoliated multiwall carbon nanotubes (Co_3O_4/N-p-MCNTs)—for oxygen reduction reaction (ORR) and oxygen evolution reaction (OER) for the rechargeable and flexible solid-state Zn–air battery. The Co_3O_4/N-p-MCNTs demonstrates good catalytic performance with the ORR half-wave potential of 0.760 V (vs RHE). Additionally, the Co_3O_4/N-p-MCNTs exhibits superior limiting current density with higher stability than Pt/C in alkaline solutions. The catalyst obtains a low operating potential (E_{j10}) of 1.62 V (vs RHE) to achieve a 10 mA cm^{-2} current density for OER. The potential difference (ΔE) between E_{j10} of OER and ORR half-wave potential is 0.86 V, which is smaller than that of many highly active bifunctional catalysts reported recently. Moreover, a Zn–air battery utilizing Co_3O_4/N-p-MCNTs as the catalyst in cathode could successfully generate a specific capacity of 768 mAh g^{-1} at 10 mA cm^{-2}, and there is no voltage loss after a continuous discharge of 135 h. The fabricated solid-state rechargeable Zn–air battery displays a high power density and superior long-term cycling stability. Furthermore, first-principles density functional theory simulations were conducted to explore the interfacial properties of the hybrid catalyst, hinting that the N-p-MCNTs could significantly enhance the electrical conductivity of Co_3O_4 nanoparticles. The free energy diagrams generated from our simulations suggest that the N-p-MCNTs influence the superior ORR performance, while cobalt oxide affects the favored performance of OER. The obtained results confirm that the Co_3O_4/N-p-MCNTs catalyst would have a broad impact and could be used for renewable energy conversion devices.
xvii. **Open access status** *(Immediate open access / Embargoed open access / Non-open access)*	*Non-open access*
xviii. **Embargo end date (month, year) (if any)**	
xix. **Accessible from the institutional repository** *(Yes or No)*	yes
xx. **Hyperlink to the publication (the link to institutional repository if preferred) (if any)**	https://repository.ust.hk/ir/Record/1783.1-98454
xxi. **Other affordable means for access (if any)** *(Individual article purchase offered by the publisher / Access through the university libraries (on membership) / Contacting the corresponding author(s))*	

xxii. **Article Processing Charge (APC) for publishing the article in an open access journal*** *(Required / Not required / Not applicable)*	Not required
xxiii. **Total amount of associated APC* (in Hong Kong dollars, if any)**	
xxiv. **Amount of associated APC paid by university* (or universities, in case it is borne by more than one university) (in Hong Kong dollars, if any)**	
xxv. **Copyright retained by author(s)** *(Yes or No)*	No
xxvi. **Number(s) and jurisdiction(s) of the granted patents associated with the article (if any)**	
xxvii. **Submitted to RGC (indicate the year ending of the relevant progress report)**	2019
xxviii. **Attached to this report** *(Yes or No)*	yes
xxix. **Acknowledged the support of RGC** *(Yes or No)*	yes

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ii. **Author(s)** *(denote the corresponding author with an asterisk*)*	J.-C. Li, F. Xiao, H. Zhong, T. Li, M.J. Xu d, L. Ma, M. Cheng, D. Liu. S. Feng, Q.R. Shi, H.-M. Cheng, C. Liu*, D. Du, S.P. Beckman, X.Q. Pan, Y.H. Lin*, M.H. Shao*			
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	M.H.Shao	0000-0003-4496-0057	kemshao@ust.hk	
iv. **Title (in published language)**	Secondary-atom-assisted synthesis of single iron atoms anchored on N-doped carbon nanowires for oxygen reduction reaction			
v. **Title in other language (if any)**				
vi. **Full name of journal/book**	ACS Catalysis			
vii. **Volume**	9			
viii. **Issue number**	7			
ix. **Pages**	5929-5934			
x. **Article Number**	N/A			
xi. **Other necessary publishing details (if any)**				
xii. **Year of publication / Year of acceptance**	2019			
xiii. **Original language of the publication**	English			
xiv. **Publisher or equivalent**	American Chemical Society			
xv. **Digital object identifier (DOI)**	10.1021/acscatal.9b00869			

xvi. **Abstract (as set out in the journal article)**	The development of efficient Fe–N–C materials enriched with single-atom Fe sites toward the oxygen reduction reaction (ORR) is still a great challenge because Fe atoms are mobile and easily aggregate into nanoparticles during the high-temperature treatment. Herein, we proposed a facile and universal secondary-atom-assisted strategy to prepare atomic iron sites with high density hosted on porous nitrogen-doped carbon nanowires (Fe–NCNWs). The Fe–NCNWs showed an impressive half-wave potential ($E_{1/2}$) of 0.91 V and average kinetic current density (J_K) of 6.0 mA cm^{-2} at 0.9 V in alkaline media. They also held a high ORR activity in acidic solution with the $E_{1/2}$ of 0.82 V and average J_K of 8.0 mA cm^{-2} at 0.8 V. Density functional theory calculations demonstrated that the high ORR activity achieved is originated from single-atom iron sites that decrease the energy barrier in the reaction path efficiently.
xvii. **Open access status** *(Immediate open access / Embargoed open access / Non-open access)*	*Non-open access*
xviii. **Embargo end date (month, year) (if any)**	
xix. **Accessible from the institutional repository** *(Yes or No)*	yes
xx. **Hyperlink to the publication (the link to institutional repository if preferred) (if any)**	https://repository.ust.hk/ir/Record/1783.1-98416
xxi. **Other affordable means for access (if any)** *(Individual article purchase offered by the publisher / Access through the university libraries (on membership) / Contacting the corresponding author(s))*	
xxii. **Article Processing Charge (APC) for publishing the article in an open access journal*** *(Required / Not required / Not applicable)*	Not required
xxiii. **Total amount of associated APC* (in Hong Kong dollars, if any)**	
xxiv. **Amount of associated APC paid by university* (or universities, in case it is borne by more than one university) (in Hong Kong dollars, if any)**	
xxv. **Copyright retained by author(s)** *(Yes or No)*	No
xxvi. **Number(s) and jurisdiction(s) of the granted patents associated with the article (if any)**	
xxvii. **Submitted to RGC (indicate the year ending of the relevant progress report)**	2019
xxviii. **Attached to this report** *(Yes or No)*	yes
xxix. **Acknowledged the support of RGC** *(Yes or No)*	yes

i. **The Latest Status of Publication**	**Published**	**Accepted but not yet published^**	**Under Review^**	**Under Preparation^** (optional)
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ii. **Author(s)** *(denote the corresponding author with an asterisk*)*	X.P. Qin, S.Q. Zhu, F. Xiao, L.L. Zhang, M.H. Shao*			
iii. **Contact information of the corresponding author(s)**	Name	ORCID (if any)	Email	
	M.H.Shao	0000-0003-4496-0057	kemshao@ust.hk	
iv. **Title (in published language)**	Active Sites on Heterogeneous Single-Iron-Atom Electrocatalysts in CO_2 Reduction Reaction			
v. **Title in other language (if any)**				
vi. **Full name of journal/book**	ACS Energy Letters			
vii. **Volume**	4			
viii. **Issue number**	7			
ix. **Pages**	1778-1783			
x. **Article Number**	N/A			
xi. **Other necessary publishing details (if any)**				
xii. **Year of publication / Year of acceptance**	2019			
xiii. **Original language of the publication**	English			
xiv. **Publisher or equivalent**	American Chemical Society			
xv. **Digital object identifier (DOI)**	10.1021/acsenergylett.9b01015			
xvi. **Abstract (as set out in the journal article)**	Nitrogen-coordinated single-metal-atom catalysts (Me–N–C) are promising candidates for CO_2-to-CO electrocatalytic conversion. The nature of real active sites in this type of electrocatalyst, however, is not clear. In this Letter, we study the specific interactions between the reaction intermediates and a model single-iron-atom catalyst (Fe–N–C) by combining in situ infrared absorption spectroscopy and density functional theory (DFT) calculations. For the first time, we confirm that the Fe centers in $Fe–N_4$ moieties hosted by the complete graphitic layer are poisoned by strongly adsorbed CO and should not be the real active sites for gaseous CO production. Further DFT calculation results suggest that the high CO selectivity and reaction rate may originate from $Fe–N_4$ moieties embedded in a defective graphitic layer that have balanced binding energies of adsorbed COOH and CO species. These findings add significant new insights into the mechanisms of CO_2 reduction on carbon-based single-atom electrocatalysts.			

xvii. **Open access status** *(Immediate open access / Embargoed open access / Non-open access)*	*Non-open access*
xviii. **Embargo end date (month, year) (if any)**	
xix. **Accessible from the institutional repository** *(Yes or No)*	yes
xx. **Hyperlink to the publication (the link to institutional repository if preferred) (if any)**	https://repository.ust.hk/ir/Record/1783.1-97916
xxi. **Other affordable means for access (if any)** *(Individual article purchase offered by the publisher / Access through the university libraries (on membership) / Contacting the corresponding author(s))*	
xxii. **Article Processing Charge (APC) for publishing the article in an open access journal*** *(Required / Not required / Not applicable)*	Not required
xxiii. **Total amount of associated APC* (in Hong Kong dollars, if any)**	
xxiv. **Amount of associated APC paid by university* (or universities, in case it is borne by more than one university) (in Hong Kong dollars, if any)**	
xxv. **Copyright retained by author(s)** *(Yes or No)*	No
xxvi. **Number(s) and jurisdiction(s) of the granted patents associated with the article (if any)**	
xxvii. **Submitted to RGC (indicate the year ending of the relevant progress report)**	2019
xxviii. **Attached to this report** *(Yes or No)*	yes
xxix. **Acknowledged the support of RGC** *(Yes or No)*	yes

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ii. **Author(s)** *(denote the corresponding author with an asterisk*)*	F. Xiao , G.L. Xu, C.J. Sun, M.J. Xu , W. Wen, Q. Wang, M. Gu, S.Q. Zhu , Y.Y. Li, Z.D. Wei, X.Q. Pan, J.G. Wang, K. Amine*, M.H. Shao*			
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iv. **Title (in published language)**	Nitrogen-coordinated single iron atom catalysts derived from metal organic frameworks for oxygen reduction reaction			
v. **Title in other language (if any)**				
vi. **Full name of journal/book**	Nano Energy			
vii. **Volume**	61			
viii. **Issue number**	N/A			
ix. **Pages**	60-68			
x. **Article Number**	N/A			
xi. **Other necessary publishing details (if any)**				
xii. **Year of publication / Year of acceptance**	2019			
xiii. **Original language of the publication**	English			
xiv. **Publisher or equivalent**	Elsevier Ltd			
xv. **Digital object identifier (DOI)**	10.1016/j.nanoen.2019.04.033			
xvi. **Abstract (as set out in the journal article)**	Iron and nitrogen co-doped carbon (Fe-*N*-C) catalysts hold great promise to replace platinum group metal used for the oxygen reduction reaction (ORR) in low-temperature fuel cells. However, general synthesis routes require tedious acid washing and extensive heat treatment, usually resulting in uncontrollable morphologies and undesirable compounds. In this work, a zeolitic imidazolate framework (ZIF-8) was employed as a self-template for one-pot synthesis of a Fe-*N*-C catalyst consisting of uniformly dispersed Fe single atoms. Atomically dispersed Fe atoms were well distributed along the edges of the porous carbon matrix. Each of the Fe atoms was coordinated with four N atoms in the plane and two O atoms in the axial direction. The optimized Fe-*N*-C catalyst showed excellent ORR activities with half-wave potentials of 0.81 and 0.90 V in acidic and alkaline solutions, respectively. The results may be important for the optimization of single-atom-based catalysts for various reactions.			

xvii. **Open access status** *(Immediate open access / Embargoed open access / Non-open access)*	*Non-open access*
xviii. **Embargo end date (month, year) (if any)**	
xix. **Accessible from the institutional repository** *(Yes or No)*	yes
xx. **Hyperlink to the publication (the link to institutional repository if preferred) (if any)**	https://repository.ust.hk/ir/Record/1783.1-96984
xxi. **Other affordable means for access (if any)** *(Individual article purchase offered by the publisher / Access through the university libraries (on membership) / Contacting the corresponding author(s))*	
xxii. **Article Processing Charge (APC) for publishing the article in an open access journal*** *(Required / Not required / Not applicable)*	Not required
xxiii. **Total amount of associated APC* (in Hong Kong dollars, if any)**	
xxiv. **Amount of associated APC paid by university* (or universities, in case it is borne by more than one university) (in Hong Kong dollars, if any)**	
xxv. **Copyright retained by author(s)** *(Yes or No)*	No
xxvi. **Number(s) and jurisdiction(s) of the granted patents associated with the article (if any)**	
xxvii. **Submitted to RGC (indicate the year ending of the relevant progress report)**	2019
xxviii. **Attached to this report** *(Yes or No)*	yes
xxix. **Acknowledged the support of RGC** *(Yes or No)*	yes

xxx. **The Latest Status of Publication**	**Published**	**Accepted but not yet published^**	**Under Review^**	**Under Preparation^** (optional)
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^ For not-yet-published publication, items (vi) to (xxvi) can be left blank if information is not yet available.				
xxxi. **Author(s)** *(denote the corresponding author with an asterisk*)*	J.-C. Li, D. Liu, D. Du, Y.H. Lin, Z.D. Wei, M.H. Shao*			
xxxii. **Contact information of the corresponding author(s)**	Name	ORCID (if any)	Email	
	M.H.Shao	0000-0003-4496-0057	kemshao@ust.hk	
xxxiii. **Title (in published language)**	Dispersive single-atom metals anchored on functionalized nanocarbons for electrochemical reactions			
xxxiv. **Title in other language (if any)**				
xxxv. **Full name of journal/book**	Topics in Current Chemistry			
xxxvi. **Volume**	377			
xxxvii. **Issue number**	1			
xxxviii. **Pages**	127-148			
xxxix. **Article Number**	4			
xl. **Other necessary publishing details (if any)**				
xli. **Year of publication / Year of acceptance**	2019			
xlii. **Original language of the publication**	English			
xliii. **Publisher or equivalent**	Springer Nature Switzerland AG.			
xliv. **Digital object identifier (DOI)**	10.1007/978-3-030-43294-2_5			
xlv. **Abstract (as set out in the journal article)**	The use of dispersive single-atom metals anchored on functionalized carbon nanomaterials as electrocatalysts for electrochemical energy conversion reactions represents a burgeoning area of research, due to their unique characteristics of low coordination number, uniform coordination environment, and maximum atomic utilization. Here we highlight the advanced synthetic methods, characterization techniques, and electrochemical applications for carbon-based single-atom metal catalysts, and provide illustrative correlations between molecular/electronic structures and specific catalytic activity for O_2 reduction, water splitting, and other emerging reactions including CO_2 reduction, H_2O_2 production, and N_2 reduction. We also discuss fundamental principles for the future design of carbon-based single-atom metal catalysts for specific electrochemical reactions. In addition, we explore the challenges and opportunities that lie ahead in further work with carbon-based single atom metal electrocatalysts.			
xlvi. **Open access status** *(Immediate open access / Embargoed open access / Non-open access)*	*Non-open access*			

xlvii. **Embargo end date (month, year) (if any)**	
xlviii. **Accessible from the institutional repository** *(Yes or No)*	yes
xlix. **Hyperlink to the publication (the link to institutional repository if preferred) (if any)**	https://repository.ust.hk/ir/Record/1783.1-95613
l. **Other affordable means for access (if any)** *(Individual article purchase offered by the publisher / Access through the university libraries (on membership) / Contacting the corresponding author(s))*	
li. **Article Processing Charge (APC) for publishing the article in an open access journal*** *(Required / Not required / Not applicable)*	Not required
lii. **Total amount of associated APC* (in Hong Kong dollars, if any)**	
liii. **Amount of associated APC paid by university* (or universities, in case it is borne by more than one university) (in Hong Kong dollars, if any)**	
liv. **Copyright retained by author(s)** *(Yes or No)*	No
lv. **Number(s) and jurisdiction(s) of the granted patents associated with the article (if any)**	
lvi. **Submitted to RGC (indicate the year ending of the relevant progress report)**	2019
lvii. **Attached to this report** *(Yes or No)*	yes
lviii. **Acknowledged the support of RGC** *(Yes or No)*	yes

i. **The Latest Status of Publication**	**Published**	**Accepted but not yet published^**	**Under Review^**	**Under Preparation^** (optional)
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ii. **Author(s)** *(denote the corresponding author with an asterisk*)*	J.-C. Li , X.P. Qin , P.-X. Hou, M. Cheng, C. Shi, C. Liu*, H.-M. Cheng, M.H. Shao*			
iii. **Contact information of the corresponding author(s)**	Name	ORCID (if any)	Email	
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iv. **Title (in published language)**	Identification of active sites in nitrogen and sulfur co-doped carbon-based oxygen reduction catalysts			
v. **Title in other language (if any)**				
vi. **Full name of journal/book**	Carbon			
vii. **Volume**	147			
viii. **Issue number**	N/A			
ix. **Pages**	303-311			
x. **Article Number**	N/A			
xi. **Other necessary publishing details (if any)**				
xii. **Year of publication / Year of acceptance**	2019			
xiii. **Original language of the publication**	English			
xiv. **Publisher or equivalent**	Elsevier Ltd			
xv. **Digital object identifier (DOI)**	10.1016/j.carbon.2019.01.018			
xvi. **Abstract (as set out in the journal article)**	Different heteroatoms co-doped carbons are a burgeoning class of metal-free catalysts to replace Pt for the oxygen reduction reaction (ORR), but the lack of understanding of active sites delays their further improvement. Here we combined experimental designs and theoretical simulations with attempts to understand the correlation between N and/or S doping configurations and their catalytic activities. The results indicated that there is no obvious synergistic effect between N and S co-doping, in contrast with previous observations. S doping followed by N doping contributes to a large pyridinic N content in the catalyst due to the low formation energy for N to substitute doped S, leading to greatly enhanced ORR activity. Inversely, N doping followed by S doping takes pyridinic N away, resulting in an obvious ORR performance loss. Therefore, the doping sequence of S and N is crucial for the ORR activity of the co-doped catalysts. Furthermore, the pyridinic N is determined as the active functional group in N, S co-doped carbons by first-principle density functional theory calculations.			

xvii. **Open access status** *(Immediate open access / Embargoed open access / Non-open access)*	*Non-open access*
xviii. **Embargo end date (month, year) (if any)**	
xix. **Accessible from the institutional repository** *(Yes or No)*	yes
xx. **Hyperlink to the publication (the link to institutional repository if preferred) (if any)**	https://repository.ust.hk/ir/Record/1783.1-96268
xxi. **Other affordable means for access (if any)** *(Individual article purchase offered by the publisher / Access through the university libraries (on membership) / Contacting the corresponding author(s))*	
xxii. **Article Processing Charge (APC) for publishing the article in an open access journal*** *(Required / Not required / Not applicable)*	Not required
xxiii. **Total amount of associated APC* (in Hong Kong dollars, if any)**	
xxiv. **Amount of associated APC paid by university* (or universities, in case it is borne by more than one university) (in Hong Kong dollars, if any)**	
xxv. **Copyright retained by author(s)** *(Yes or No)*	No
xxvi. **Number(s) and jurisdiction(s) of the granted patents associated with the article (if any)**	
xxvii. **Submitted to RGC (indicate the year ending of the relevant progress report)**	2019
xxviii. **Attached to this report** *(Yes or No)*	yes
xxix. **Acknowledged the support of RGC** *(Yes or No)*	yes

i. **The Latest Status of Publication**	**Published**	**Accepted but not yet published^**	**Under Review^**	**Under Preparation^** (optional)
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ii. **Author(s)** *(denote the corresponding author with an asterisk*)*	J.-C. Li, M. Cheng, L. Ma, T. Li, X.F. Ruan, D. Liu, H.-M. Cheng, C. Liu*, D. Du, Z.D. Wei, Y.H. Lin*, M.H. Shao*			
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	C. Liu	0000-0003-3016-3997	cliu@imr.ac.cn	
	M.H.Shao	0000-0003-4496-0057	kemshao@ust.hk	
iv. **Title (in published language)**	Carbon nanotube-linked hollow carbon nanospheres doped with iron and nitrogen as single-atom catalysts for the oxygen reduction reaction in acidic solution			
v. **Title in other language (if any)**				
vi. **Full name of journal/book**	Journal of Materials Chemistry A			
vii. **Volume**	7			
viii. **Issue number**	24			
ix. **Pages**	14478-14482			
x. **Article Number**	N/A			
xi. **Other necessary publishing details (if any)**				
xii. **Year of publication / Year of acceptance**	2019			
xiii. **Original language of the publication**	English			
xiv. **Publisher or equivalent**	The Royal Society of Chemistry			
xv. **Digital object identifier (DOI)**	10.1039/C9TA00508K			
xvi. **Abstract (as set out in the journal article)**	Non-noble metal electrocatalysts toward the oxygen reduction reaction (ORR) are highly required to substitute expensive Pt/C as the cathode of proton exchange membrane fuel cells. However, the relatively low ORR activity of Pt-free catalysts under acidic conditions is the major issue. Herein, we engineered a three-dimensional structure consisting of atomically dispersed Fe, N-doped hollow carbon nanospheres linked by carbon nanotubes as an electrocatalyst for the ORR. Benefiting from the unique structure and high-density atomic Fe–N_x sites, this new type of electrocatalyst showed an impressive ORR half-wave potential of 0.84 V and kinetic current density of 13.1 mA cm^{-2} at a potential of 0.8 V in acidic media, which was even better those of commercial Pt/C.			

xvii. **Open access status** *(Immediate open access / Embargoed open access / Non-open access)*	*Non-open access*
xviii. **Embargo end date (month, year) (if any)**	
xix. **Accessible from the institutional repository** *(Yes or No)*	yes
xx. **Hyperlink to the publication (the link to institutional repository if preferred) (if any)**	https://repository.ust.hk/ir/Record/1783.1-98793
xxi. **Other affordable means for access (if any)** *(Individual article purchase offered by the publisher / Access through the university libraries (on membership) / Contacting the corresponding author(s))*	
xxii. **Article Processing Charge (APC) for publishing the article in an open access journal*** *(Required / Not required / Not applicable)*	Not required
xxiii. **Total amount of associated APC* (in Hong Kong dollars, if any)**	
xxiv. **Amount of associated APC paid by university* (or universities, in case it is borne by more than one university) (in Hong Kong dollars, if any)**	
xxv. **Copyright retained by author(s)** *(Yes or No)*	No
xxvi. **Number(s) and jurisdiction(s) of the granted patents associated with the article (if any)**	
xxvii. **Submitted to RGC (indicate the year ending of the relevant progress report)**	2019
xxviii. **Attached to this report** *(Yes or No)*	yes
xxix. **Acknowledged the support of RGC** *(Yes or No)*	yes

i. **The Latest Status of Publication**	**Published**	**Accepted but not yet published^**	**Under Review^**	**Under Preparation^** (optional)
	√			
^ For not-yet-published publication, items (vi) to (xxvi) can be left blank if information is not yet available.				
ii. **Author(s)** *(denote the corresponding author with an asterisk*)*	J.-C. Li, P.-X. Hou, M. Cheng, C. Liu*, H.-M. Cheng*, M.H. Shao*			
iii. **Contact information of the corresponding author(s)**	Name	ORCID (if any)	Email	
	C. Liu	0000-0003-3016-3997	cliu@imr.ac.cn	
	M.H.Shao	0000-0003-4496-0057	kemshao@ust.hk	
iv. **Title (in published language)**	Carbon nanotube encapsulated in nitrogen and phosphorus co-doped carbon as a bifunctional electrocatalyst for oxygen reduction and evolution reaction			
v. **Title in other language (if any)**				
vi. **Full name of journal/book**	Carbon			
vii. **Volume**	139			
viii. **Issue number**	N/A			
ix. **Pages**	156-163			
x. **Article Number**	N/A			
xi. **Other necessary publishing details (if any)**				
xii. **Year of publication / Year of acceptance**	2018			
xiii. **Original language of the publication**	English			
xiv. **Publisher or equivalent**	Elsevier Ltd			
xv. **Digital object identifier (DOI)**	10.1016/j.carbon.2018.06.023			
xvi. **Abstract (as set out in the journal article)**	The development of inexpensive and robust bifunctional reversible oxygen electrocatalysts is critical to rechargeable metal-air batteries and regenerative fuel cells. Here we reported a single-wall carbon nanotube (SWCNT) conductive network embedded in porous N, P co-doped carbon (SWCNT@NPC) as a bifunctional oxygen electrocatalyst. The SWCNT@NPC material showed excellent electrocatalytic activity with an oxygen reduction half-wave potential of 0.85 V and oxygen evolution potential of 1.678 V at 10 mA cm^{-2}. When used to assemble rechargeable Zn-air batteries, SWCNT@NPC exhibited better catalytic activity as well as durability compared to commercial noble-metal catalysts. In particular, it is demonstrated that mutual promotion between N and P doping induces ultrahigh ORR activity while N doping is identified as the primary active sites for the OER.			

xvii. **Open access status** *(Immediate open access / Embargoed open access / Non-open access)*	*Non-open access*
xviii. **Embargo end date (month, year) (if any)**	
xix. **Accessible from the institutional repository** *(Yes or No)*	yes
xx. **Hyperlink to the publication (the link to institutional repository if preferred) (if any)**	https://repository.ust.hk/ir/Record/1783.1-91652
xxi. **Other affordable means for access (if any)** *(Individual article purchase offered by the publisher / Access through the university libraries (on membership) / Contacting the corresponding author(s))*	
xxii. **Article Processing Charge (APC) for publishing the article in an open access journal*** *(Required / Not required / Not applicable)*	Not required
xxiii. **Total amount of associated APC* (in Hong Kong dollars, if any)**	
xxiv. **Amount of associated APC paid by university* (or universities, in case it is borne by more than one university) (in Hong Kong dollars, if any)**	
xxv. **Copyright retained by author(s)** *(Yes or No)*	No
xxvi. **Number(s) and jurisdiction(s) of the granted patents associated with the article (if any)**	
xxvii. **Submitted to RGC (indicate the year ending of the relevant progress report)**	2019
xxviii. **Attached to this report** *(Yes or No)*	yes
xxix. **Acknowledged the support of RGC** *(Yes or No)*	yes

i. **The Latest Status of Publication**	**Published**	**Accepted but not yet published^**	**Under Review^**	**Under Preparation^** (optional)
	√			
^ For not-yet-published publication, items (vi) to (xxvi) can be left blank if information is not yet available.				
ii. **Author(s)** *(denote the corresponding author with an asterisk*)*	Z.X. Huang, X.P. Qin , X.F. Gu, G.Z. Li, Y.C. Mu, N.G. Wang, K. Ithisuphalap, H.X. Wang, Z.P. Guo, Z.C. Shi*, G. Wu*, M.H. Shao*			
iii. **Contact information of the corresponding author(s)**	Name	ORCID (if any)	Email	
	M.H.Shao	0000-0003-4496-0057	kemshao@ust.hk	
iv. **Title (in published language)**	Mn_3O_4 quantum dots supported on nitrogen-doped partially exfoliated multiwall carbon nanotubes as oxygen reduction electrocatalysts for high-performance Zn-air batteries			
v. **Title in other language (if any)**				
vi. **Full name of journal/book**	ACS Applied Materials & Interfaces			
vii. **Volume**	10			
viii. **Issue number**	28			
ix. **Pages**	23900-23909			
x. **Article Number**	N/A			
xi. **Other necessary publishing details (if any)**				
xii. **Year of publication / Year of acceptance**	2018			
xiii. **Original language of the publication**	English			
xiv. **Publisher or equivalent**	American Chemical Society			
xv. **Digital object identifier (DOI)**	10.1021/acs.nanolett.1c01493			

xvi. **Abstract (as set out in the journal article)**	Highly efficient and low-cost nonprecious metal electrocatalysts that favor a four-electron pathway for the oxygen reduction reaction (ORR) are essential for high-performance metal–air batteries. Herein, we show an ultrasonication-assisted synthesis method to prepare Mn_3O_4 quantum dots (QDs, ca. 2 nm) anchored on nitrogen-doped partially exfoliated multiwall carbon nanotubes (Mn_3O_4 QDs/N-p-MCNTs) as a high-performance ORR catalyst. The Mn_3O_4 QDs/N-p-MCNTs facilitated the four-electron pathway for the ORR and exhibited sufficient catalytic activity with an onset potential of 0.850 V (vs reversible hydrogen electrode), which is only 38 mV less positive than that of Pt/C (0.888 V). In addition, the Mn_3O_4 QDs/N-p-MCNTs demonstrated superior stability than Pt/C in alkaline solutions. Furthermore, a Zn–air battery using the Mn_3O_4 QDs/N-p-MCNTs cathode catalyst successfully generated a specific capacity of 745 mA h g^{-1} at 10 mA cm^{-2} without the loss of voltage after continuous discharging for 105 h. The superior ORR activity of Mn_3O_4 QDs/N-p-MCNTs can be ascribed to the homogeneous Mn_3O_4 QDs loaded onto the N-doped carbon skeleton and the synergistic effects of Mn_3O_4 QDs, nitrogen, and carbon nanotubes. The interface binding energy of −3.35 eV calculated by the first-principles density functional theory method illustrated the high stability of the QD-anchored catalyst. The most stable adsorption structure of O_2, at the interface between Mn_3O_4 QDs and the graphene layer, had the binding energy of −1.17 eV, greatly enhancing the ORR activity. In addition to the high ORR activity and stability, the cost of production of Mn_3O_4 QDs/N-p-MCNTs is low, which will broadly facilitate the real application of metal–air batteries.
xvii. **Open access status** *(Immediate open access / Embargoed open access / Non-open access)*	*Non-open access*
xviii. **Embargo end date (month, year) (if any)**	
xix. **Accessible from the institutional repository** *(Yes or No)*	yes
xx. **Hyperlink to the publication (the link to institutional repository if preferred) (if any)**	https://repository.ust.hk/ir/Record/1783.1-92194
xxi. **Other affordable means for access (if any)** *(Individual article purchase offered by the publisher / Access through the university libraries (on membership) / Contacting the corresponding author(s))*	

xxii. **Article Processing Charge (APC) for publishing the article in an open access journal*** *(Required / Not required / Not applicable)*	Not required
xxiii. **Total amount of associated APC* (in Hong Kong dollars, if any)**	
xxiv. **Amount of associated APC paid by university* (or universities, in case it is borne by more than one university) (in Hong Kong dollars, if any)**	
xxv. **Copyright retained by author(s)** *(Yes or No)*	No
xxvi. **Number(s) and jurisdiction(s) of the granted patents associated with the article (if any)**	
xxvii. **Submitted to RGC (indicate the year ending of the relevant progress report)**	2019
xxviii. **Attached to this report** *(Yes or No)*	yes
xxix. **Acknowledged the support of RGC** *(Yes or No)*	yes

* *This information will be for the Secretariat's reference only and not be disclosed to the public.*

9. Recognized international conference(s) in which paper(s) related to this research project was/were delivered

(Please attach a copy of each delivered paper. All listed papers must acknowledge RGC's funding support by quoting the specific grant reference.)

Month/Year/ Place	Title	Conference Name	Submitted to RGC *(indicate the year ending of the relevant progress report)*	Attached to this report *(Yes or No)*	Acknowledged the support of this Joint Research Scheme *(Yes or No)*	Accessible from the institutional repository *(Yes or No)*
05/2019/Dallas, USA	Theoretical and Experimental Investigations in Metal−N−C Composites for Oxygen Reduction Reaction and Hydrogen Evolution Reaction at Universal pHs	235th ECS Meeting	2019	yes	Yes (funding information was mentioned in the presentation)	Yes
10/2020/ Honolulu, Hawaii, USA	Durable Hybrid Electrocatalysts for Proton Exchange Membrane Fuel Cells	PRiME 2020, Pacific Rim Meeting on Electrochemical and Solid State Science	2020	yes	Yes (funding information was mentioned in the presentation)	Yes

08/2021/ Jeju Island, Korea	Solid-State Synthesis of Highly Dispersed Nitrogen-Coordinated Single Iron Atom Electrocatalysts for Proton Exchange Membrane Fuel cells	Solid-State Synthesis of Highly Dispersed Nitrogen-Coordinated Single Iron Atom Electrocatalysts for Proton Exchange Membrane Fuel cells	2021	yes	Yes (funding information was mentioned in the presentation)	yes

10. Student(s) trained *(Please attach a copy of the title page of the thesis.)*

Name	Degree registered for	Date of registration	Date of thesis submission/ graduation
Fei Xiao	Mphil	2016	2018
Fei Xiao	PhD	2018	2021
Xueping Qin	PhD	2015	2019

11. Other impact *(e.g. award of patents or prizes, collaboration with other research institutions, technology transfer, etc.)*

Patent applications:

1. **M.H. Shao**, F. Xiao, "Catalysts consisting of active supports and nanoparticles for fuel cells", US provisional patent application, 63/100,244, filed on 04/03/2020.
2. **M.H. Shao**, F. Xiao, "Durable hybrid electrocatalysts for fuel cells", PCT/US2020/017240, filed on 07/02/2020.
3. **M.H. Shao**, J.C. Li, "A high efficient M-N-C electrocatalyst and its synthesis method", China patent application, 201911414571.9, filed on 12/31/2019.

12. Statistics on Research Outputs *(Please ensure the summary statistics below are consistent with the information presented in other parts of this report.)*

	Peer-reviewed journal publications	Conference papers	Scholarly books, monographs and chapters	Patents awarded	Other research outputs (Please specify)
No. of outputs arising directly from this research project [or conference]	24	3	0	3	0