Curriculum Vitae

Dr. Zhongfang CHEN

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EDUCATION

1997.9 – 2000.7	Ph. D. in Physical Chemistry, Dept. of Chemistry, Nankai University, P. R. China; Supervisor: Prof. Auchin Tang and Prof. Xuezhuang Zhao
1994.9 – 1997.7	M. S. in Physical Chemistry, Dept. of Chemistry, Nankai University, P. R. China, Supervisor: Prof. Xuezhuang Zhao
1990.9 – 1994.7	B. S. in Organic Chemistry, Dept. of Chemistry, Nankai University, P. R. China

PROFESSIONAL EXPERIENCE

2014.7-	Full professor, Department of Chemistry, University of Puerto Rico, Río Piedras campus
2008.8-2014.6	Associate Professor (tenured in 2013), Department of Chemistry, University of Puerto Rico, Río Piedras campus
2008.1-2008.7	Research Associate Professor, Department of Physics, Applied Physics, and Astronomy, Rensselaer Polytechnic Institute
2006.1-2007.12	Associate Research Scientist, Department of Chemistry, University of Georgia
2003.10– 2005.12	Postdoc, Department of Chemistry, Center for Computational Chemistry, University of Georgia, with Prof. Paul von Ragué Schleyer
2002.10 – 2003.9	Institut für Organische Chemie, Universität Erlangen-Nürnberg, Germany, with Prof. Andreas Hirsch and Prof. Paul von Ragué Schleyer
2001.04 – 2002.9	Humboldt Fellow, Institut für Organische Chemie, Universität Erlangen-Nürnberg, Germany, with Prof. Andreas Hirsch
2000.04 – 2001.03	Postdoc, Max-Planck-Institut für Kohlenforschung, Mülheim an der Ruhr, Germany, with Prof. Walter Thiel
1999.12 – 2000.02	Humboldt Fellow, Institut für Organische Chemie, Universität Erlangen-Nürnberg, Germany, with Prof. Andreas Hirsch

CURRENT MAIN RESEARCH TOPICS

- Carbon graphene and inorganic graphene analogues – *Towards molecular electronics, nano-devices and advanced materials for energy storage and conversion*
- Nanocatalysis – *Towards more efficient and environmentally benign catalysts, especially for electrocatalysis*
- Computational nanotoxicity – *Towards understanding and predicting nano-safety and toxicity*
- Computational environmental chemistry – *Removal of emerging pollutants from water system*

OTHER RESEARCH TOPICS

- One-dimensional nanomaterials (nanotubes, nanocables, peapods, etc.)
- Novel materials for hydrogen and lithium storage
- Endohedral metallofullerenes and related endohedral clusters
- Molecules with novel bonding patterns
  - ✧ Planar hypercoordinate carbon and other elements
  - ✧ Novel aromaticity

PUBLICATIONS (see the publication list for details)

- 322 journal articles, including *Chem. Rev.* (3), *Acc. Chem. Res.* (1), *Coord. Chem. Rev.* (3), *Chem. Soc. Rev.* (1), *J. Am. Chem. Soc.* (21), *Angew. Chem. Int. Ed.* (12), *Phys. Rev. Lett.* (2), *Nature Commun.* (2), *ACS Nano* (5), *Adv. Funct. Mater.* (5), *Nano Lett.* (5), *Energy Environ. Sci*. (1), and 14 book chapters; 1 co-edited book for Wiley.
- 50 first-authored, 206 corresponding-authored; over 25,800 citations and h-index of 78 by Web of Science (over 29,900 citations and h-index of 86 by Google Scholar). Over 75 papers received over 100 citations each.
- Eleven (11) papers were highlighted or feature by scientific news journals (*Nature*, *Nature Chemistry, Chem. & Eng. News* and/or *Nachrichten aus der Chemie, Nature China*); over 30 were highlighted as cover pictures or frontispiece of scientific journals

STUDENTS/POSTDOCS SUPERVISED AT UPR

- Postdocs
  Wei Chen (female), Yafei Li, Xin Tan, Fengyu Li (female), Haijun Zhang, Xiaoxuan Wei (female), Yinghe Zhao
- Graduate students
  Fengyu Li (female), Yunlong Liao, Kaixiong Tu, Bay Allen Pantoja (Hispanic), Keily Gutierrez (Hispanic), Fuzhao Yi, Si Yang, Siru Lin (female), Jinxing Gu, Saneliswa Magagula (female, African), Ziyuan Zhao (female), Amanda Alvarado Torres (female, Hispanic), Linguo Lu, Biao Liu
- Undergraduate students (all Hispanic)
  Keysha Melendez Cuadrado (female),Keyra Melendez Cuadrado (female), Clara Leticia Cruz (female), Valerie Lopez (female), Juan Corchado, Jessica M. Gonzalez Delgado (female), Maxier Acosta, Cristian Morales, Gabriel Reilly
- REU Undergraduate students
  Jayro Rivera, Kaitlyn A. Jacoby (female), Colby J. Agostino
- High school students
  Jack Feng, Esmarline De Leon Peralta (female, Hispanic), Michelle Gao (female), Angel Vergara, Karen Gao (female)

COMMITTEE MEMBER IN THE DEPARTMENT AND OTHER SERVICES

- Faculty Committee
- Academic Affairs Committee
- Admission Committee
- Volunteer as the web master and editor of departmental website
- AD Hoc Committee, Faculty of Natural Sciences, UPR

PROFESSIONAL SERVICES

Editor and Member of Editorial Board

- *Green Energy & Environment (Associate Editor)*
- *Journal of Materials Informatics (Associate Editor)*
- Journal of Hazardous Materials Letters *(Associate Editor)*

Membership in Professional Associations

- American Chemical Society (ACS)
- American Physical Society (APS)
- Materials Research Society (MRS)
- Royal Society of Chemistry (RSC)
- Alexander von Humboldt Association of America

PROFESSIONAL REFERENCES

- Prof. Waldemar Adam
  Department of Chemistry,
  University of Puerto Rico, San Juan PR 00931
  Email: wadam@chemie.uni-wuerzburg.de
- Prof. Shengbai Zhang
  Department of Physics, Applied Physics, and Astronomy, Rensselaer Polytechnic Institute,
  110 Eighth Street, Troy, New York, 12180
  Email: zhangs9@rpi.edu
- Prof. Xiao Cheng Zeng
  Department of Chemistry, University of Nebraska-Lincoln, Lincoln, Nebraska 68588
  Email: xzeng1@unl.edu
- Prof. Shigeru Nagase
  Fukui Institute for Fundamental Chemistry
  Kyoto University, Kyoto 606-8103, Japan
  Email: nagase@ims.ac.jp

PUBLICATIONS OF DR. ZHONGFANG CHEN

Edited Book and Special Issues

- Guest Co-editor, A Special Issue on Structures, Properties, and Applications of Nanomaterials: a Computational Exploration, *J. Comput. Theor. Nanosci.* **2**011
- "Graphene Chemistry: Theoretical Perspectives", John Wiley & Sons, 2013, edited by De-en Jiang and Zhongfang Chen.

Full Publication List (337)

(* indicates the corresponding authorship)

A. Reviews articles (18)

18. Structures and Functions of Two-Dimensional Materials: from Theoretical Prediction to Experimental Realization
Lijuan Zhang, Jinxing Gu, **Zhongfang Chen***
Science Bulletin, **2021**, *66*，563-579

17. Planar Hypercoordinate Motifs in Two-dimensional Materials
Yu Wang, Yafei Li,* **Zhongfang Chen***
Acc. Chem. Res. **2020**, *53*, 887-895.

16. Exohedral Functionalization of Endohedral Metallofullerenes: Interplay Between Inside and Outside
Peng Jin, Ying Li, Saneliswa Magagula, Zhongfang Chen*
Coordination Chemistry Reviews **2019**, 388, 406-439.

15. Recent Advances in Aromatic Antimony Clusters
Lei-Jiao Li, Basharat Ali, **Zhongfang Chen***, Zhong-Ming Sun*
Chinese Journal of Chemistry, **2018**, 36, 955-960.

14. Aromaticity and Antiaromaticity in Zintl Clusters
Chao Liu, Ivan A. Popov, **Zhongfang Chen**, Alexander I. Boldyrev, and Zhong−Ming Sun*
Chem. Eur. J. **2018,** *24*, 14583-14597.
Highlighted as Frontispiece

13. Recent progress in 2D group-VA semiconductors: From theory to experiment
Shengli Zhang, Shiying Guo, **Zhongfang Chen**, Yeliang Wang, Hongjun Gao, Julio Gómez-Herrero, Pablo Ares, Félix Zamora,* Zhen Zhu, Haibo Zeng*
Chem. Soc. Rev. **2018**, 47, 982-1021.

12. Innovation and Discovery of Graphene-Like Materials via DFT Computations
Qing Tang, Zhen Zhou,* **Zhongfang Chen***
WIREs Computational Molecular Science, **2015**, *5*, 360-379.

11. Four Decades of the Chemistry of Planar Hypercoordinate Compounds
Li-Ming Yang,* Eric Ganz, **Zhongfang Chen,*** Zhi-Xiang Wang, Paul von Ragué Schleyer
Angew. Chem. Int. Ed. **2015**, 54, 9468-9501.
Angew. Chem. **2015**, *127*, 9602-9637.

10. Magnetic Properties of Atomic Clusters and Endohedral Metallofullerenes
Jijun Zhao,* Xiaoming Huang, Peng Jin, **Zhongfang Chen***
Coord. Chem. Rev. **2015**, *289-290*, 315-340.

9. Graphene, Inorganic Graphene Analogs and Their Composites for Lithium Ion Batteries
Yu Jing, Zhen Zhou,* Carlos R. Cabrera, **Zhongfang Chen***
J. Mater. Chem. A. **2014**, *2*, 12104-12122.
Highlighted as a cover picture

8. Carbon Atoms Trapped in Cages: Metal Carbide Clusterfullerenes
Peng Jin*, Chengchun Tang, **Zhongfang Chen***
Coord. Chem. Rev. **2014**, *270-271*, 89–111.

7. Graphene-related Nanomaterials: Tuning Properties by Functionalization
Qing Tang, Zhen Zhou,* **Zhongfang Chen***

Nanoscale, **2013**, 5, 4541-4583.
Highlighted as a cover picture

6. Theoretical Insights into the Structures of Graphene Oxide and Its Chemical Conversions between Graphene
Xingfa Gao, De-en Jiang,* Yuliang Zhao, Shigeru Nagase, Shengbai B. Zhang, **Zhongfang Chen***
J. Comput. Theor. Nanosci. **2011***, 8,* 2406-2422.

5. The Evaluation of Aromaticity in Inorganic Clusters and Related Compounds by Nucleus-Independent Chemical Shifts
Zhongfang Chen,* R. Bruce King*
ChemTracts-Inorganic Chemistry, **2006**, *19*, 45-65.

4. Curved π-Conjugation, Aromaticity and the Related Chemistry of Small Fullerenes (<C_{60}) and Single-Walled Carbon Nanotubes
Xin Lu,* **Zhongfang Chen***
Chem. Rev. **2005**, *105*, 3463-3496.
Most-Accessed Article: October-December, 2005

3. Spherical Aromaticity: Recent Work on Fullerenes, Polyhedral Boranes, and Related Structures
Zhongfang Chen,* R. Bruce King
Chem. Rev. **2005**, *105*, 3613-3642.

2. Nucleus-Independent Chemical Shifts (NICS) as an Aromaticity Criterion
Zhongfang Chen,* Chaitanya S. Wannere, Clémence Corminboeuf, Ralph Puchta, Paul. v. R. Schleyer*
Chem. Rev. **2005**, *105*, 3842-3888.
Ranked as No. 1 "hot paper" of Chemical Reviews in Jan., 2008 by ACS publications as recognized by Thomson ISI®'s Essential Science Indicators (former rankings in 2007 were No. 21 in Jan, No. 18 in March, No. 13 in May, No. 12 in July, No. 5 in Sept. and No. 3 in Nov.), the most- cited article

1. Recent Progress on the Theoretical Studies of Heterofullerenes
Zhongfang Chen, Xuezhuang Zhao, Auchin Tang
Chinese Journal of Structural Chemistry **1999**, *18*, 463. (in Chinese)

B. Research Papers in Peer-Reviewed Journals

At University of Puerto Rico as An Associate Professor

304. Particle Swarm Predictions of a SrB_8 Monolayer with 12-Fold Metal Coordination
Xin Qu, Lihua Yang, Jian Lv*, Yu Xie, Jinghai Yang, Yukai Zhang, Yanchao Wang*, Jijun Zhao, **Zhongfang Chen*,** and Yanming Ma
J. Am. Chem. Soc. **2022**, https://doi.org/10.1021/jacs.1c13654

303. Atomically Dispersed Uranium Enables an Unprecedentedly High NH3 Yield RateYinghe Zhao, Jingyu Qu, Haobo Li, Pengyu Li, Teng Liu, **Zhongfang Chen***, Tianyou Zhai*
Nano Lett. **2022**, *22*, 4475–4481.

302. Understanding the CH_4 Conversion over Metal Dimers from First Principles
Haihong Meng, Bing Han, Fengyu Li*, Jingxiang Zhao*， **Zhongfang Chen***
Nanomaterials, **2022**, *12*, 1518.

301. Constructing two-dimensional holey-graphyne with unusual annulative π-extension
Xinghui Liu, Soo Min Cho, Shiru Lin, **Zhongfang Chen**, Wooseon Choi, Young-Min Kim, Eunbhin Yun, Eun Hee Baek, Do Hyun Ryu*, Hyoyoung Lee*
Matters，**2022**, https://doi.org/10.1016/j.matt.2022.04.033
Highlighted by *ScienceDaily*,
https://www.sciencedaily.com/releases/2022/05/220518113832.htm
Phys.org, https://phys.org/news/2022-05-synthesis-two-dimensional-holey-graphyne.html
https://www.azonano.com/news.aspx?newsID=39157
https://blingeach.com/synthesis-of-two-dimensional-holey-graphyne/

300. Tailoring 2-electron oxygen reduction reaction selectivity on h-BN-based single-atom catalysts from superoxide dismutase: A DFT investigation

Yu Zou, Xiangyu Guo, Xiaoqiong Bian, Yongfan Zhang, Wei Lin, Shuping Huang, **Zhongfang Chen**, Kaining Ding
Applied Surface Science, **2022**, *592*, 153233.

299. Novel 2D porous C_3N_2 framework as promising anode material with ultra-high specific capacity for lithium-ion batteries
Xinyong Cai, Wencai Yi, Jiao Chen, Linguo Lu, Bai Sun, Yuxiang Ni, Simon A. T. Redfern,* Hongyan Wang, **Zhongfang Chen**,* Yuanzheng Chen*
J. Mater. Chem. A. **2022**, 10, 6551-6559.

298. Revisiting the Catalytic Performance of Supported Metal Dimers for Oxygen Reduction Reaction via Magnetic Coupling from First Principles
Linke Yu, Fengyu Li, Jingxiang Zhao, **Zhongfang Chen***
Advanced Powder Materials, **2022**, *1*, 100031.

297. 2D Auxetic Material with Intrinsic Ferromagnetism: Copper Halide ($CuCl_2$) Monolayer
Haifei Qin, Jiao Chen, Bai Sun, Yongliang Tang, Yuxiang Ni, **Zhongfang Chen,*** Hongyan Wang, Yuanzheng Chen*
Phys. Chem. Chem. Phys., **2021**, *23*, 22078-22085.

296. Single-atom catalysts with anionic metal centers: promising electrocatalysts for the oxygen reduction reaction and beyond
Jinxing Gu, Yinghe Zhao, Shiru Lin, Jingsong Huang,* Carlos R. Cabrera, Bobby G. Sumpter, **Zhongfang Chen***
J. Energy Chem. **2021**, *63*, 285-293.

295. Controllable CO_2 Electrocatalytic Reduction via Fer-roelectric Switching on In_2Se_3 Monolayer Anchoring Atomically Dispersed Transition Metal Atoms
Lin Ju, Xin Tan, Xin Mao, Yuantong Gu, Sean Smith, Aijun Du, **Zhongfang Chen,** Changfeng Chen, Liangzhi Kou*
Nature Comm. **2021**, 12, 5128.

294. Molecular Crowding Effect in Aqueous Electrolytes to Suppress Hydrogen Reduction Reaction and Enhance Electrochemical Nitrogen Reduction
Ying Guo, Jinxing Gu, Rong Zhang, Shaoce Zhang, Zhen Li, Yuwei Zhao, Zhaodong Huang, Jun Fan, **Zhongfang Chen,*** Chunyi Zhi*
Adv. Energy Mater. **2021**, *11*, 2101699.

293. Tunable Electronic Properties and Enhanced Ferromagnetism in Cr2Ge2Te6 Monolayer by Strain Engineering
Lifei Liu, Xiaohui Hu,* Yifeng Wang, Arkady V. Krasheninnikov, Zhongfang Chen, Litao Sun
Nanotechnology **2021**, *32*, 485408.

292. C_9N_4 and $C_2N_6S_3$ Monolayers as Promising Anchoring Materials for Lithium-Sulfur Batteries: Weakening the Shuttle Effects via Optimizing Lithium Bonds
Yinan Dong, Bai Xu, Haiyu Hu, Jiashu Yang, Fengyu Li,* Jian Gong,* **Zhongfang Chen***
Phys. Chem. Chem. Phys, **2021**,*23*, 12958-12967 .
Highlighted by front cover

291. Enhancing ferromagnetism and tuning electronic properties of CrI_3 monolayers by adsorption of transition metal atoms
Qiang Yang, Xiaohui Hu,* Xiaodong Shen, Arkady V. Krasheninnikov, **Zhongfang Chen,** Litao Sun
ACS Appl. Mater. Interfaces **2021**, *13*, 18, 21593–21601.

290. MX Anti-MXenes from Non-van der Waals Bulks for Electrochemical Applications：The Merit of Metallicity and Active Basal Plane
Jinxing Gu, Ziyuan Zhao, Jingsong Huang,* Bobby G. Sumpter, **Zhongfang Chen***
ACS Nano **2021**, *15*, 6233–6242.

289. Identifying the Activity Origin of a Cobalt Single-Atom Catalyst for Hydrogen Evolution Using Supervised Learning
Liu, X.; Zheng, L.; Han, C.; Zong, H.; Yang, G.; Lin, S.; Kumar, A.; Jadhav, A. R.; Tran, N. Q.;

Hwang, Y.; Lee, J.; Vasimalla, S.; **Chen, Z.;** Kim, S. G.; Lee, H.*
Adv. Funct. Mater. **2021**, *31*, 2100547.

288. Underlying mechanisms of reactive oxygen species and oxidative stress photoinduced by graphene and its surface-functionalized derivatives†
Hongye Yao, Yang Huang, Xuan Li, Xuehua Li,* Hongbin Xie, Tianlie Luo, Jingwen Chen, **Zhongfang Chen**
Environ. Sci.: Nano, **2020**, *7*, 782-792

287. Enhanced performance of Mo_2P monolayer as lithium-ion battery anode materials by carbon and nitrogen doping: a first principles study
Liu, X.; Lin, S.; Gao, J.; Shi, H.; Kim, S. G.; **Chen, Z**.*; Lee, H.*
Phys. Chem. Chem. Phys., **2021**, *23*, 4030-4038.

286. Predicting Adsorption of Organic Pollutants on Boron Nitride Nanosheets via in silico Techniques: DFT Computations and QSAR Modeling
Wang, Y.; Tang, W.; Peng, Y.*, **Chen, Z.*;** Chen, J.*; Xiao, Z,; Zhao, X.; Qu, Y.; Li, J.,
Environ. Sci.: Nano, **2021**, *8*, 795-805.

285. In Situ Observation of Non-Classical 2-Norbornyl Cation in Confined Zeolites at Ambient Temperature
Tang, X.; Chen, W.; Yi, X.; Liu, Z.; Xiao, Y.; **Chen, Z.*;** Zheng, A.*
Angew. Chem. Int. Ed. **2021**, *60*, 4581-4587.
Highlighted by back cover

284. Establishing a Theoretical Landscape for Identifying Basal Plane Active 2D Metal Borides (MBenes) toward Nitrogen Electroreduction
Guo, X.; Lin, S.; Gu, J.; Zhang, S.*; **Chen, Z.*;** Huang, S.*
Adv. Funct. Mater. **2021**, *31*, 2008056.
Highlighted by Nanowerk: https://www.nanowerk.com/spotlight/spotid=56645.php

283. Understanding Activity Origin for Oxygen Reduction Reaction on Bi-Atom Catalysts by DFT Study and Machine-Learning
Chaofang Deng, Yang Su, Jinxing Gu, Fuhua Li, Weifeng Shen, **Zhongfang Chen*,** Qing Tang*
J. Mater. Chem. A. **2020**, *8*, 24563-24571.

282. Scalable synthesis of 2D hydrogen-substituted graphdiyne on Zn substrate for high-yield N_2 fixation
Qi Yang, Ying Guo, Jinxing Gu, Na Li, Changda Wang, Zhuoxin Liu, Xinliang Li, Zhaodong Huang, Shiqiang Wei, Suying Xu, Li Song, Jun Fan,* **Zhongfang Chen**,* Jieshan Qiu, Chunyi Zhi*
Nano Energy **2020**, 105283.

281. Evaluation Procedure of Photocatalysts for VOCs Degradation from the View of Density Functional Theory Calculations: g-C_3N_4 Dots/Graphene as an Example
Binghua Jing, Zhimin Ao,* Weina Zhao, Ying Xu, **Zhongfang Chen**, Taicheng Ao
J. Mater. Chem. A. **2020**,*8*, 20363-20372.

280 Zeolite-Templated Carbons as Effective Sorbents to Remove Methylsiloxanes and Derivatives: A Computational Screening
Shiru Lin, Kaitlyn A. Jacoby, Jinxing Gu, Dariana R. Vega-Santander, Arturo J. Hernández-Maldonado,* **Zhongfang Chen***
Green Energy & Environment, **2021**, 6, 884-892.

279. Double-sided surface functionalization: An effective approach to stabilize and modulate the electronic structure of graphene-like borophene
Xiao Tang, Jinxing Gu, Jing Shang, **Zhongfang Chen*,** and Liangzhi Kou*
InfoMat. **2021**,*3*,327–336.

278. Rational Prediction of Single Metal Atom Supported on Two-Dimensional Metal Diborides for Electrocatalytic N_2 Reduction Reaction with Integrated DescriptorLei Ge, Weiwei Xu, Chongyang Chen, Chao Tang, Lai Xu*, and Zhongfang Chen*
J. Phys. Chem. Lett. **2020**, *11*, 5241–5247.

277. Ultrahigh Capacity 2D Anode Materials for Lithium/Sodium-Ion Batteries: Entirely Planar B_7P_2 monolayer with Proper Pore Size and Distribution

Changyan Zhu, Shiru Lin, Min Zhang,* Quan Li, Zhongmin Su, **Zhongfang Chen***
J. Mater. Chem. A. **2020**, 8, 10301-10309.

276. Metallic FeSe Monolayer as Anode Materials for Li and and Non-Li Ion Batteries: A DFT Study
Xiaodong Lu, Fengyu Li,* Jian Gong,* Jinxing Gu, Shiru Lin, **Zhongfang Chen***
Phys. Chem. Chem. Phys., **2020**, 22, 8902-8912

275. Polymorphism of Low Dimensional Boron Nanomaterials Driven by Electrostatic Gating: A Computational Discovery
Yalong Jiao,* Fengxian Ma, Jinxing Gu, **Zhongfang Chen***, and Aijun Du*
Nanoscale **2020, 12,** 10543-10549.

274. Tackling the Activity and Selectivity Challenges of Electrocatalysts towards Nitrogen Reduction Reaction via Atomically Dispersed Biatomic Catalysts
Xiangyu Guo, Jinxing Gu, Shiru Lin, Shengli Zhang,* **Zhongfang Chen***, Shiping Huang*
J. Am. Chem. Soc. **2020**, 142, 5709-5721.

273. Directly Predicting Limiting Potentials from Easily Obtainable Physical Properties of Graphene-Supported Single-Atom Electrocatalysts by Machine Learning
Shiru Lin, Haoxiang Xu, Yekun Wang, Xiao Cheng Zeng, **Zhongfang Chen***
J. Mater. Chem. A. **2020**, *8*, 5663 – 5670.
Highlighted by Nanowerk: https://www.nanowerk.com/spotlight/spotid=54551.php

272. Machine-Learning-Assisted Screening of Pure-Silica Zeolites for Effective Removal of Linear Siloxanes and Derivatives
Shiru Lin, Yekun Wang, Yinghe Zhao, Luis R. Pericchi, Arturo J. Hernández-Maldonado,* **Zhongfang Chen***
J. Mater. Chem. A. **2020**, *8*, 3228 – 3237.
Correction: *J. Mater. Chem. A*. **2020**, *8*, 6372 – 6374.
Highlighted by Nanowerk: https://www.nanowerk.com/spotlight/spotid=54968.php

271. N-heterocyclic carbene as a promising metal-free electrocatalyst with high-efficiency for nitrogen reduction to ammonia
Hongyan Li, Le Yang, Zhongxu Wang, Peng Jin,* Jingxiang Zhao,* **Zhongfang Chen***
J. Energy Chemistry, **2020**, *46*, 78-86.

270. Relative Efficacy of Co-X_4 embedded graphene(X=N, S, B, and P) Electrocatalysts towards Hydrogen Evolution Reaction: Is Nitrogen Really the Best Choice?
Chunjin Ren, Yongli Zhang, Saneliswa Magagula, Qianyu Jiang, Yongfan Zhang, **Zhongfang Chen***, Kaining Ding*
ChemCatChem, **2020**, *12*, 536-543.

269. Semiconducting SN_2 Monolayer with Three-Dimensional Auxetic Properties: A Global Minimum with Tetracoordinated Sulfurs
Fengyu Li,* Xiaodong Lv, Jinxing Gu, Kaixiong Tu, Jian Gong, Peng Jin,* Zhongfang Chen*
Nanoscale **2020**, *12*, 85-92.

268. Coordination Tailoring Towards Efficient Single-Atom Catalysts for N_2 Fixation: A Case Study of Iron-Nitrogen-Carbon (Fe@N-C) Systems
Xiangyu Guo, Jinxing Gu, Shengli Zhang,* Zhongfang Chen,* Shiping Huang*
Catalysis Today, **2020**, *50*, 91-99.

267. Simultaneously Achieving High Activity and Selectivity towards Two-Electron O_2 Electroreduction: the Power of Single-Atom Catalysts
Xiangyu Guo, Shiru Lin, Jinxing Gu, Shengli Zhang,* **Zhongfang Chen,*** Shiping Huang*
ACS Catal. **2019**, *9*, 11042-11054.

266. Frustrated Lewis Pairs Photocatalyst for Visible Light-Driven Reduction of CO into Multi-Carbon Chemicals
Zhe Chen, Jia Zhao, Jingxiang Zhao,* **Zhongfang Chen,*** Lichang Yin*
Nanoscale, **2019**,*11*, 20777-20784.

265. Identifying the Ground-State NP Sheet through a Global Structure Search in Two-Dimensional Space and Its Promising High-Efficiency Photovoltaic Properties

Yuanzheng Chen,* Zebin Lao, Bai Sun, Xiaolei Feng,* Simon A.T. Redfern, Hanyu Liu, Jian Lv, Hongyan Wang, **Zhongfang Chen***
ACS Materials Lett. **2019**, *1*, 375-382

264. Oxygen Evolution Reaction on 2D Ferromagnetic Fe_3GeTe_2: Boosting the Reactivity by the Self-Reduction of Surface Hydroxy
Yinghe Zhao, Jinxing Gu, and Zhongfang Chen*
Adv. Funct. Mater. **2019**, *29*, 1904782.

263. Highly Porous, Low Band-gap $Ni_xMn_{3-x}O_4$ ($0.55 \leq x \leq 1.2$) Spinel Nanoparticles with In-situ Coated Carbon as Advanced Cathode Materials for Zinc-ion Batteries
Jun Long, Jinxing Gu, Zhanghong Yan,* Jianfeng Mao, Juannan Hao, **Zhongfang Chen,*** Zaipping Guo*
J. Mater. Chem. A, **2019**, *7*, 17854-17866.

262. Predicting Novel 2D MB_2 (M=Ti, Hf, V, Nb, Ta) Monolayers with Ultrafast Dirac Transport Channel and Electron-Orbital Controlled Negative Poisson's Ratio
Chunmei Zhang, Tianwei He, Sri Kasi Matta, Ting Liao, Liangzhi Kou, **Zhongfang Chen**, Aijun Du*
J. Phys. Chem. Lett., **2019**, *10*, 2567–2573.

261. B-Terminated (111) Polar Surface of BP and BAs: Promising Metal-Free Electrocatalysts with Large Reaction Regions for Nitrogen Fixation
Zhe Chen, Jingxiang Zhao,* Lichang Yin,* **Zhongfang Chen***
J. Mater. Chem. A. **2019**, *7*, 13284 - 13292

260. Boosting ORR/OER Activity of Graphdiyne by Simple Heteroatom Doping
Jinxing Gu, Saneliswa Magagula, Jingxiang Zhao,*, **Zhongfang Chen***
Small Methods, **2019**, https://doi.org/10.1002/smtd.201800550

259. Non-Volatile Electrical Control and Heterointerface-Induced Half-Metallicity of 2D Ferromagnets
Yinghe Zhao, Jun-Jie Zhang, Shijun Yuan, **Zhongfang Chen***
Adv. Funct. Mater. **2019**, 29, 1901420.

258. Two-dimensional Blue-AsP Monolayers with Tunable Direct Band Gap and Ultrahigh Carrier Mobility Show Promising High-performance Photovoltaic Properties
Xingyong Cai, Yuanzheng Chen,* Bai Sun, Jiao Chen, Shouhui Zhu, Hongyan Wang, Li Tao, Yuxiang Ni, Hui Wang, Jian Lv, Xiaolei Feng, Simon A. T. Redfern, **Zhongfang Chen**
Nanoscale **2019**, 11, 8260-8269.

257. 1+1′ > 2: Heteronuclear Bi-atom Catalyst Outperforms Its Homonuclear Counterparts for CO Oxidation
Fengyu Li,* Xinying Liu, **Zhongfang Chen***
Small Methods **2019**, *3*, 1800480

256. Defect-rich and ultrathin N doped carbon nanosheets as advanced trifunctional metal-free electrocatalysts for ORR, OER and HER
Hao Jiang, Jinxing Gu, Xusheng Zheng, Min Liu, Xiaoqing Qiu, Liangbing Wang, Wenzhang Li,* **Zhongfang Chen,*** Xiaobo Ji, Jie Li*
Energy Environ. Sci., **2019**, *12*, 322-333.

255. Computational Screening of Efficient Single-atom Catalysts based on Graphitic Carbon Nitride ($g\text{-}C_3N_4$) for Nitrogen Electroreduction
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