

## Curriculum Vitae

### Dr. Zhongfang CHEN

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University of Puerto Rico  
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<https://orcid.org/0000-0002-1445-9184>

### EDUCATION

- 1997.9 – 2000.7 Ph. D. in Physical Chemistry, Dept. of Chemistry, Nankai University, P. R. China; Supervisor: Prof. Auchin Tang and Prof. Xuezhuan Zhao
- 1994.9 – 1997.7 M. S. in Physical Chemistry, Dept. of Chemistry, Nankai University, P. R. China, Supervisor: Prof. Xuezhuan 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 analogs – *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)

- 333 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.* (3), *ACS Nano* (6), *Adv. Funct. Mater.* (5), *Nano Lett.* (5), *Energy Environ. Sci.* (1), and 14 book chapters; 1 co-edited book for Wiley.
- 50 first-authored, 215 corresponding-authored; over 34,500 citations and an h-index of 89 by Google Scholar. Over 80 papers received over 100 citations each.
- Eleven (11) papers were highlighted or featured 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, Alvaro J Guerrero
- 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), Jerry Chen, Saleh Yassin, Kevin Shan

## **COMMITTEE MEMBER IN THE DEPARTMENT AND OTHER SERVICES**

- Faculty Committee
- Academic Affairs Committee
- Admission Committee
- Volunteer as the webmaster and editor of the departmental website (2008-2018)
- 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)
- *Carbon Neutralization* (Editorial board member)

### 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](mailto: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](mailto:zhangs9@rpi.edu)
- Prof. Xiao Cheng Zeng  
Department of Chemistry, University of Nebraska-Lincoln, Lincoln, Nebraska 68588  
Email: [xzeng1@unl.edu](mailto:xzeng1@unl.edu)
- Prof. Shigeru Nagase  
Fukui Institute for Fundamental Chemistry  
Kyoto University, Kyoto 606-8103, Japan  
Email: [nagase@ims.ac.jp](mailto: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.* 2011
- "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, Shiyong 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  $\pi$ -Conjugation, Aromaticity and the Related Chemistry of Small Fullerenes (<C<sub>60</sub>) 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,** Xuezhuan 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*

315. Double-Atom Catalysts Featuring Inverse Sandwich Structure for CO<sub>2</sub> Reduction Reaction: A Synergetic First-Principles and Machine Learning Investigation  
 Linke Yu, Fengyu Li,\* Jingsong Huang,\* Bobby G. Sumpter, William E. Mustain, **Zhongfang Chen\***  
*ACS Catalysis*, **2023**, ASAP  
[Highlighted by front cover](#)
314. New Platinum Complexes from Salen- and Hydroxy-Substituted Salpn-Naphthalene Ligands with CO<sub>2</sub>Reduction Activity  
 Javier Rivera, Joesene Soto-Pérez, Miguel Sepulveda Pagán, Lingup Lu, Justin Borrero, Alanys Luna, Pedro Trinidad, Yomaira Pagan, **Zhongfang Chen**, Carlos Cabrera, William West, John Jones, Dalice Marie Piñero Cruz \*  
*Catalysts* **2023**, 13, 911.
313. Suppressed Fermi Level Pinning and Wide-Range Tunable Schottky Barrier in CrI<sub>3</sub> (CrBr<sub>3</sub>)/2D Metal Contacts  
 Yanmei Hu, Xiaohui Hu,\* Yifeng Wang, Chunhua Lu, Arkady V. Krashennnikov, **Zhongfang Chen**, Litao Sun  
*J. Phys. Chem. Lett.* **2023**, 14, 2807–2815
312. A polymeric hydrogel electrocatalyst for direct water oxidation.  
 Zengxia Pei,\* Hao Tan, Jinxing Gu, Linguo Lu, Xin Zeng, Tianqi Zhang, Cheng Wang, Luyao Ding, Patrick Cullen, **Zhongfang Chen\***, and Shenlong Zhao\*  
*Nature Commun* **2023**, 14, 818.

311. Trinuclear and Cyclometallated Organometallic Dinuclear Pt-Pyrazolato Complexes: A Combined Experimental and Theoretical Study  
Zhi-Chun Shi, Fengyu Li, Hong Zhao, Indranil Chakraborty, **Zhongfang Chen**,\* Raphael G. Raptis\*  
*Chemistry* **2023**, *5*, 187-200.
310. Narrowing the Band Gap and Suppressing Electron–Hole Recombination in  $\beta$ -Fe<sub>2</sub>O<sub>3</sub> by Chlorine Doping  
Gaoxiang He, Linguo Lu, Ningsi Zhang, Wangxi Liu, **Zhongfang Chen**\*, Zhaosheng Li\*, Zhigang Zou  
*Phys. Chem. Chem. Phys.*, **2023**, *25*, 3695-3701.
309. Protonated Methyl-Cyclopropane is an Intermediate Providing Complete <sup>13</sup>C-label Scrambling at C<sub>4</sub> Olefin Isomerization in Zeolite  
Wei Chen, Mengdi Huang, Xianfeng Yi,\* Yu Hui, Pan Gao, Guangjin Hou,\* Alexander G. Stepanov, Yucai Qin, Lijuan Song, Shang-Bin Liu, **Zhongfang Chen**\* and Anmin Zheng\*  
*Chem Catalysis*, **2023**, *3*, 100503.
308. Two-dimensional Ruthenium Boride: A Dirac Nodal Loop Quantum Electrocatalyst for Efficient Hydrogen Evolution Reaction  
Zhen Gao, Fengxian Ma,\* Hongbo Wu, Yongheng Ge, Ziming Zhu, Ying Liu, Yalong Jiao,\* **Zhongfang Chen**\*  
*J. Mater. Chem. A*, **2023**, *11*, 3717-3724.
307. Boosting the efficiency of urea synthesis *via* cooperative electroreduction of N<sub>2</sub> and CO<sub>2</sub> on MoP†  
Dongxu Jiao, Yilong Dong, Xiaoqiang Cui, Qinghai Cai, Carlos R. Cabrera, Jingxiang Zhao,\* **Zhongfang Chen**\*  
*J. Mater. Chem. A*, **2023**, *11*, 232-240.
306. Two-dimensional Be<sub>2</sub>Au Monolayer with Planar Hexacoordinate s-Block Metal Atoms: A Superconducting Global Minimum Dirac Material with Two Perfect Dirac Node-Loops  
Meng-hui Wang, Zhong-hua Cui\*, Sheng Wang, Quan Li, Jijun Zhao, **Zhongfang Chen**\*  
*Chemical Sciences* **2022**, *13*, 11099-11109.
305. CuB Monolayer: A novel 2D anti-van't Hoff/Le Bel nanostructure with planar hyper-coordinate boron/copper and superconductivity  
Kaixiong Tu, Jinxing Gu, Linguo Lu, Shijun Yuan, Long Zhou, **Zhongfang Chen**\*  
*J. Mater. Inf.* **2022**, *2*, 13.
304. Particle Swarm Predictions of a SrB<sub>8</sub> 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 NH<sub>3</sub> Yield Rate  
Yinghe Zhao, Jingyu Qu, Haobo Li, Pengyu Li, Teng Liu, **Zhongfang Chen**\*, Tianyou Zhai\*  
*Nano Lett.* **2022**, *22*, 4475–4481.
302. Understanding the CH<sub>4</sub> 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  $\pi$ -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-hole-graphyne.html>  
<https://www.azonano.com/news.aspx?newsID=39157>  
<https://blingeach.com/synthesis-of-two-dimensional-hole-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<sub>3</sub>N<sub>2</sub> 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<sub>2</sub>) 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<sub>2</sub> Electrocatalytic Reduction via Fer-roelectric Switching on In<sub>2</sub>Se<sub>3</sub> 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 Cr<sub>2</sub>Ge<sub>2</sub>Te<sub>6</sub> Monolayer by Strain Engineering  
Lifei Liu, Xiaohui Hu,\* Yifeng Wang, Arkady V. Krasheninnikov, Zhongfang Chen, Litao Sun  
*Nanotechnology* **2021**, 32, 485408.
292. C<sub>9</sub>N<sub>4</sub> and C<sub>2</sub>N<sub>6</sub>S<sub>3</sub> 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<sub>3</sub> 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<sub>2</sub>P 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<sub>2</sub> 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<sub>3</sub>N<sub>4</sub> 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<sub>2</sub> Reduction Reaction with Integrated Descriptor  
 Lei 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<sub>7</sub>P<sub>2</sub> 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 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\***  
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